Finite-temperature lattice methods
Lecture 4.

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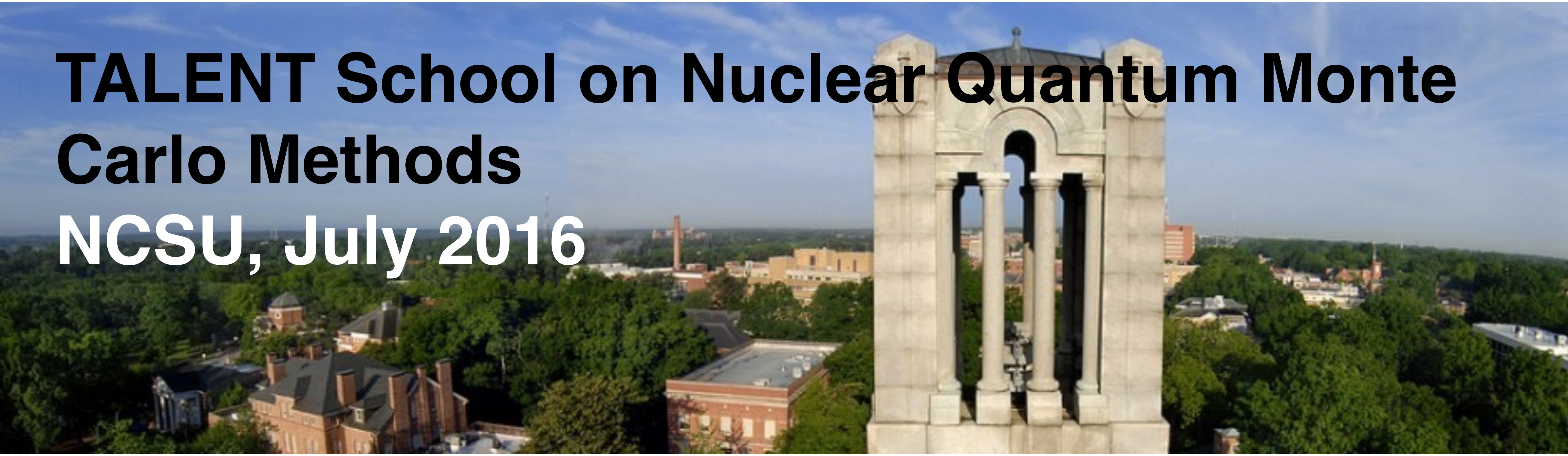
at CHAPEL HILL



TALENT School on Nuclear Quantum Monte Carlo Methods
NCSU, July 2016

Goals

- **Lecture 1**:
  General motivation. Review of thermodynamics and statistical mechanics. Non-interacting quantum gases at finite temperature.

- **Lecture 2**:
  QRL1. Formalism at finite temperature: Trotter-Suzuki decompositions; Hubbard-Stratonovich transformations. From traces to determinants. Bosons and fermions. The sign problem.

- **Lecture 3**:
  QRL2. Computing expectation values (finally!). Particle number. Energy. Correlation functions: static and dynamic. Sampling techniques. Signal-to-noise issues and how to overcome them.

Goals

- **Lecture 4**:
  Quantum phase transitions and quantum information. Entanglement entropy. Reduced density matrix. Replica trick. Signal-to-noise issues.

- **Lecture 5**:
  QRL3. Finite systems. Particle-number projection. The virial expansion. Signal-to-noise issues. Trapped systems.

- **Lecture 6**:
  QRL5. Spacetime formulation. Finite-temperature perturbation theory on the lattice.

- **Lecture 7**:
  Applications to ultracold atoms in a variety of situations. Beyond equilibrium thermodynamics.

Quantum phase transitions
&
quantum information

TOWARD UNITARY ENTANGLEMENT

William J. Porter

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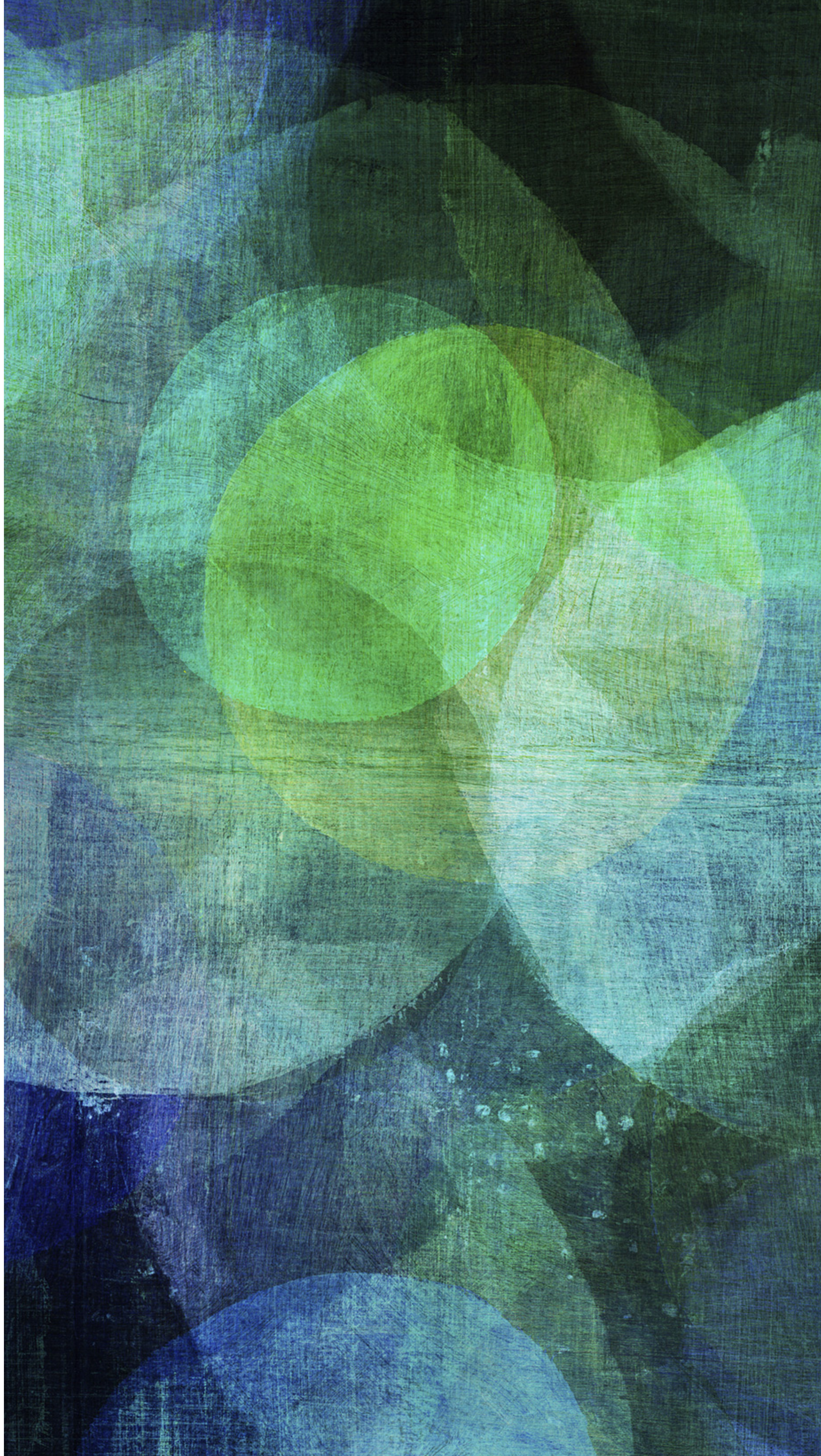
January 20, 2016



OVERVIEW

- Introduction: What is entanglement?
  Why is it interesting?
- How is it calculated?
- Results: What's new?
- Summary, conclusions, and future work

WHAT IS ENTANGLEMENT?

- Entanglement comprises inherently quantum mechanical correlations.
- It characterizes the degree to which a state **fails** to factor.
- Contrast, for example the two-spin system (writing $|s\,m\rangle$ for the state with total spin s and z-component m), the pure state

$$|11\rangle = |\uparrow\uparrow\rangle$$

and the spin singlet

$$|10\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right).$$

J. Preskill, J. Mod. Opt. **47**, 127 (2000).

WHAT IS ENTANGLEMENT?

❖ Another example is the **Slater determinant** encapsulating the ground-state properties of N non-interacting fermions.

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_N(\mathbf{x}_N) \end{vmatrix}$$

J. Preskill, J. Mod. Opt. **47**, 127 (2000).

WHAT IS ENTANGLEMENT?

- Consider a quantum state $|\Psi\rangle$ with density matrix $\hat{\rho} = |\Psi\rangle\langle\Psi|$.
- For a subset $\bar{A}$ of quantum numbers, we can compute a **reduced density matrix**

$$\hat{\rho}_A \equiv \mathrm{Tr}_{\bar{A}}\, \hat{\rho},$$

which is an operator defined on the Hilbert space corresponding to the remaining degrees of freedom.

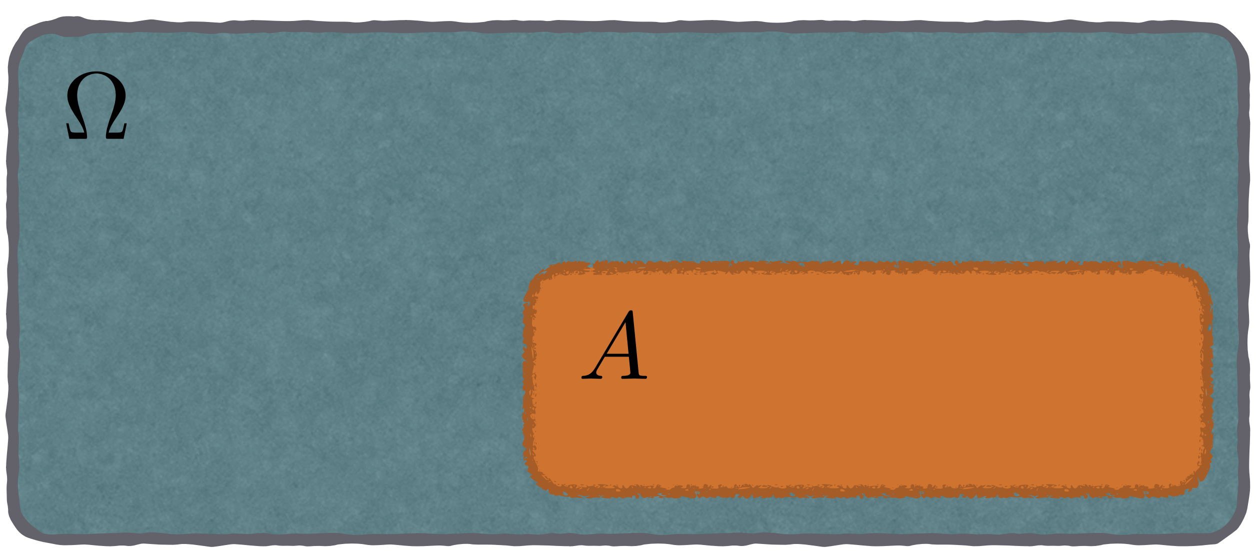


Figure: A complete set of quantum numbers Ω along with a restriction to a subset $A \subseteq \Omega$ of them.

R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki, Rev. Mod. Phys. **81**, 865 (2009).

WHAT IS ENTANGLEMENT?

- Our entanglement measure of interest will be the n-th order **Rényi entropy** $S_{A,n}$ for the spatial subregion A defined

$$\boxed{S_{A,n} \equiv \frac{1}{1-n} \ln \mathrm{Tr}_A\, \hat{\rho}_A^n .}$$

$$S_A \equiv -\mathrm{Tr}_A \left[\hat{\rho}_A \log_2 \hat{\rho}_A\right]$$

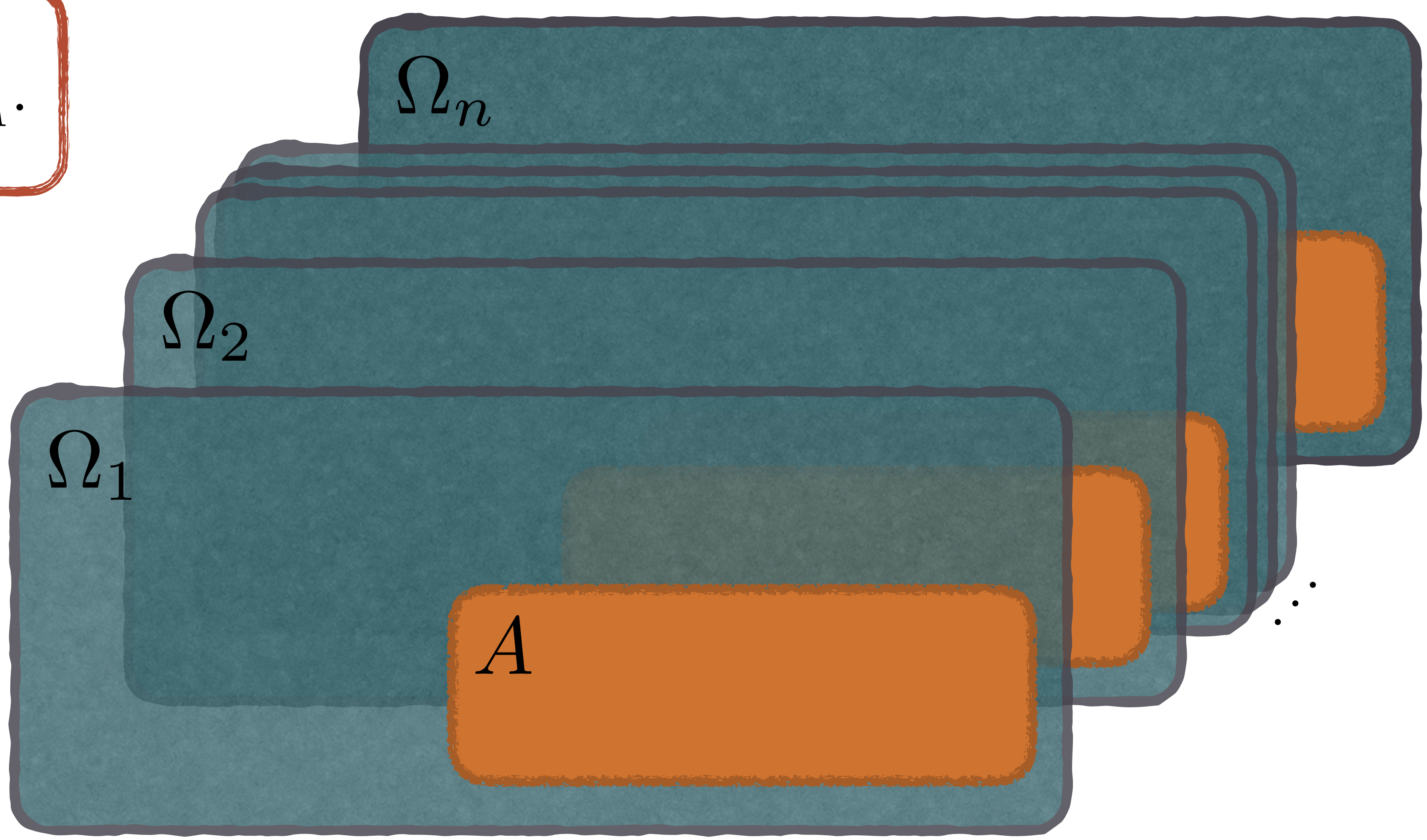


Figure: Replicas $\{\Omega_i\}_i$ of the system with the quantum numbers corresponding to the region A contracted across the collection.

P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.

WHAT IS ENTANGLEMENT?

- Ground state entanglement results in long-range (**nonlocal**) correlations at zero temperature.
- Quantifying these correlations is an essential step toward understanding **quantum phase transitions**.
- Entanglement measures show **universal** scaling in critical systems.

Osterloh, L. Amico, G. Falci, R. Fazio, Nature **416**, 608 (2002);
T.J. Osborne, M.A. Nielsen, Phys. Rev. A **66**, 032110 (2002);
G. Vindal, J.I. Latorre, E. Rico, A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).

WHY IS IT INTERESTING?

- Entanglement measures show **universal** scaling in critical systems:

$$S_L \sim \frac{c+\bar{c}}{6}\log_2 L + \text{const.}$$

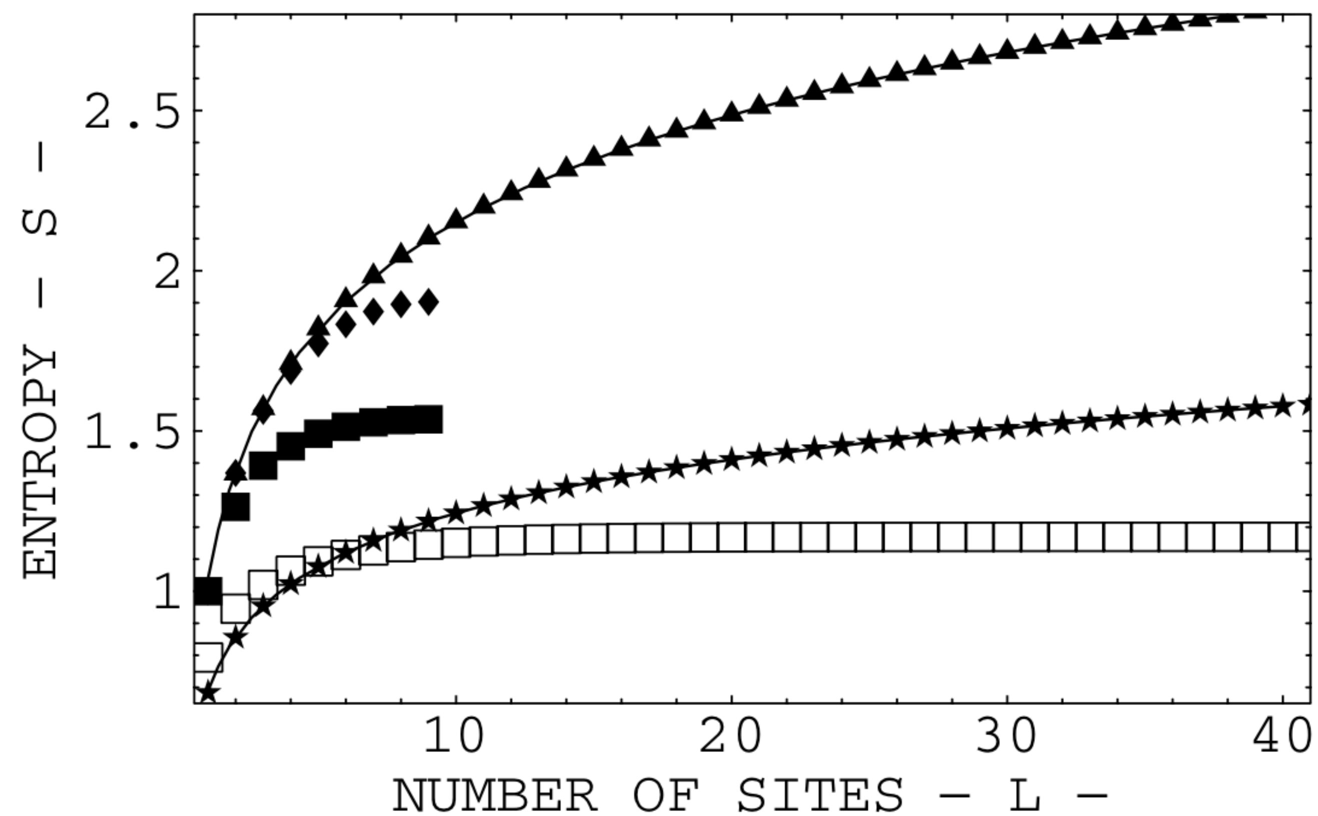
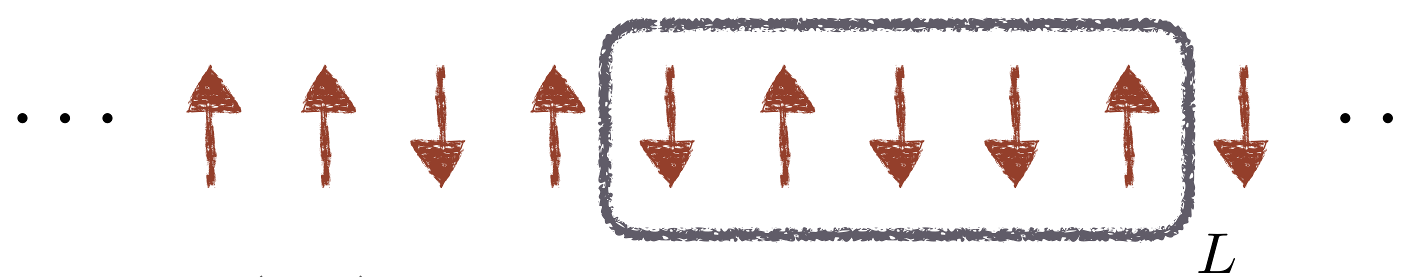


Figure: Entanglement (von Neumann) entropy for spin-chain models as a function of the number of sites. Critical systems show logarithmic divergence, whereas noncritical systems show saturation for large system sizes.



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WHY IS IT INTERESTING?

- Entanglement is a cutting-edge observable.

Measuring entanglement entropy in a quantum many-body system

Rajibul Islam, Ruichao Ma, Philipp M. Preiss, M. Eric Tai, Alexander Lukin, Matthew Rispoli & Markus Greiner

Affiliations | Contributions | Corresponding author

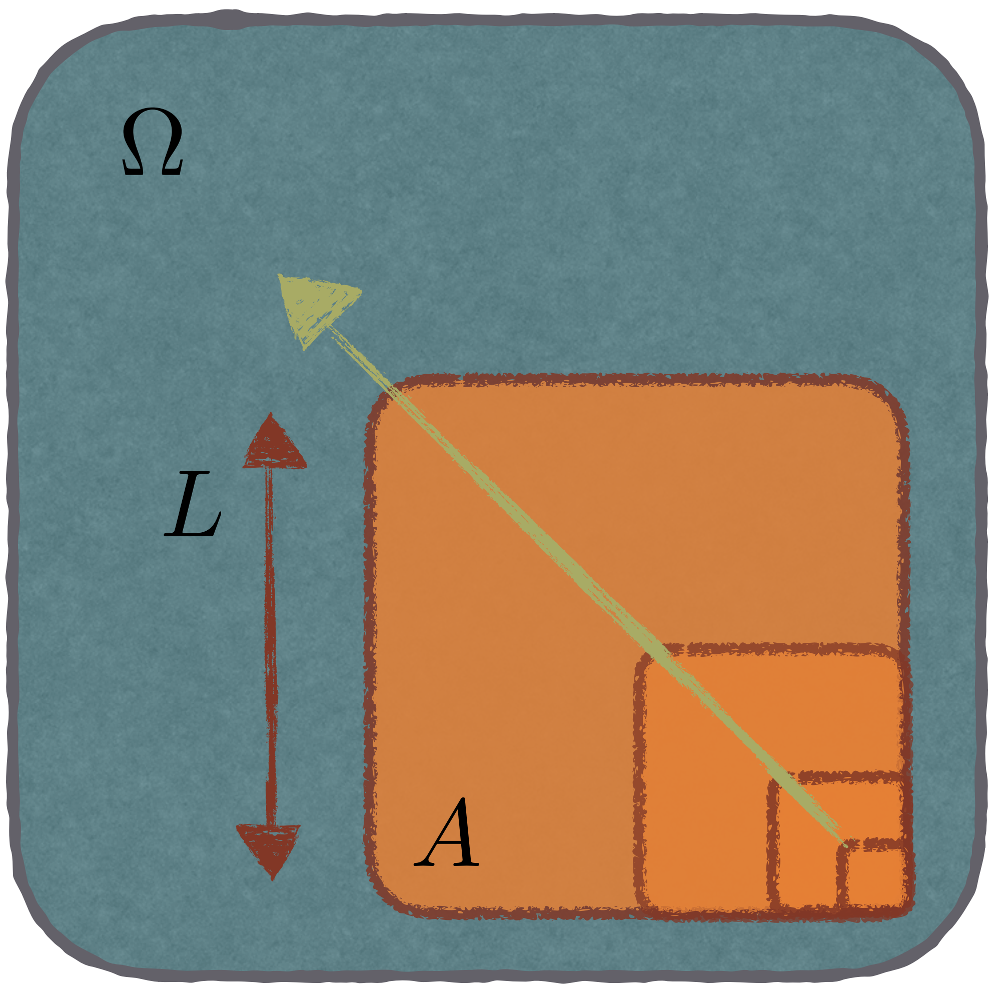
Nature **528**, 77–83 (03 December 2015) | doi:10.1038/nature15750

Received 30 July 2015 | Accepted 16 September 2015 | Published online 02 December 2015

R. Islam, R. Ma, P.M. Preiss, M.E. Tai, A. Lukin, M. Rispoli, M. Greiner, Nature **528**, 77 (2015).

WHY IS IT INTERESTING?

- Rigorous scaling results also exist for free systems, some Fermi systems showing **area-law violation**.



For **bosonic** systems,

$$S_{A,n} \sim L^{d-1},$$

but for **gapless fermions**

$$S_{A,n} \sim L^{d-1} \log L.$$

Figure: Scaling of the d-dimensional subregion with boundary of measure L^{d-1}*.*

M. Srednicki, Phys. Rev. Lett. **71**, 666 (1993);
M.W. Wolf, Phys. Rev. Lett. **96**, 010404 (2006);
D. Gioev, I. Klich, Phys. Rev. Lett. **96**, 100503 (2006);
B. Swingle, Phys. Rev. Lett. **105**, 050502 (2010);
H. Leschke, A.V. Sobolev, W. Spitzer, Phys. Rev. Lett. **112**, 160403 (2014);
H. Leschke, A.V. Sobolev, W. Spitzer, arXiv:1501.03412.

HOW IS IT CALCULATED?

- Techniques for handling **interactions** are varied and often system-dependent.
- Many approaches have foundation in the **replica trick**.

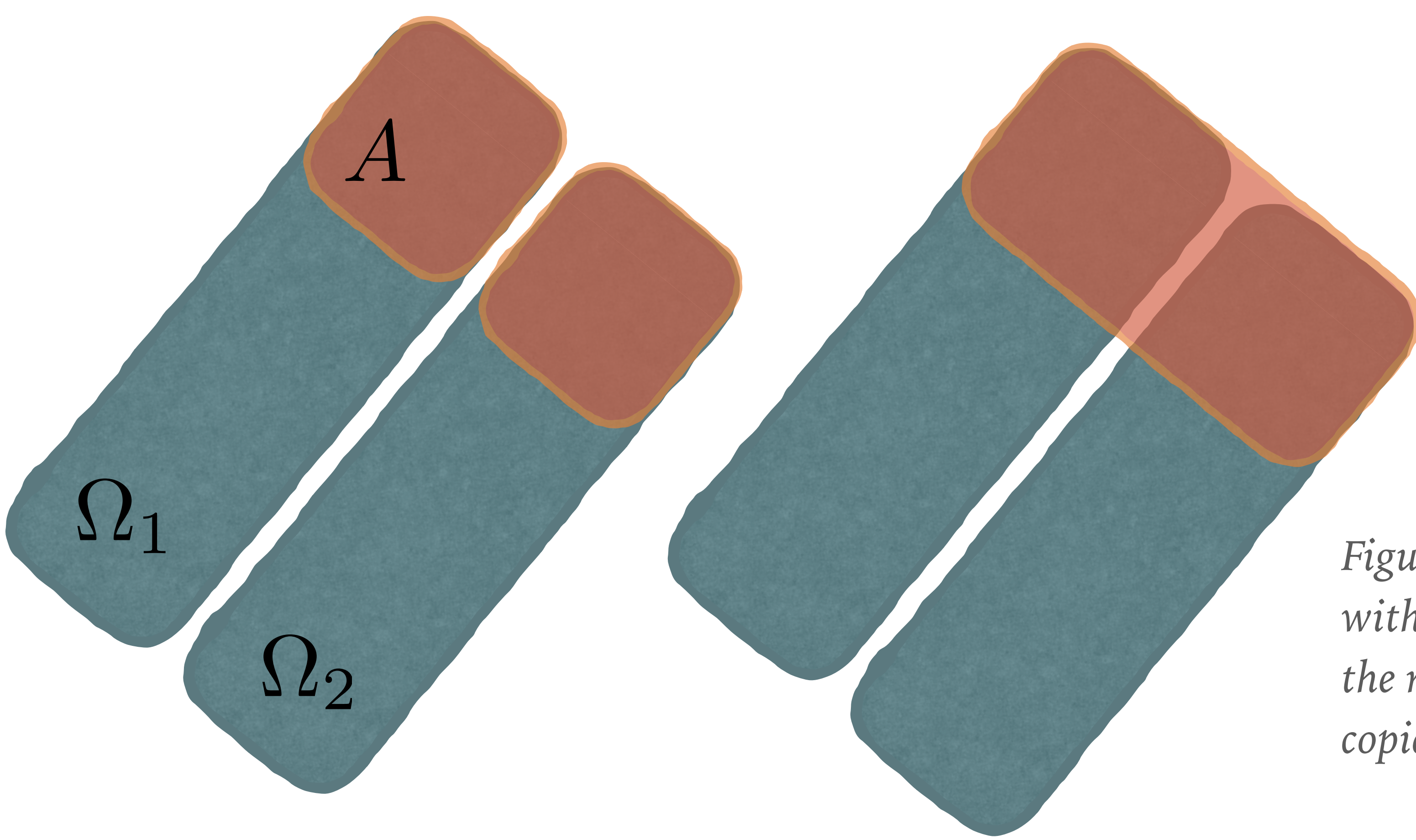


Figure: Two collections of replicas: one with independent copies and another with the region of interest identified across the copies.

P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.

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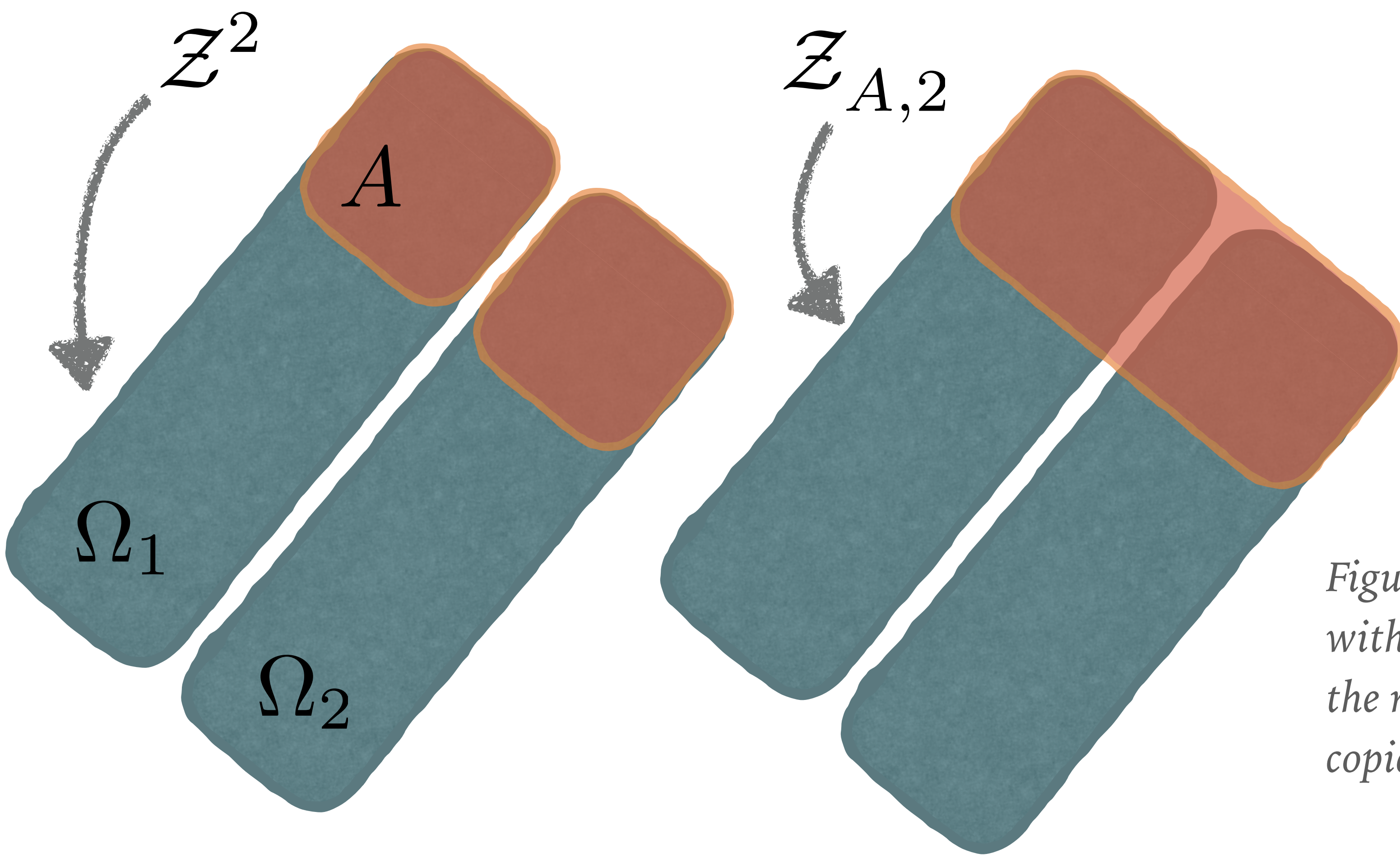
❖ Many approaches have foundation in the **replica trick**.

$$e^{(1-n)S_{A,n}} = \mathrm{Tr}\,\hat{\rho}_A^n = \frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n}$$



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HOW IS IT CALCULATED?

- The entropy can be estimated in an extended ensemble.

$$e^{(1-n)S_{A,n}} = \mathrm{Tr}\,\hat{\rho}_A^n = \frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n}$$

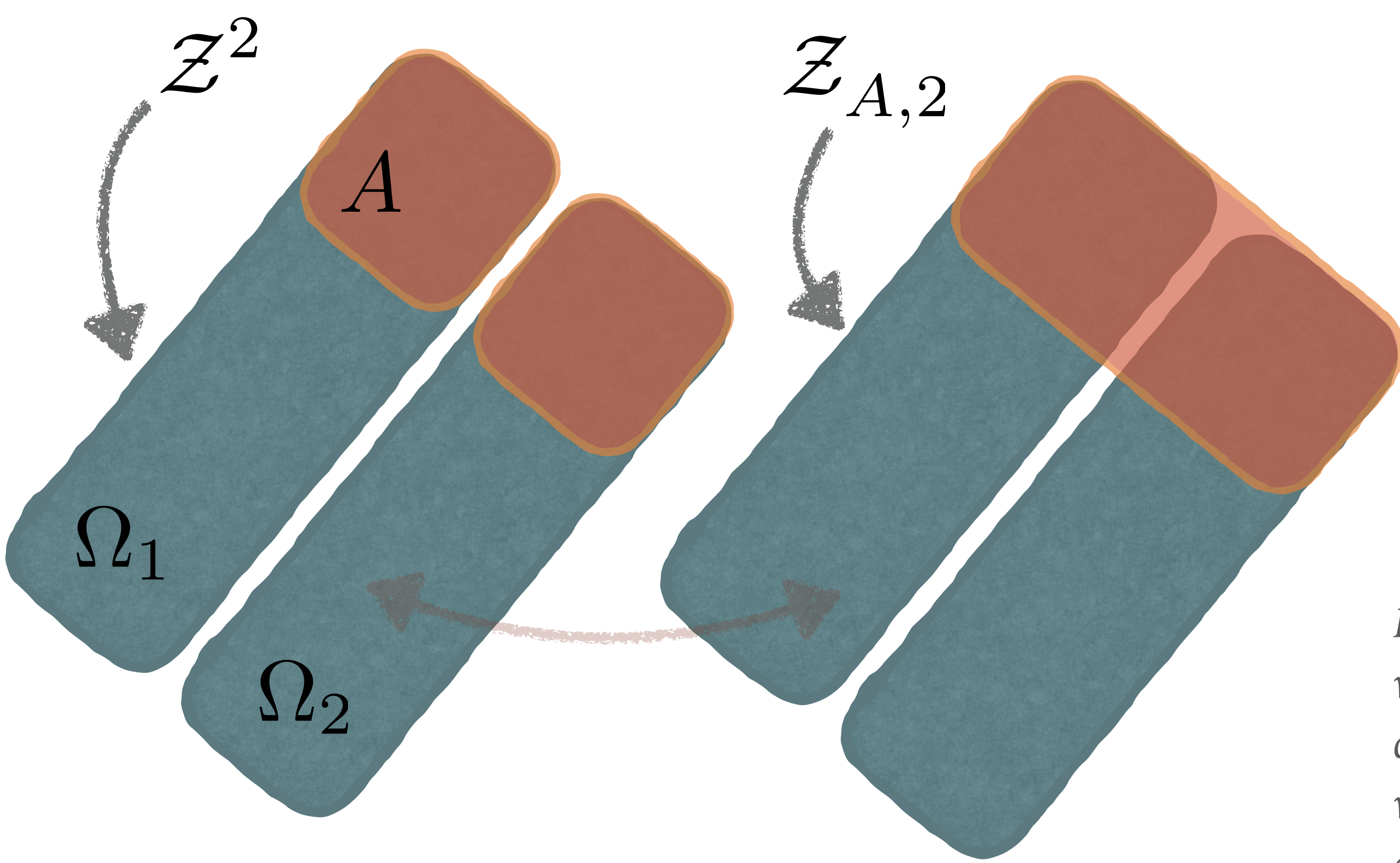


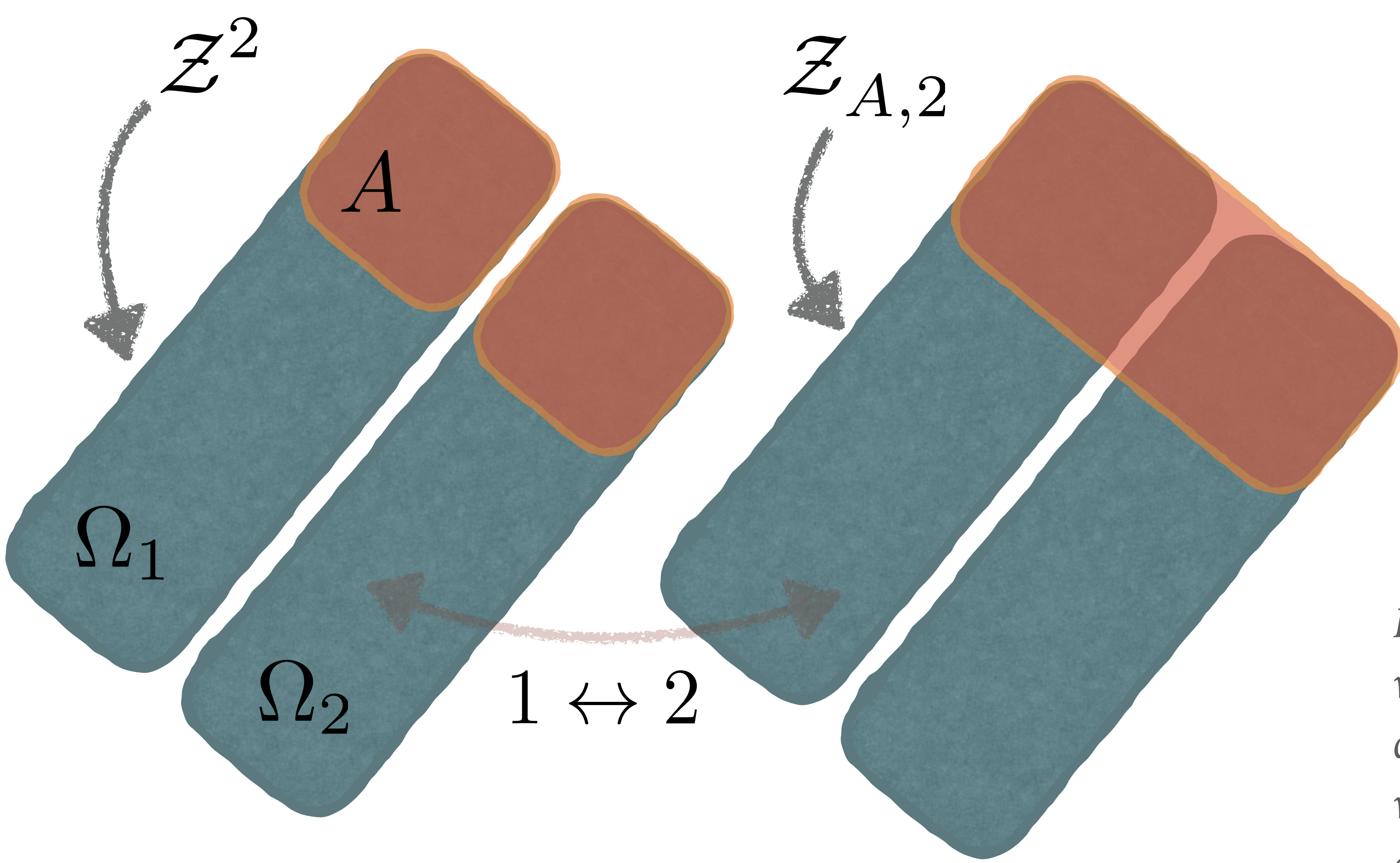
Figure: An extended ensemble with weights w_1 and w_2 comprised of two sets of replicas with different topologies in configuration $\mathcal{C}$.

S. Humeniuk, T. Roscilde, Phys. Rev. B **86**, 235116 (2012);
P. Broecker, S. Trebst, J. Stat. Mech. (2014) P08015;
L. Wang, M. Troyer, Phys. Rev. Lett. **113**, 110401 (2014).

HOW IS IT CALCULATED?

- This method can be implemented within a variety of Monte Carlo frameworks.

$$\frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n} = \frac{\langle p_{1\to 2}\rangle}{\langle p_{2\to 1}\rangle}$$



$$p_{1\to 2} = \min\left(1, \frac{w_2(\mathcal{C})}{w_1(\mathcal{C})}\right)$$

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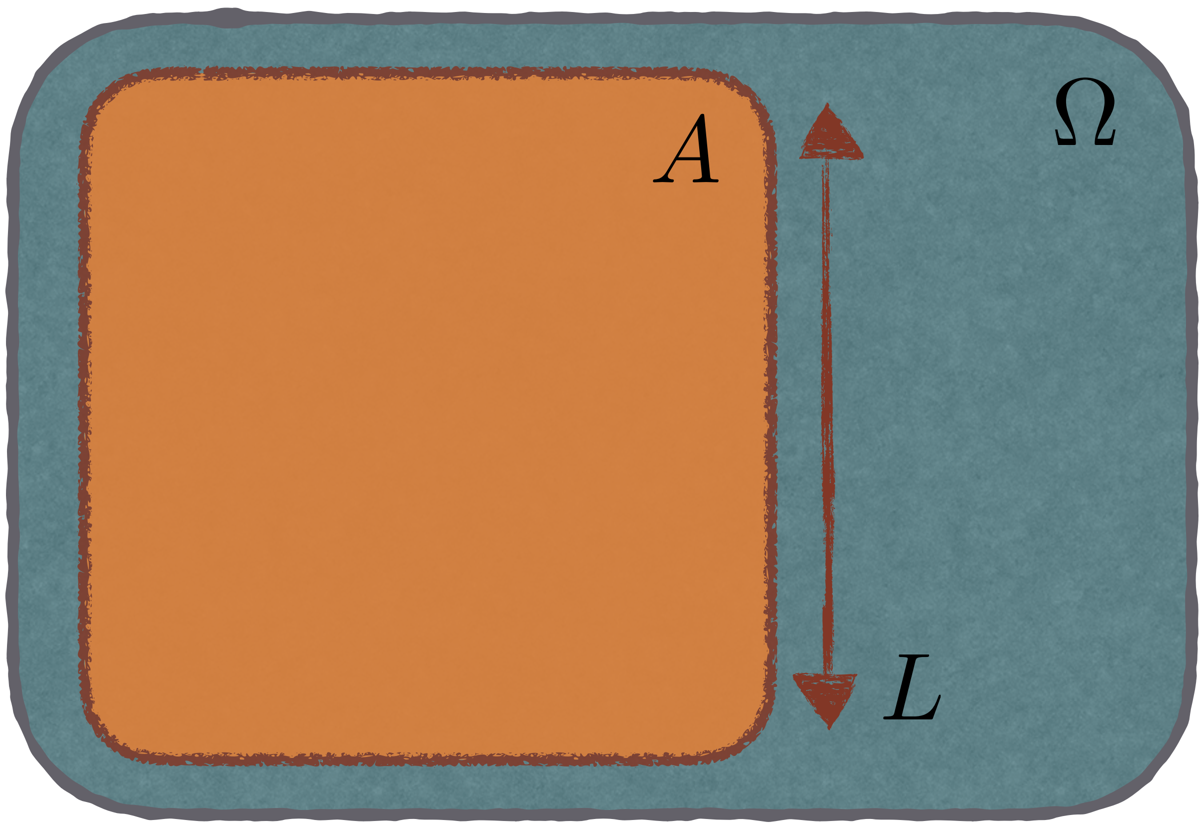
HOW IS IT CALCULATED?

- **Problem:** This ratio can be **small.**

$$\frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n} = \exp\left[(1-n)S_{n,A}\right] \sim \exp\left[(1-n)L^{d-1}\ln L\right]$$



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HOW IS IT CALCULATED?

- Introducing intermediate ratios can help avoid this problem.

$$\frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n} = \frac{\mathcal{Z}_{A,n}}{\mathcal{Z}_{A_N,n}} \frac{\mathcal{Z}_{A_N,n}}{\mathcal{Z}_{A_{N-1},n}} \cdots \frac{\mathcal{Z}_{A_2,n}}{\mathcal{Z}_{A_1,n}} \frac{\mathcal{Z}_{A_1,n}}{\mathcal{Z}^n}$$

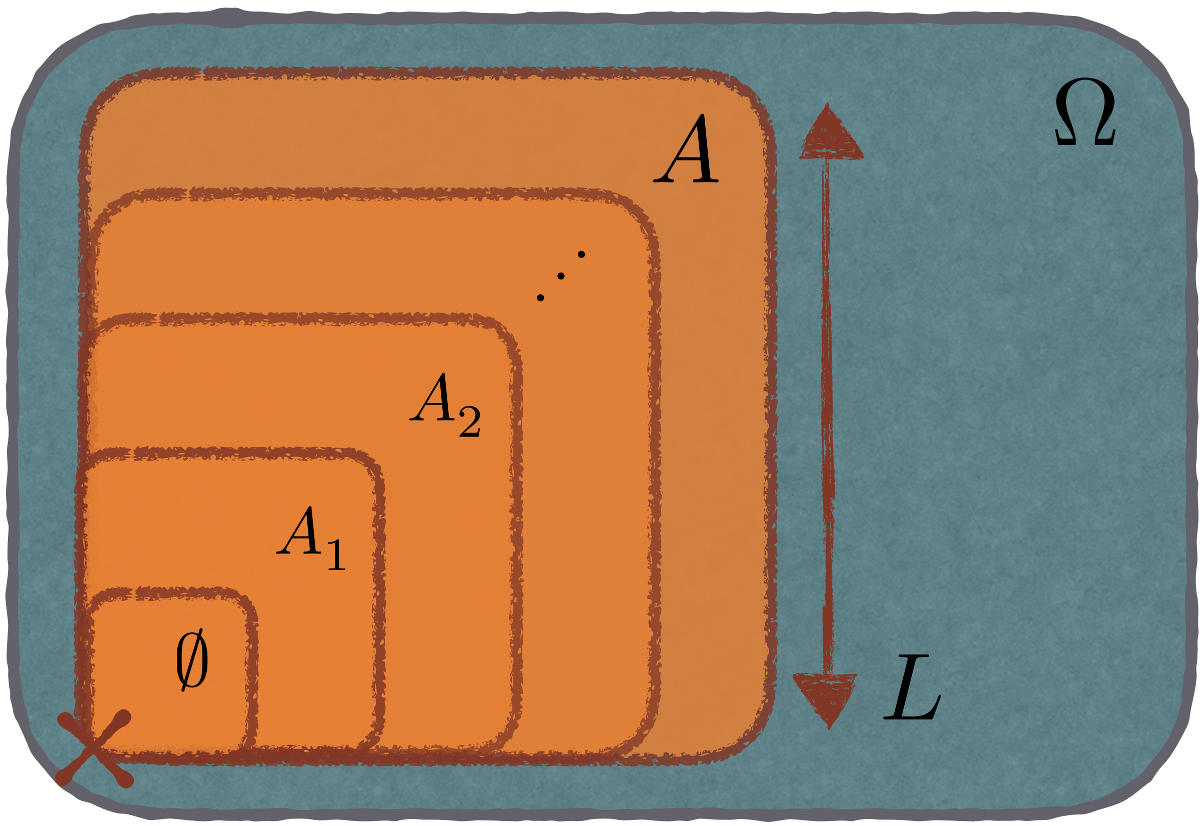

Figure: A sequence of slightly dissimilar regions $\{A_i\}_i$ *with sizes ranging from vanishing to that desired.*

M.B. Hastings, I. González, A.B. Kallin, R.G. Melko, Phys. Rev. Lett. **104**, 157201 (2010).

HOW IS IT CALCULATED?

❖ An **auxiliary field decomposition** recasts the interacting entropy as an average over free systems.

$$\hat{\rho}_A = \int \mathcal{D}\sigma \; P[\sigma]\, \hat{\rho}_{A,\sigma}$$

$$P[\sigma] \propto \det U[\sigma]$$

T. Grover, Phys. Rev. Lett. **111**, 130402 (2013).
R. L. Stratonovich, Sov. Phys. Dokl. **2**, (1958) 416;
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$$\hat{\rho}_A^n = \int \mathcal{D}\{\sigma\}\; P[\{\sigma\}] \prod_{i=1}^{n} \hat{\rho}_{A,\sigma_i}$$

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$$P[\{\sigma\}] = \prod_{i=1}^{n} P[\sigma_i]$$

$$\boxed{\begin{aligned} e^{(1-n)S_{A,n}} &= \mathrm{Tr}\, \hat{\rho}_A^n = \int \mathcal{D}\{\sigma\} \; P[\{\sigma\}] \det M_{A,n}[\{\sigma\}] \\ M_{A,n}[\{\sigma\}] &= \prod_{i=1}^{n} \left(1 - G_{A,\sigma_i}\right) \left(1 + \prod_{i=1}^{n} \frac{G_{A,\sigma_i}}{1 - G_{A,\sigma_i}}\right) \end{aligned}}$$

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J. Hubbard, Phys. Rev. Lett. **3**, (1959) 77.

HOW IS IT CALCULATED?

- An **auxiliary field decomposition** recasts the interacting entropy as an average over free systems.
- Use the probability $P[\{\sigma\}]$ to sample the σ-field and the remaining determinant as the observable.

$$\boxed{\begin{aligned} e^{(1-n)S_{A,n}} &= \mathrm{Tr}\,\hat{\rho}_A^n = \int \mathcal{D}\{\sigma\}\, P[\{\sigma\}]\, \det M_{A,n}[\{\sigma\}] \\ M_{A,n}[\{\sigma\}] &= \prod_{i=1}^{n}\left(1 - G_{A,\sigma_i}\right)\left(1 + \prod_{i=1}^{n} \frac{G_{A,\sigma_i}}{1 - G_{A,\sigma_i}}\right) \end{aligned}}$$

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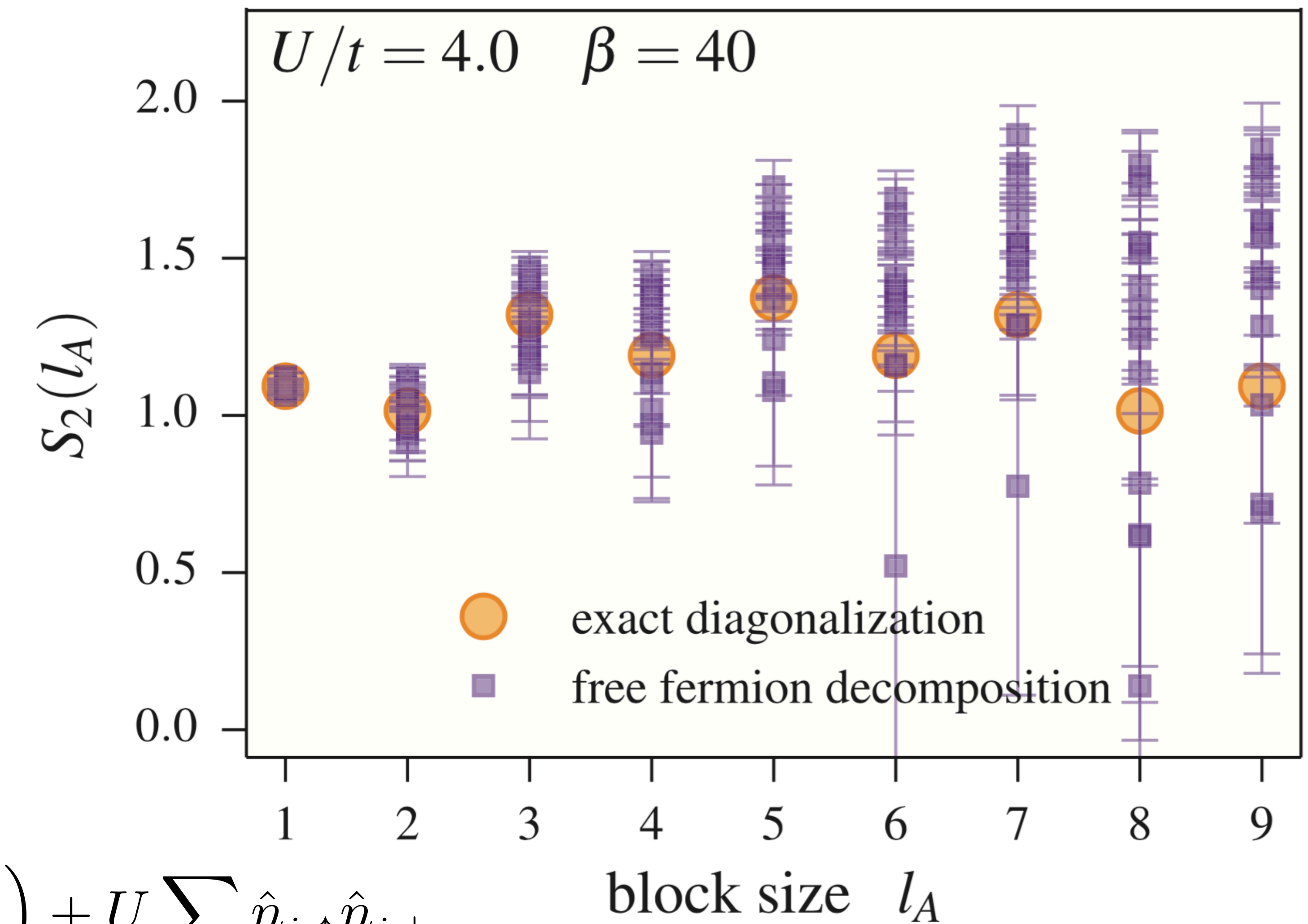
HOW IS IT CALCULATED?

- **Problem:** Fluctuations in the determinant become unmanageable for increasing subregion size.

Figure: Results for the one-dimensional Hubbard model at half-filling as a function of region size.



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

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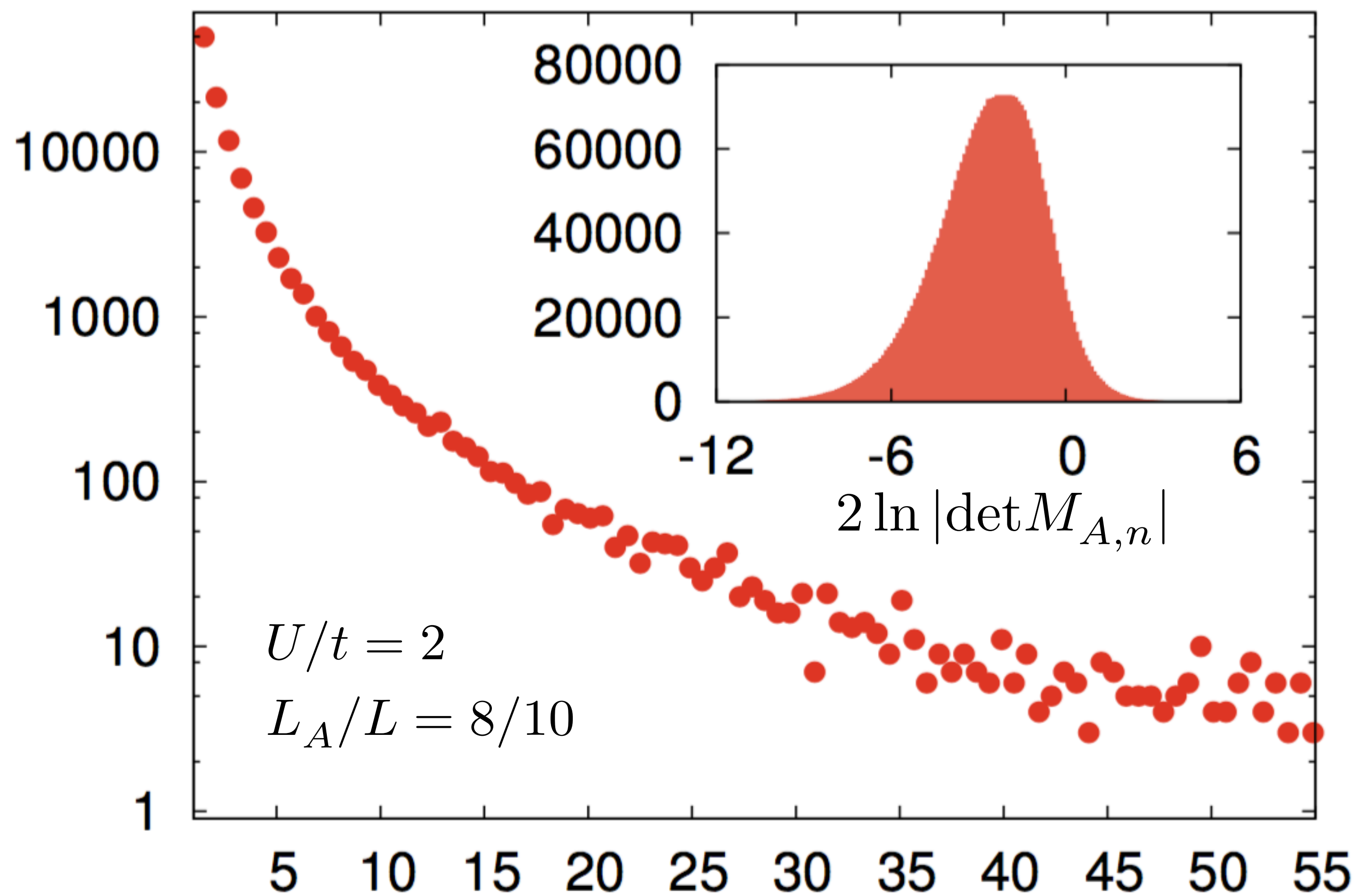
Figure: Histogram of the log of the required determinant for the one-dimensional two-species Hubbard model at half-filling as a function of region size.



$$(1-n)S_{A,n} = \ln\langle \det M_{A,n}\rangle$$

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

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

- Incorporate this determinant into the measure.

$$e^{(1-n)S_{A,n}} = \int \mathcal{D}\{\sigma\}\; P[\{\sigma\}]\, Q[\{\sigma\}]$$

$$Q[\{\sigma\}] = \det M_{A,n}[\{\sigma\}]$$

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$$g \to \lambda^2 g$$

$$\Gamma(\lambda; g) = \int \mathcal{D}\{\sigma\}\; P[\{\sigma\}]\, Q_\lambda[\{\sigma\}]$$

$$Q_\lambda[\{\sigma\}] = \det M_{A,n,\lambda}[\{\sigma\}]$$

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$$Q_\lambda[\{\sigma\}] = \det M_{A,n,\lambda}[\{\sigma\}]$$

$$\boxed{\begin{aligned} \frac{d\ln\Gamma}{d\lambda} &= \int \mathcal{D}\{\sigma\}\; \tilde{P}_\lambda[\{\sigma\}]\, \tilde{Q}_\lambda[\{\sigma\}] \\ \tilde{P}_\lambda[\{\sigma\}] &= \frac{1}{\Gamma(\lambda; g)} P[\{\sigma\}]\, Q_\lambda[\{\sigma\}] \\ \tilde{Q}_\lambda[\{\sigma\}] &= \mathrm{Tr}\left[M^{-1}_{A,n,\lambda}[\{\sigma\}] \frac{\partial M_{A,n,\lambda}}{\partial \lambda} \right] \end{aligned}}$$

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

- This expectation can be evaluated with Monte Carlo methods.

$$\frac{d \ln \Gamma}{d\lambda} = \int \mathcal{D}\{\sigma\}\ \tilde{P}_\lambda[\{\sigma\}]\, \tilde{Q}_\lambda[\{\sigma\}]$$

$$\tilde{P}_\lambda[\{\sigma\}] = \frac{1}{\Gamma(\lambda; g)} P[\{\sigma\}]\, Q_\lambda[\{\sigma\}]$$

$$\tilde{Q}_\lambda[\{\sigma\}] = \mathrm{Tr}\left[M^{-1}_{A,n,\lambda}[\{\sigma\}] \frac{\partial M_{A,n,\lambda}}{\partial \lambda}\right]$$

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

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$$\frac{d \ln \Gamma}{d\lambda} = \langle \tilde{Q}_\lambda[\{\sigma\}] \rangle_\Gamma$$

$$\frac{1}{1-n} \ln \Gamma(0; g) = S^{(0)}_{n,A}$$

$$\frac{1}{1-n} \ln \Gamma(1; g) = S_{n,A}$$

$$\frac{d \ln \Gamma}{d\lambda} = \int \mathcal{D}\{\sigma\} \, \tilde{P}_\lambda[\{\sigma\}] \, \tilde{Q}_\lambda[\{\sigma\}]$$

$$\tilde{P}_\lambda[\{\sigma\}] = \frac{1}{\Gamma(\lambda; g)} P[\{\sigma\}] \, Q_\lambda[\{\sigma\}]$$

$$\tilde{Q}_\lambda[\{\sigma\}] = \mathrm{Tr}\left[M^{-1}_{A,n,\lambda}[\{\sigma\}] \frac{\partial M_{A,n,\lambda}}{\partial \lambda} \right]$$

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$$\tilde{Q}_\lambda[\{\sigma\}] = \mathrm{Tr}\left[M^{-1}_{A,n,\lambda}[\{\sigma\}]\frac{\partial M_{A,n,\lambda}}{\partial\lambda}\right]$$

$$\boxed{S_{n,A} = S^{(0)}_{n,A} + \frac{1}{1-n}\int_0^1 d\lambda\, \langle \tilde{Q}_\lambda[\{\sigma\}]\rangle_\Gamma}$$

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

❖ Variation with system size is quite benign, and the resulting surface is remarkably smooth.

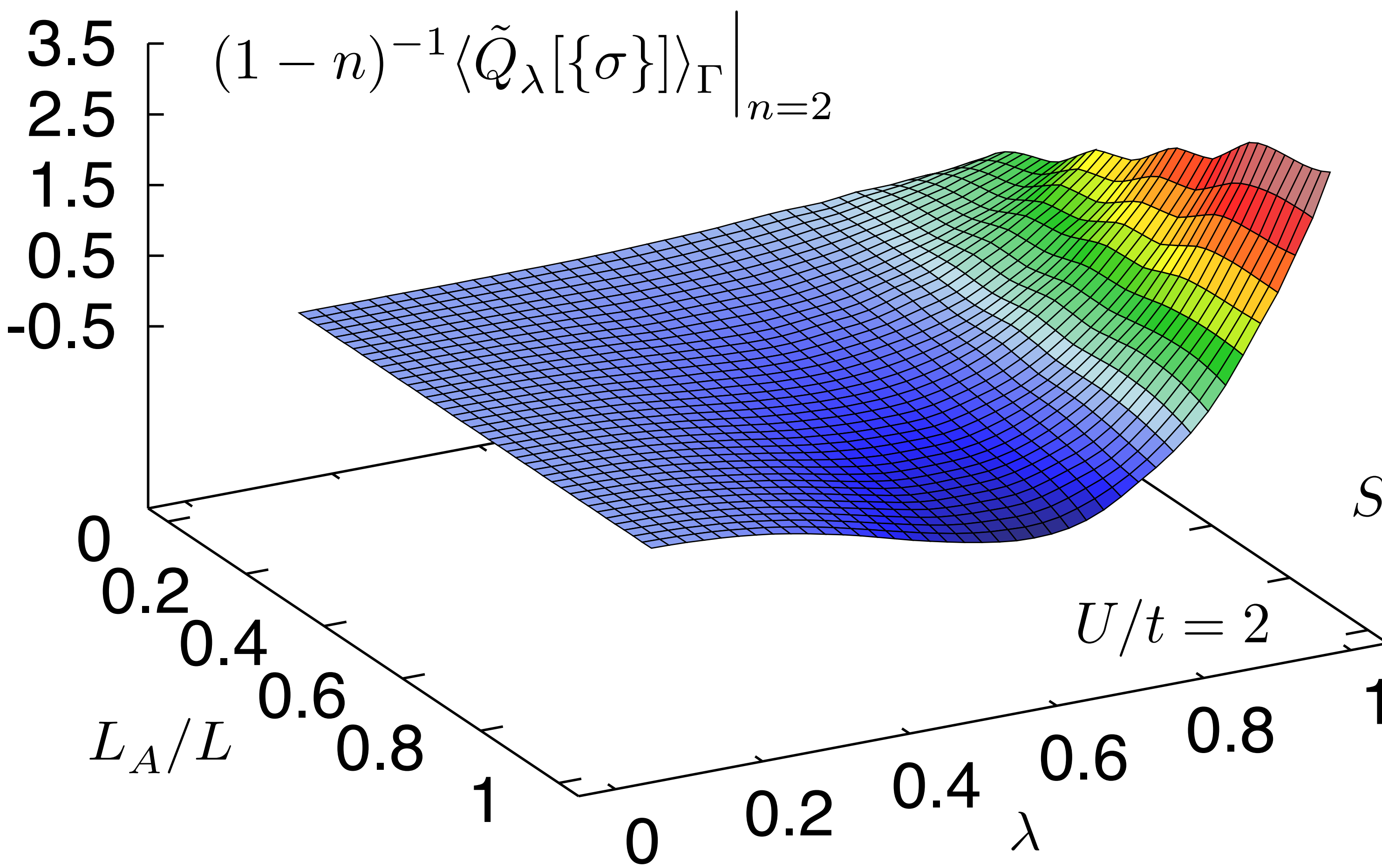

Figure: Monte Carlo results for the integrand for the Hubbard model at half-filling.

$$S_{n,A} = S_{n,A}^{(0)} + \frac{1}{1-n}\int_0^1 d\lambda\, \langle\tilde{Q}_\lambda[\{\sigma\}]\rangle_\Gamma$$

$$\frac{d\ln\Gamma}{d\lambda} = \langle\tilde{Q}_\lambda[\{\sigma\}]\rangle_\Gamma$$

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

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

- Most of the total variation is for larger values of the parameter λ.

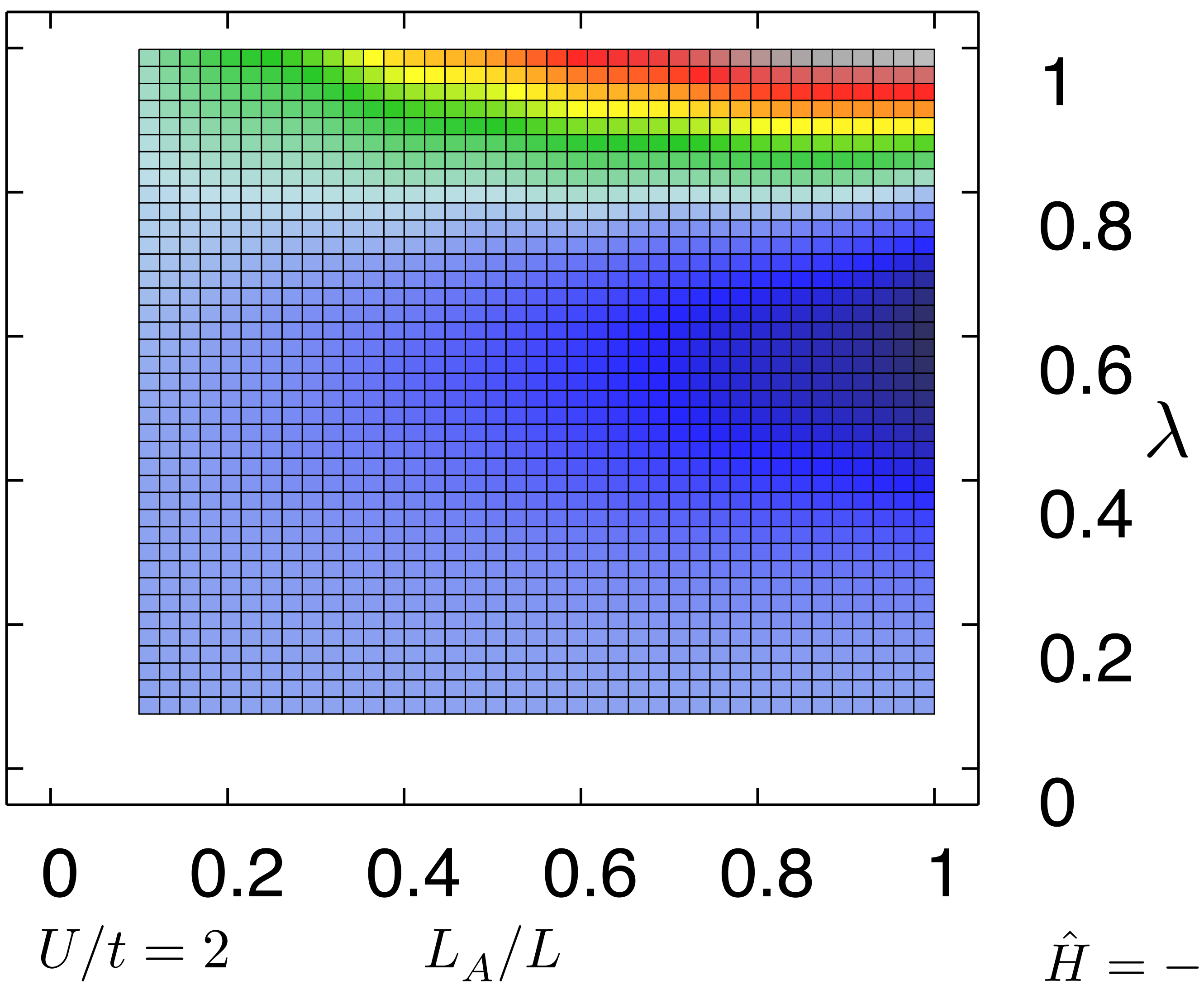

Figure: Monte Carlo results for the integrand $(1-n)^{-1}\langle \tilde{Q}_\lambda[\{\sigma\}]\rangle_\Gamma$ *for the Hubbard model at half-filling for order* $n = 2$.

$$S_{n,A} = S_{n,A}^{(0)} + \frac{1}{1-n}\int_0^1 d\lambda \, \langle \tilde{Q}_\lambda[\{\sigma\}]\rangle_\Gamma$$

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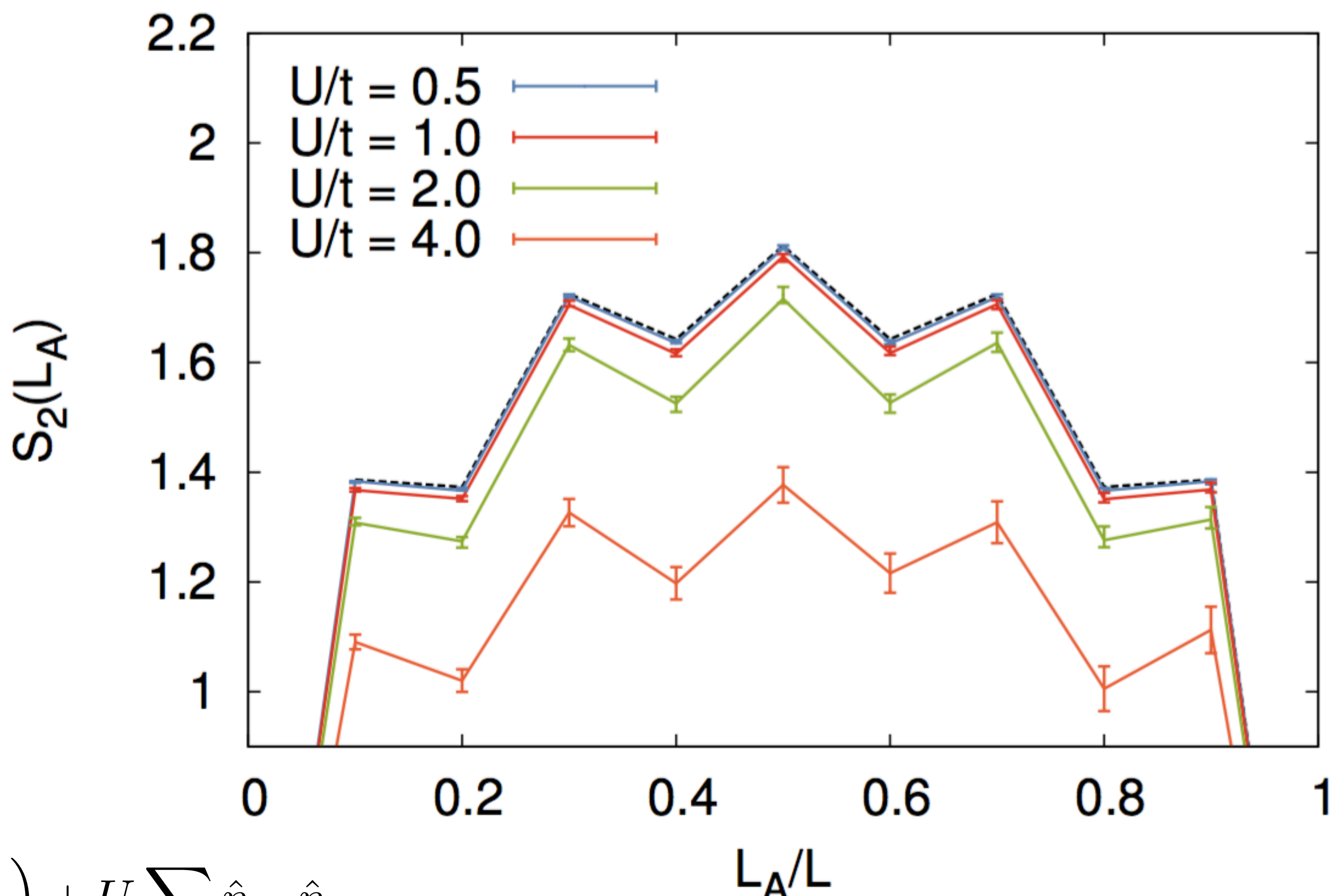
J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

❖ Our formalism successfully reproduces exact results for one-dimensional fermions.

Figure: Results for a strongly coupled, one-dimensional Hubbard model at half-filling. Error bars show the Monte Carlo results, whereas solid lines show the values obtained by exact diagonalization. The noninteracting case is shown dashed.



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$$S_{A,n} = S_{A,n}^{(0)} + \frac{1}{1-n} \int_0^1 d\lambda \, \langle \tilde{Q}_\lambda[\{\sigma\}] \rangle_\Gamma$$

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- The auxiliary parameter plays the role of the area increment.
- The partition of $\lambda \in [0,1]$ is **not unique**, and refinement allows for factors arbitrarily close to unity at the cost of linear scaling.

J.E. Drut, **W.J. Porter**, Phys. Rev. B **92**, 125126 (2015).

HOW IS IT CALCULATED?

- Other parameterizations will include these correlations differently changing the **cross sections.**

$$\Gamma(\lambda; g) = \int \mathcal{D}\{\sigma\}\; P[\{\sigma\}]\, Q^{\lambda}[\{\sigma\}]$$

$$\frac{1}{1-n} \ln \Gamma(1; g) = S_{A,n}$$

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J.E. Drut, **W.J. Porter**, arXiv:1508.04375.

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J.E. Drut, **W.J. Porter**, arXiv:1508.04375.

HOW IS IT CALCULATED?

- This second method produces much more predictable variation in the auxiliary parameter.

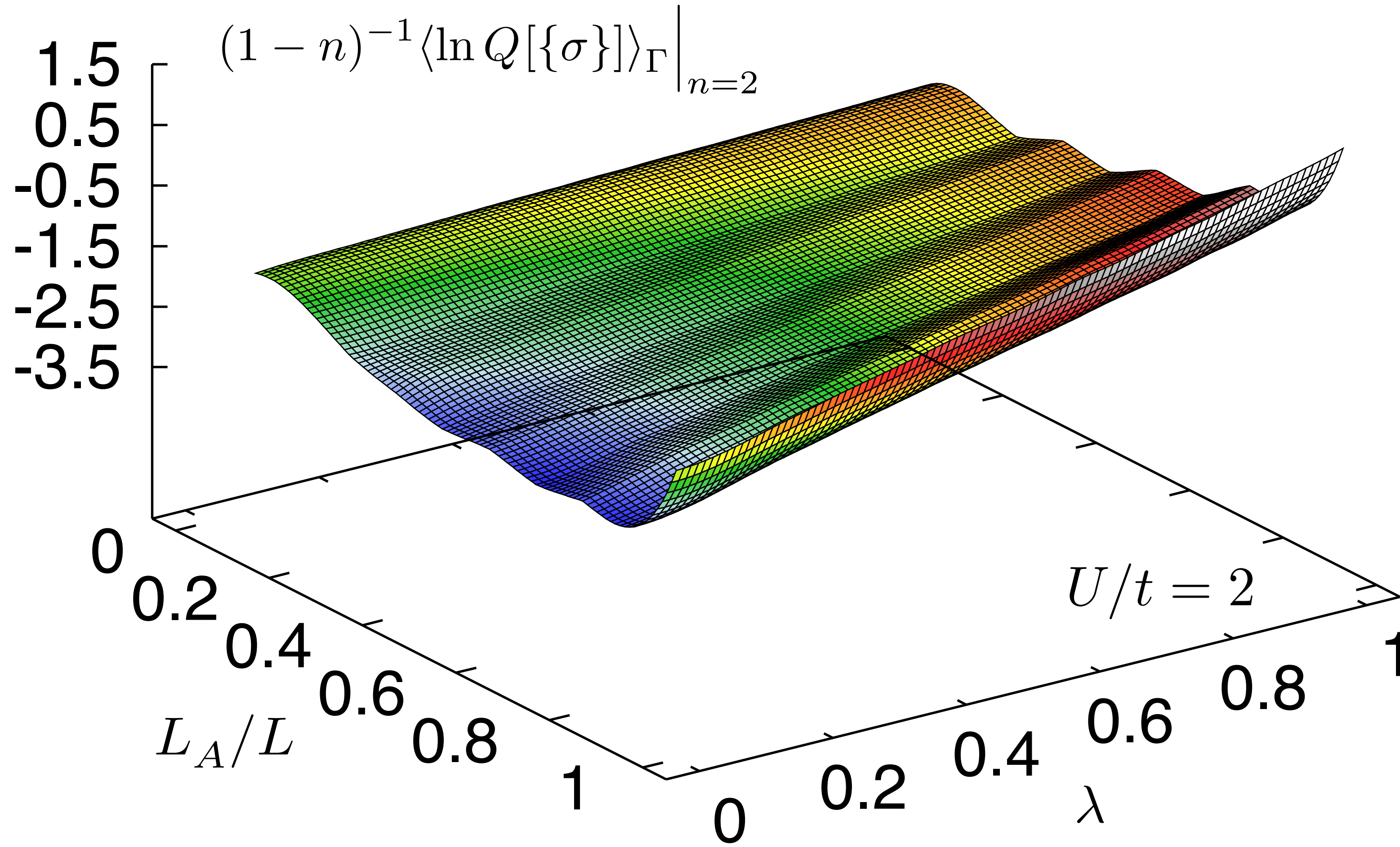

Figure: Monte Carlo results for the integrand for the Hubbard model at half-filling.

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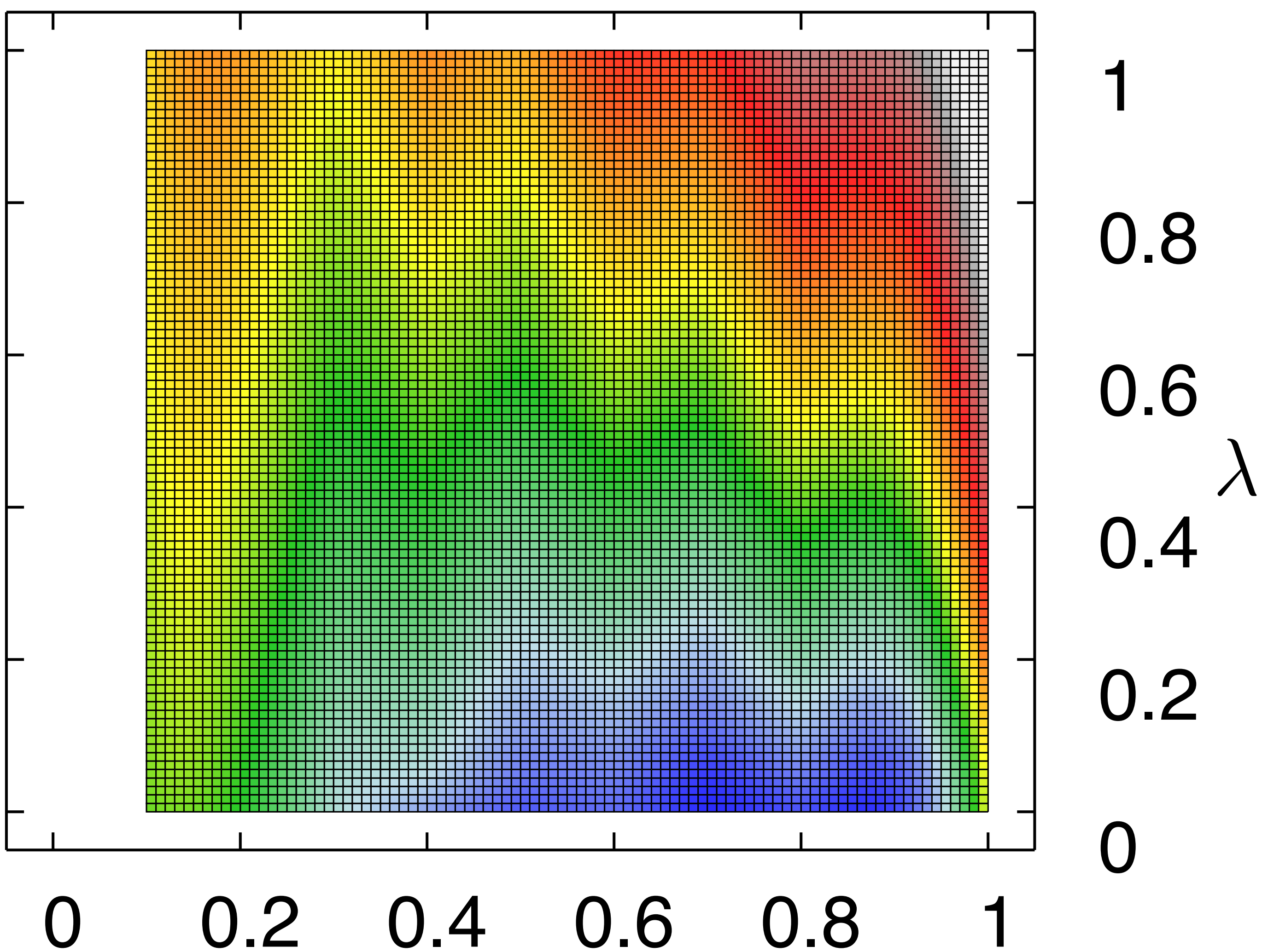
J.E. Drut, **W.J. Porter**, arXiv:1508.04375.

HOW IS IT CALCULATED?

- Much less resolution is required to obtain a reasonable uncertainty for the entanglement entropy.



$U/t = 2$ $\qquad L_A/L$

J.E. Drut, **W.J. Porter**, arXiv:1508.04375.

Figure: Monte Carlo results for the integrand for the Hubbard model at half-filling and for second order.

$$S_{A,n} = \frac{1}{1-n}\int_0^1 d\lambda \, \langle \ln Q[\{\sigma\}]\rangle_\Gamma$$

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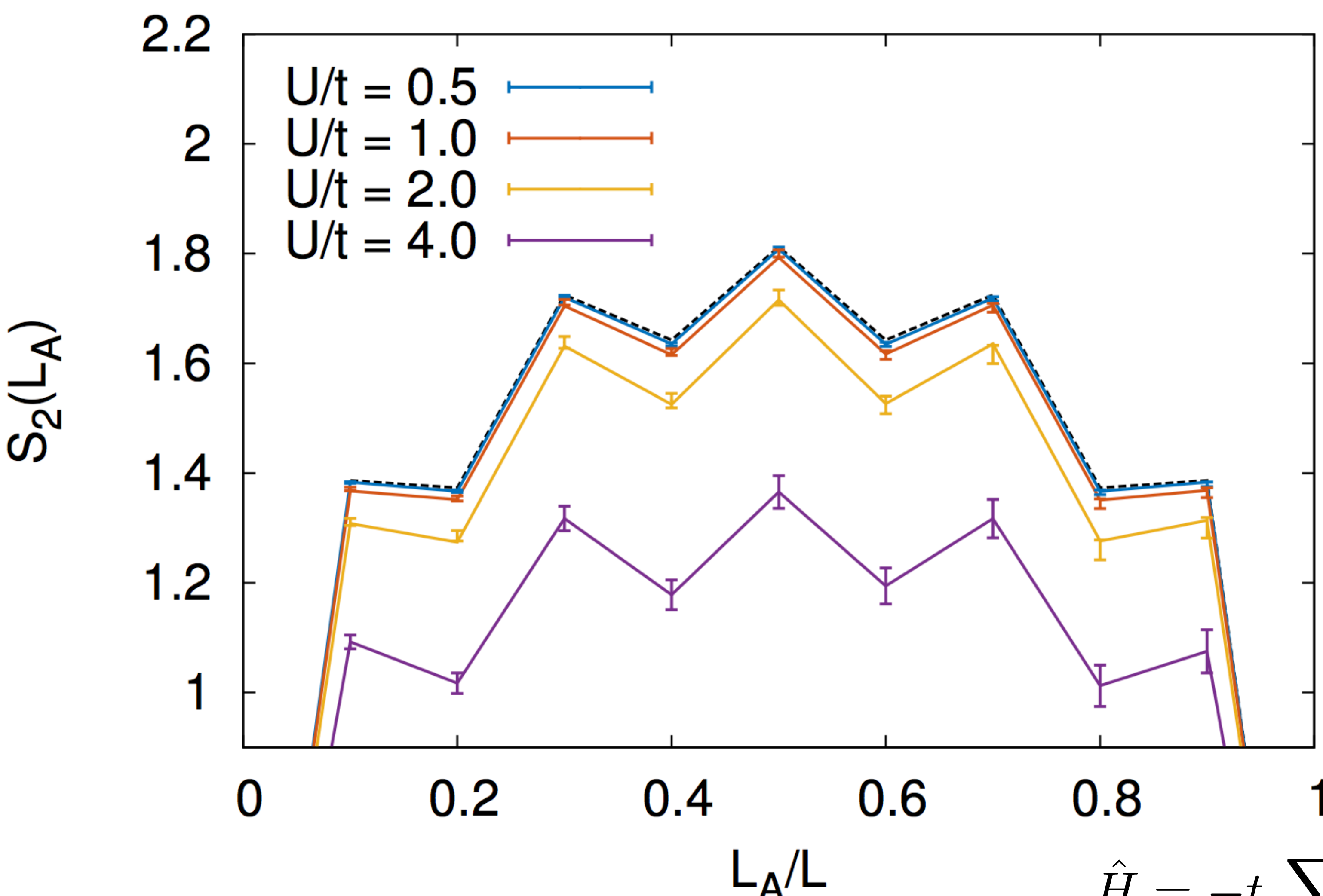
HOW IS IT CALCULATED?

- Relaxed discretization requirements for the auxiliary parameter produce results similar in quality to those seen earlier.



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J.E. Drut, **W.J. Porter**, arXiv:1508.04375.

WHAT'S NEW?

- We want to look at the **unitary Fermi gas.**
- This system has seen **staggering experimental attention.**

$$\hat{H} = \int d^3x \left[\sum_{s=\uparrow,\downarrow} \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) - g\, \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \hat{\psi}_\uparrow(\mathbf{x}) \hat{\psi}_\downarrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow(\mathbf{x}) \right]$$

$$0 \leftarrow k_F r_0 \ll 1 \ll k_F a \to \infty$$

$$k_F = \left(3\pi^2 n\right)^{1/3}$$

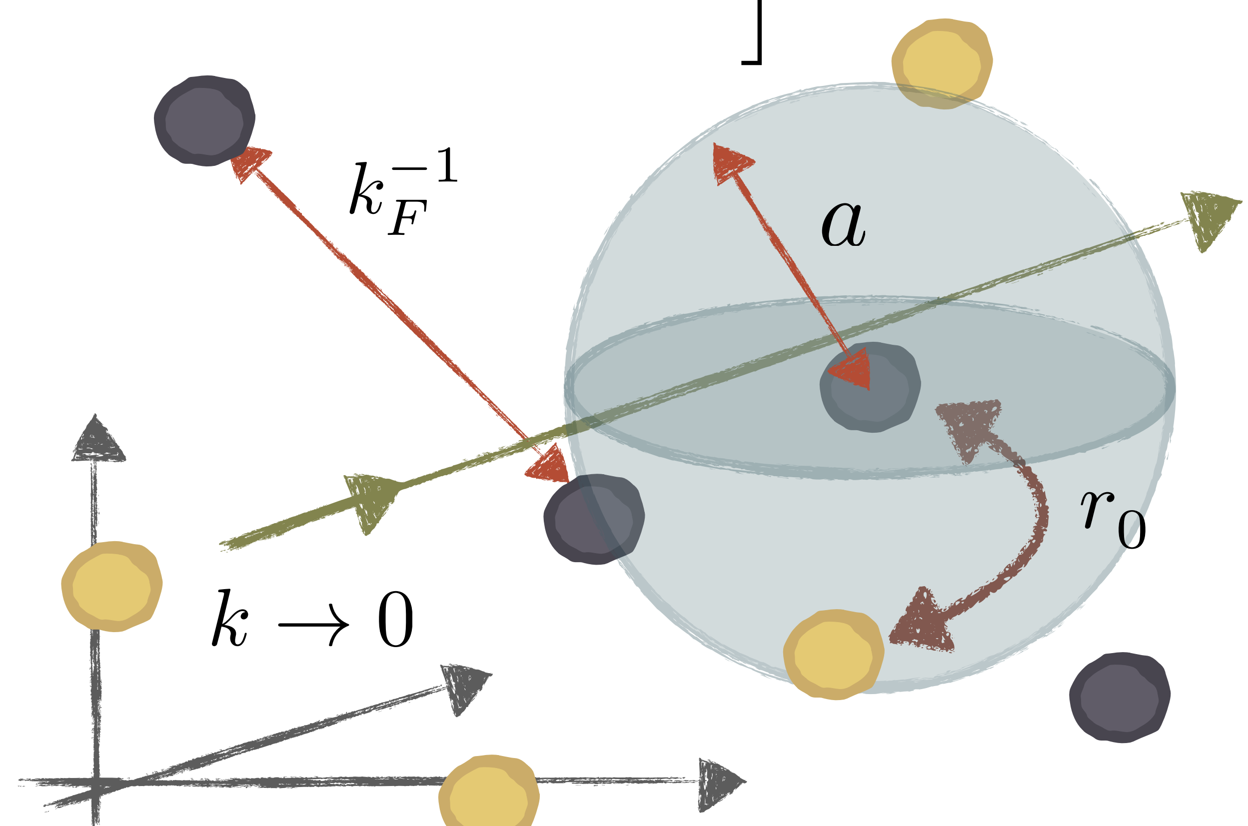

Figure: An interacting Fermi gas with two species and a finite range.

I. Bloch, J. Dalibard, W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
S. Giorgini, L.P. Pitaevskii, S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. Lett. **96**, 090404 (2006).
C. Cao, E. Elliott, J. Joseph, H. Wu, J. Petricka, T. Schäfer, J.E. Thomas, Science 331 (6013), 58-61.

WHAT'S NEW?

- The resonant Fermi gas is a **strongly interacting** system.
- Lacking small dimensionless parameters, this regime is **difficult to attack with perturbation theory**.
- It has the same number of scales as the noninteracting gas.
- The Fermi gas demonstrates **nonrelativistic scale invariance**.

E. Braaten, L. Platter, Phys. Rev. Lett. **100,** 205301 (2008).
Y. Nishida, D.T. Son, Phys. Rev. D **76**, 086004 (2007).
Y. Nishida, D.T. Son, Lecture Notes in Physics **836**, 233-275 (2012).

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- **Universality** implies the results enjoy applicability across a **vast range of length scales.**

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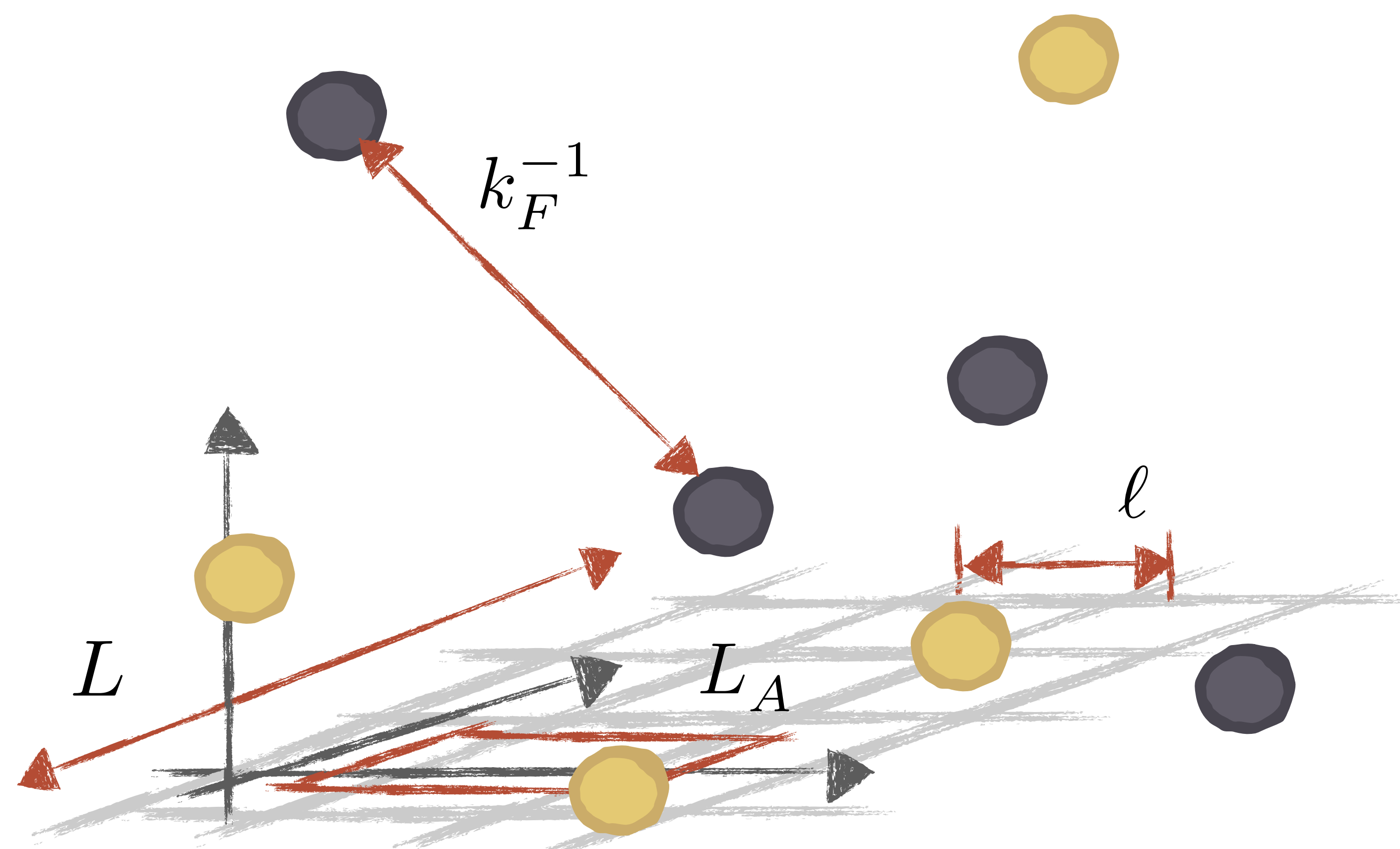

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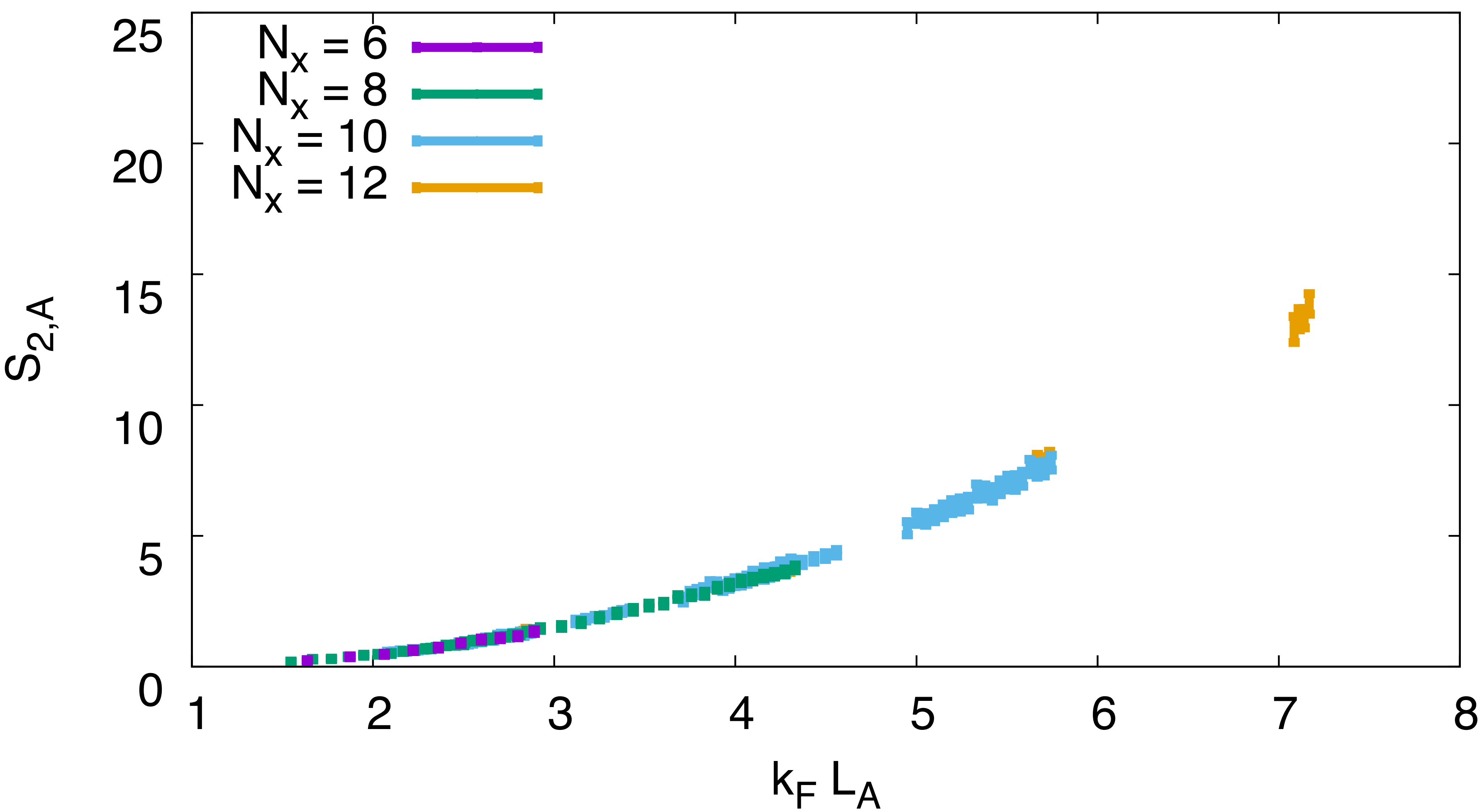

Figure: The second-order Rényi entanglement entropy for several volumes as a function of the region size.

J.E. Drut, **W.J. Porter**, Unpublished.

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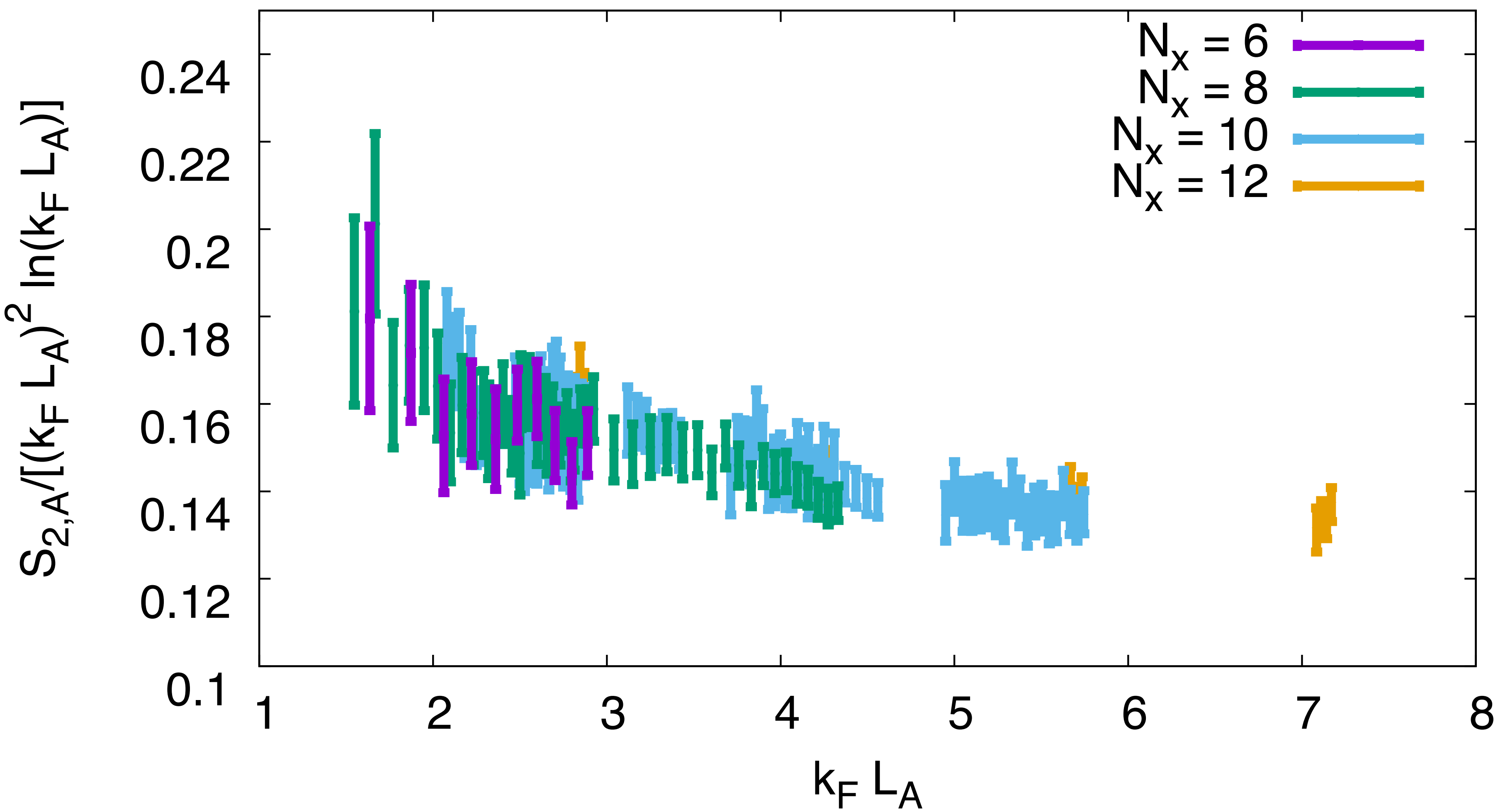

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J.E. Drut, **W.J. Porter**, Unpublished.

WHAT'S NEW?

- Results suggest that the leading behavior is **very similar to that of the noninteracting gas**.
- This result isn't entirely surprising due to the diminishing effect of interactions with increasing dimension.
- More data taken with **larger lattice sizes** is required to see differences residing largely in the **subleading behavior**.

J.E. Drut, **W.J. Porter**, Unpublished.

SUMMARY AND CONCLUSIONS

- Entanglement comprises correlations in many-body quantum systems that are not only missed by conventional local order parameters but also **largely uncharacterized**.

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- ❖ Work is underway toward **refining our calculations** for the resonant Fermi gas.
- ❖ Characterizing entanglement in this system provides a meaningful **benchmark for theoretical techniques** as well as a **prediction for future experiments**.