Finite size errors and linked cluster expansions

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Aims

Finite size effects in standard ED calculations

Linked cluster and numerical linked cluster expansions

Application to disordered systems

MBL work

Quench a homogeneous thermal state of spins (or impenetrable bosons) into a disordered Hamiltonian, and look for thermalization at infinite time.

Results "in the thermodynamic limit" when converged.

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Quench a homogeneous thermal state of spins (or impenetrable bosons) into a disordered Hamiltonian, and look for thermalization at infinite time.

Results "in the thermodynamic limit" when converged.

Disorder is binary, {h,-h}

Checking for thermalization

Thermal: $$\langle\hat{\mathcal{O}}\rangle_{\rm GE} \equiv \frac{{\rm Tr} e^{-\beta\hat{H}}\hat{\mathcal{O}}}{Z(\beta)}$$

Temperature : $$\frac{{\rm Tr} e^{-\beta\hat{H}}\hat{H}}{Z(\beta)} = Tr\rho_I\hat{H}$$

Check: $$\frac{\langle\hat{\mathcal{O}}\rangle_{\rm DE} - \langle\hat{\mathcal{O}}\rangle_{\rm GE}}{\langle\hat{\mathcal{O}}\rangle_{\rm GE}} \stackrel{?}{=} 0$$

Model

Impenetrable bosons with random chemical potential

$$\hat{H} = \sum_i \left[-t(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{h.c.}) + V \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+1} - \frac{1}{2} \right) \right]$$

$$+ \sum_i h_i (\hat{n}_i - \frac{1}{2})$$

Equivalently, Heisenberg spin chain with random field.

Model

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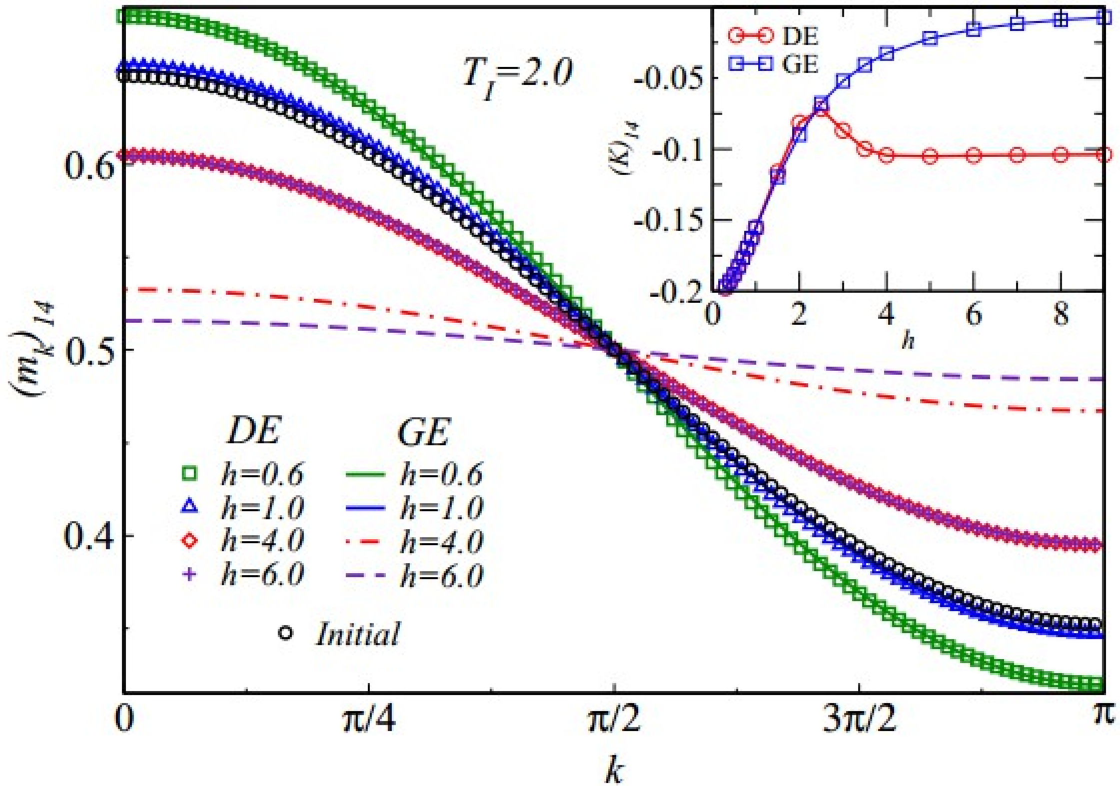
$$+ \sum_i h_i (\hat{n}_i - \frac{1}{2})$$

$$\uparrow$$

$$\{-h, h\}$$

Results

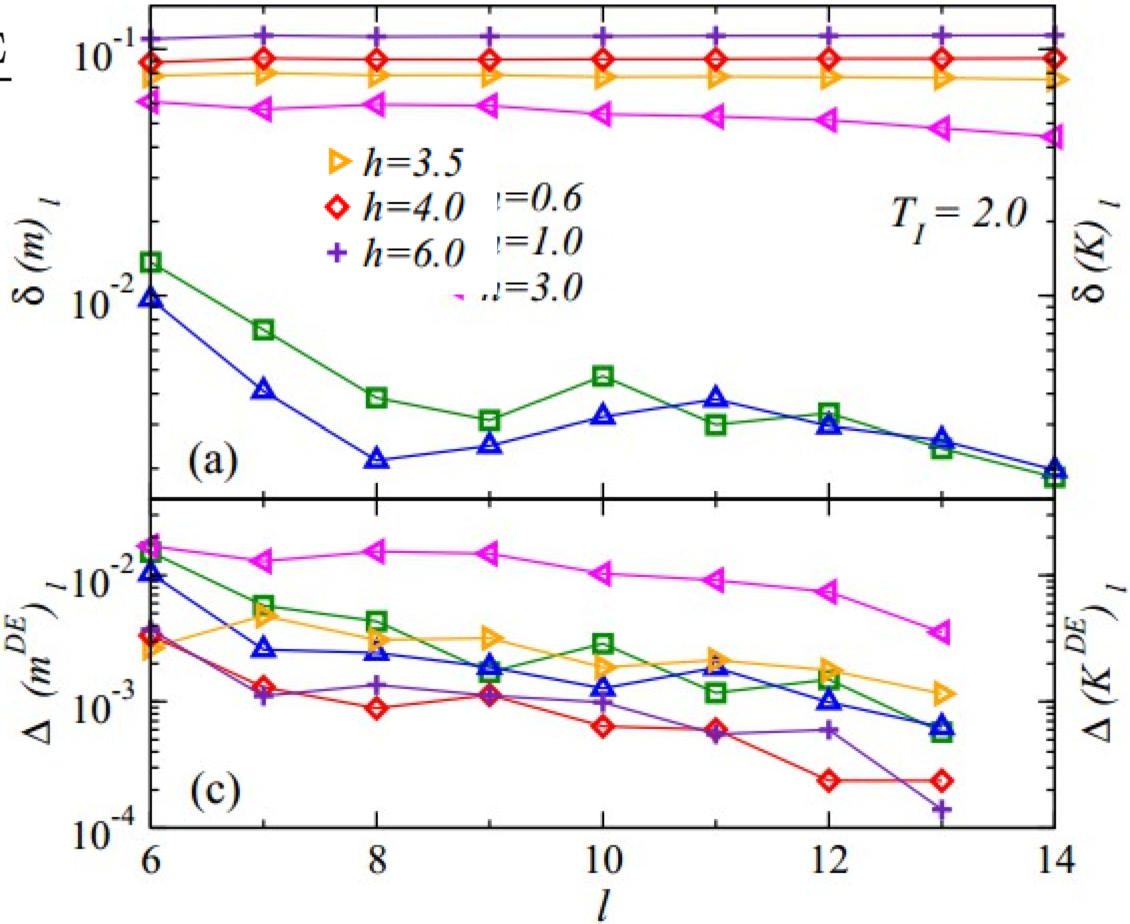
Fourier transform of single particle correlations



Tang, DI, Rigol, Phys. Rev. B 91, 161109(R)

Results

$$\delta m_l = \frac{\langle m_l \rangle_{\mathrm{DE}} - \langle m_l \rangle_{\mathrm{GE}}}{\langle m_l \rangle_{\mathrm{GE}}}$$



Tang, DI, Rigol, Phys. Rev. B 91, 161109(R)

Linked cluster expansions

… and why use them?

Finite size errors

How do finite size errors scale with system size in ED?

Finite size errors

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	Canonical	Grand Canonical
Open		
Periodic		

Finite size errors

How do finite size errors scale with system size in ED?

	Canonical	Grand Canonical
Open	$\frac{1}{L^p}$	$\frac{1}{L^p}$
Periodic	$\frac{1}{L^p}$	e^{-L}

(at finite temperature, for a phase without long range order)

DI, Srednicki, Rigol, Phys. Rev. E 91, 062142 (2015)

Why is this so?

$$\ln Z(\beta) = \ln \mathrm{Tr}(1) - \beta \frac{\mathrm{Tr}(\hat{H})}{\mathrm{Tr}(1)} + \frac{\beta^2}{2}\left[\frac{\mathrm{Tr}(\hat{H}^2)}{\mathrm{Tr}(1)} - \frac{\mathrm{Tr}(\hat{H})^2}{\mathrm{Tr}(1)^2}\right] + \cdots$$

Periodic and open boundaries

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Treat it as a cluster expansion

Finite

Infinite

Periodic and open boundaries

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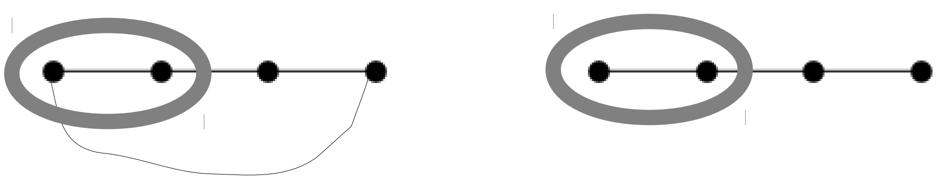


$$\frac{\ln Z}{N} \sim \frac{N}{N} \qquad \sim \frac{N-1}{N}$$

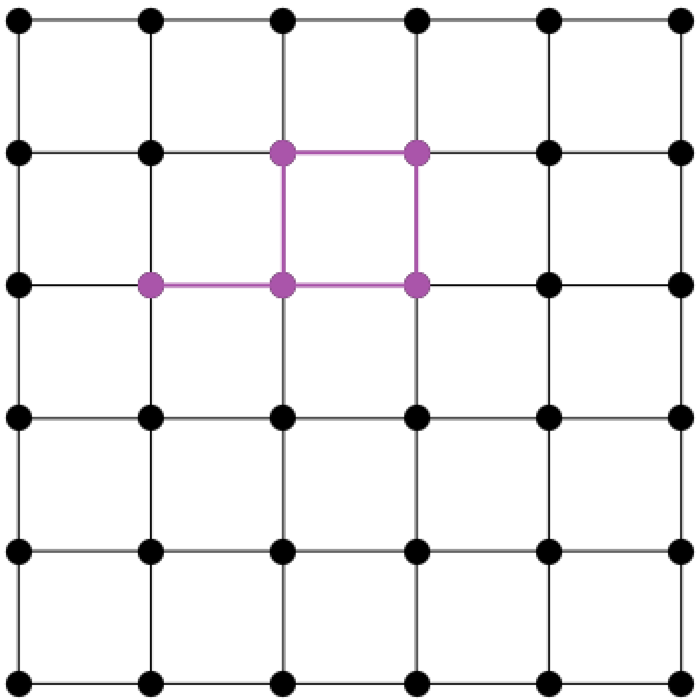
Summary of first part

$\sim O(e^{-L})$ With periodic boundaries, we produce clusters which do not exist in the infinite system, but we get the co-efficients up to order l correct.

$\sim O(1/L)$ With open boundaries, we don't produce any spurious clusters but we get the combinatoric piece of the coefficient wrong in all terms.

Can we fix the combinatorics and hope to do better than periodic boundaries?

Linked cluster expansions



Counting of various clusters embedded in a larger lattice

Extensivity is key

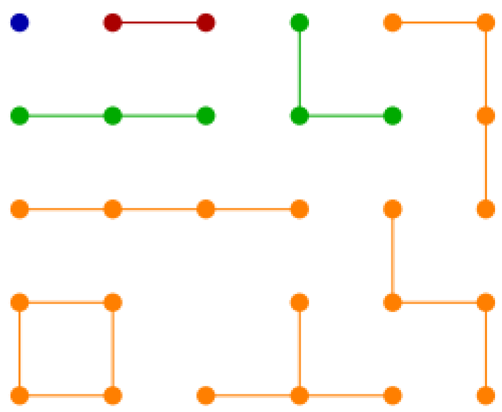
For infinite lattice, so is translational invariance

Rigol, Bryant, Singh, Phys. Rev. Lett. 97, 187202 (2006)

Tang, Khatami, Rigol, Computer Physics Communications 184, 557-564 (2013)

Linked cluster expansions

For an extensive property $\mathcal{O}$, we can calculate the "per unit volume" quantity using

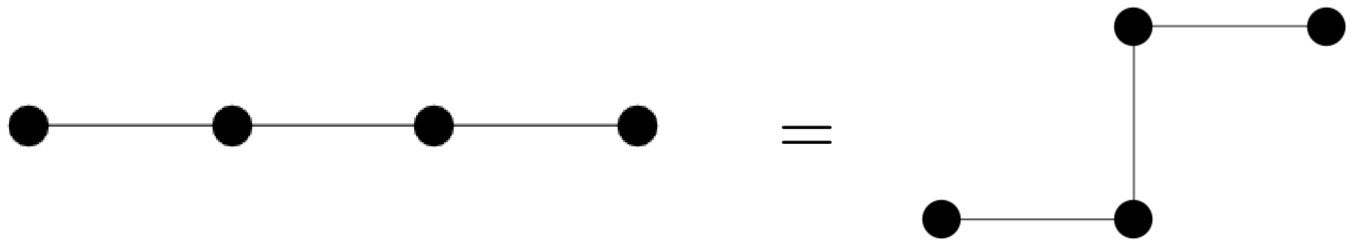


$$\frac{\mathcal{O}}{N} = \sum_{c} M(c) \times W_{\mathcal{O}}(c)$$

$$W_{\mathcal{O}}(c) = \mathcal{O}(c) - \sum_{s \subset c} W_{\mathcal{O}}(s)$$

Sykes et al, J. Math. Phys. 7 1157 (1966)

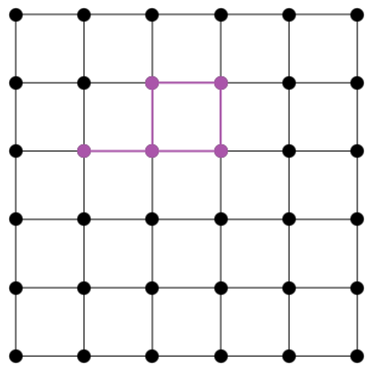
Topologically distinct clusters

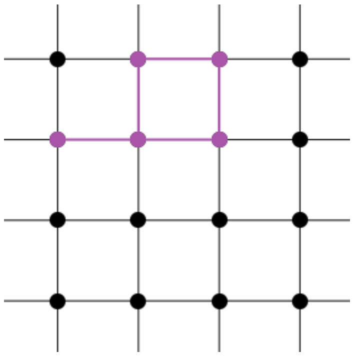


If the Hamiltonians are identical

Reduces number of distinct clusters to evaluate

Finite and infinite lattices





Clusters that involve the edges are different from clusters in the bulk

Clusters are independent of where they are on the lattice if we have translational inv.

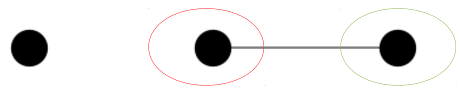
1D example

For a model with only nearest neighbor couplings.

- $$W_1 = \mathcal{O}_1$$

1D example

For a model with only nearest neighbor couplings.



$$W_1 = \mathcal{O}_1$$

$$W_2 = \mathcal{O}_2 - 2W_1 = \mathcal{O}_2 - 2\mathcal{O}_1$$

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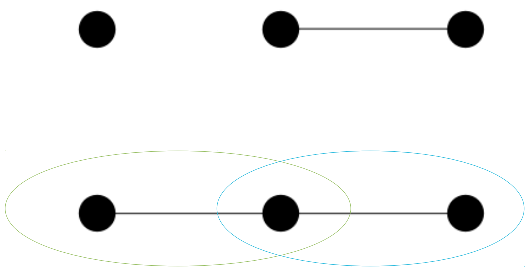

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$$W_3 = \mathcal{O}_3 - 2W_2 - 3W_1 = \mathcal{O}_3 - 2\mathcal{O}_2 + \mathcal{O}_1$$

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$$\frac{\mathcal{O}}{N} = W_1 + W_2 + W_3 = \mathcal{O}_3 - \mathcal{O}_2$$

$$(= \mathcal{O}_n - \mathcal{O}_{n-1})$$

1D Ising

$$-\frac{\beta F_{\text{exact}}}{L} = \log(e^{\beta J} + e^{-\beta J})$$

$$\mathcal{O} = -\beta F$$

$$\mathcal{O}_1 = \log(2), \qquad \mathcal{O}_2 = \log[2(e^{\beta J} + e^{-\beta J})]$$

$$\frac{\mathcal{O}}{L} = \mathcal{O}_2 - \mathcal{O}_1 = -\frac{\beta F_{\text{exact}}}{L}$$

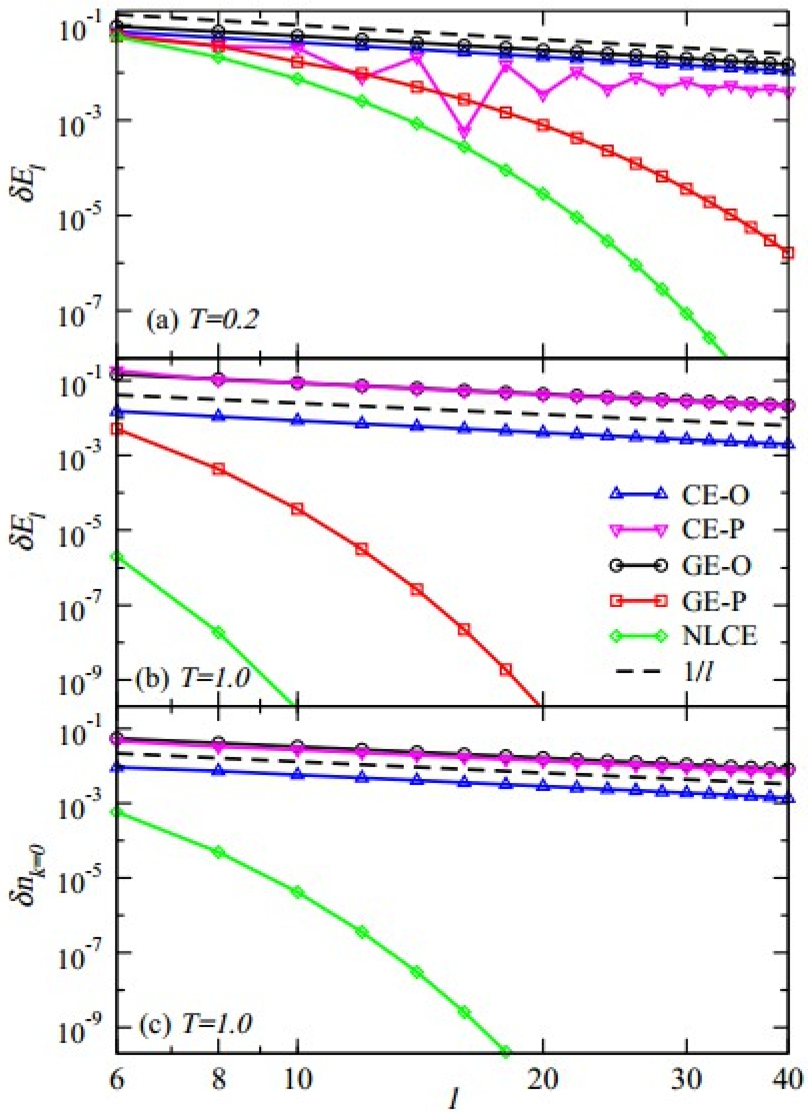
All higher weights are zero

NLCE vs Grand canonical

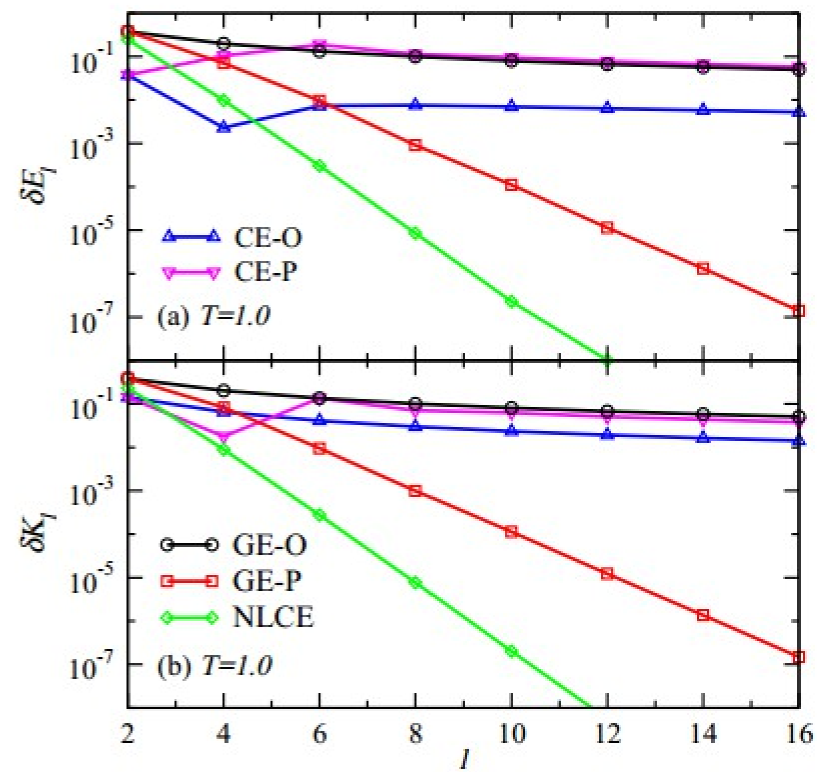
Grand canonical with periodic boundaries will always get the l-th order term in the expansion of the ln(Z) wrong.

NLCE doesn't suffer from spurious clusters and the scheme fixes the combinatorics issue in the open boundary grand canonical calculation. Can be correct beyond order l.

Examples



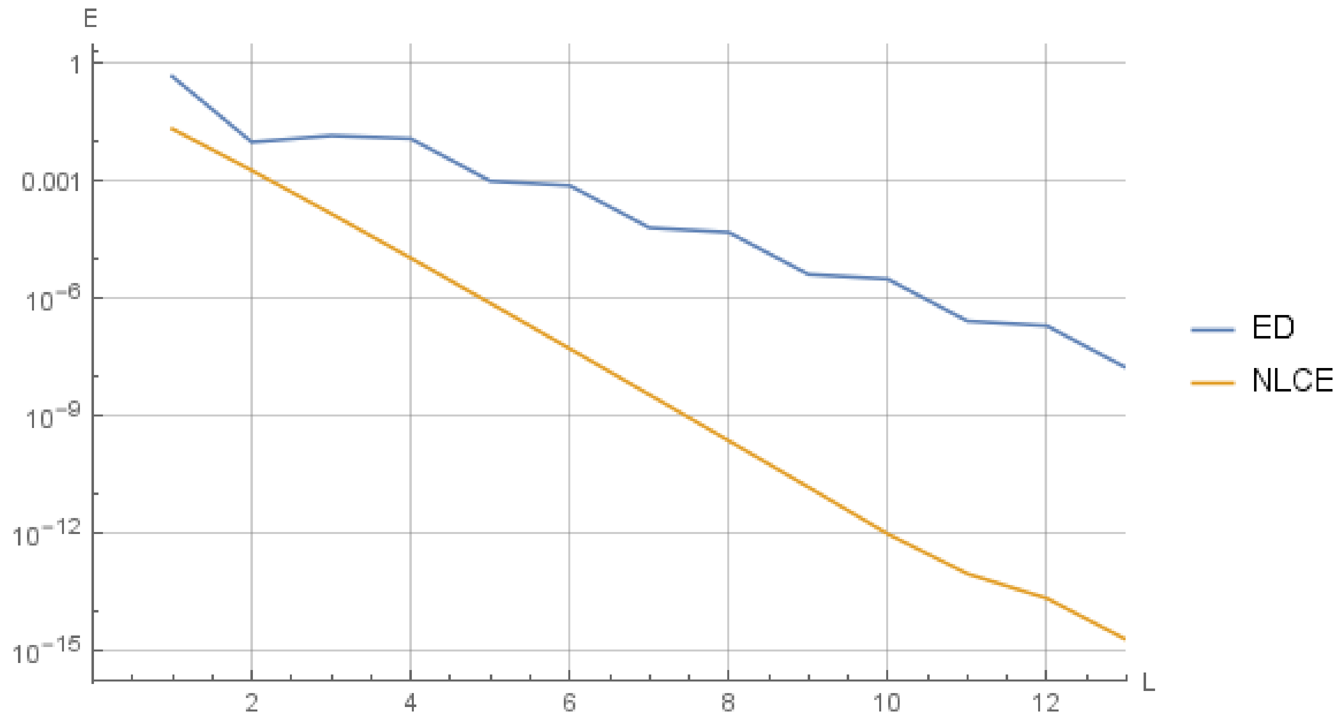
Noninteracting fermions



Interacting fermions

1D Heisenberg model

Difference in energy (at some fixed temperature) with thermodynamic limit (exact result).



Dealing with disorder

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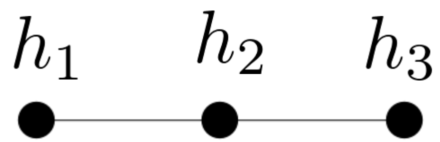
Have to restore translational invariance

Sum over **ALL** disorder realizations at each order

$$\overline{\mathcal{O}_3} = \frac{1}{2^3} \sum_{h_1, h_2, h_3}$$



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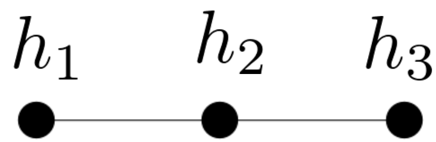


A lot of configurations, but can be parallelized

Quenches

$$\mathcal{O}(t) = \sum_{\alpha,\beta} \langle\alpha|\rho_I|\beta\rangle\langle\beta|\mathcal{O}|\alpha\rangle e^{it(E_\alpha - E_\beta)}$$

Eigenstates of the
final Hamiltonian

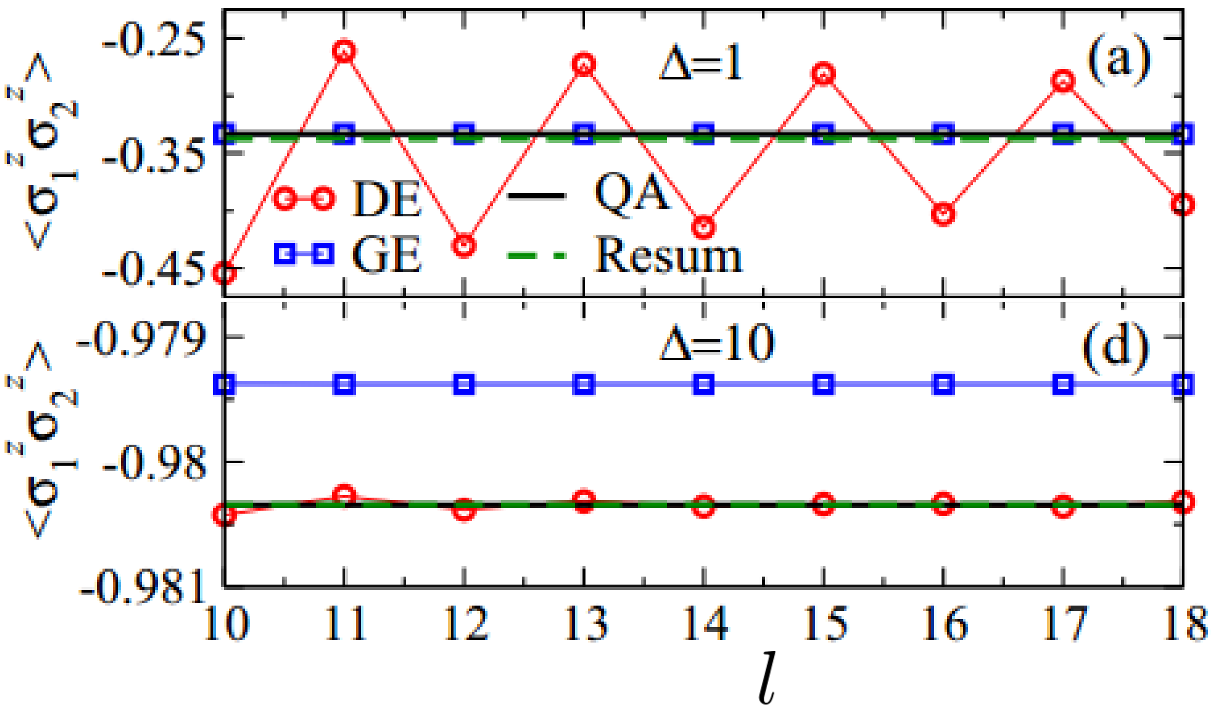
Quenches

$$\mathcal{O}(t) = \sum_{\alpha,\beta} \langle\alpha|\rho_I|\beta\rangle\langle\beta|\mathcal{O}|\alpha\rangle e^{it(E_\alpha - E_\beta)}$$

$$= \sum_{\alpha,\beta;\, E_\alpha = E_\beta} \langle\alpha|\rho_I|\beta\rangle\langle\beta|\mathcal{O}|\alpha\rangle$$

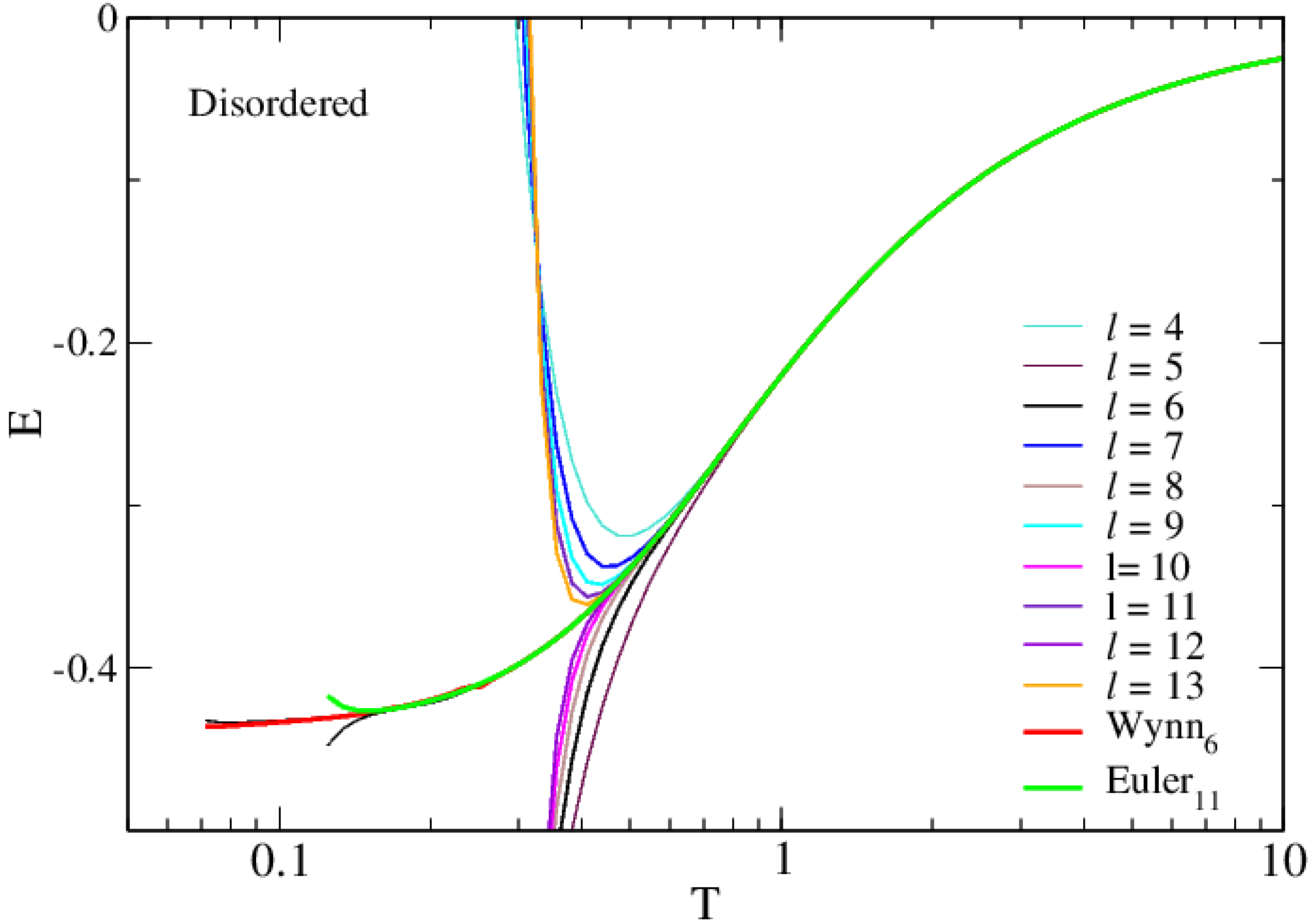
$$+ \sum_{\alpha} \langle\alpha|\rho_I|\alpha\rangle\langle\alpha|\mathcal{O}|\alpha\rangle$$

Quenches

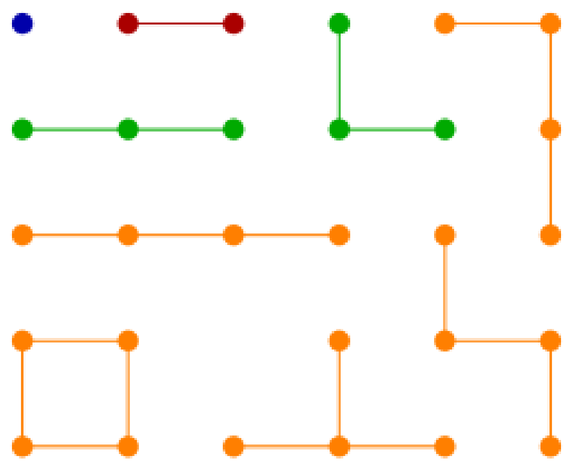


Rigol, Phys. Rev. E 90, 031301(R) (2014)

Resummation



Two dimensions



Vanilla ED gives us very few orders and large jumps – 1, 4, 9, 16, 25, …

NLCEs give us several intermediate orders and potentially allows better finite size extrapolation

Look at Tang, DI, Rigol, Phys. Rev. B 91, 174413 (2015) for an implementation to study binary disorder in 2D spin models

Summary

NLCEs work better than ED in all cases where you need to calculate extensive observables, and can be used to study disordered systems as well.