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SJSU Undergraduate Research Grants

Cluster Expansion for 1D Lattice Models

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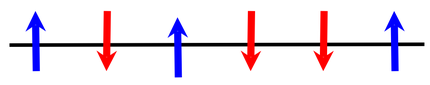
Abstract

Exact solutions of crystal lattice models of electrons in solids are often presented for a small number of atomic sites on finite clusters.

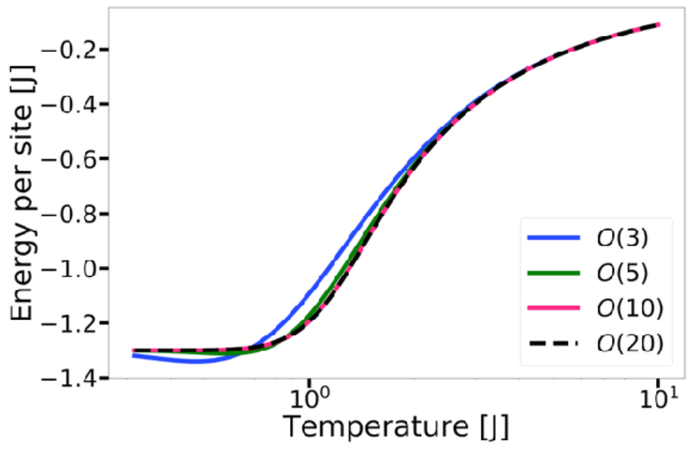
We are, however, interested in these solutions in the limit where we can explain the phenomena we observe at the macroscopic scales.

Here, we develop a method in 1D that is capable of systematically approaching that limit using properties of finite clusters. We test the method on two toy models; a model for ferromagnets and another for itinerant electrons.

Classical: Ising Model



$$E = -J \sum_{<i,j>} s_i s_j - B \sum_i s_i$$



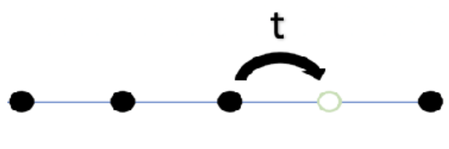
O(N) refers to the property per site in order *N*.

As the number of sites increases, the energy per site converges towards its value at the thermodynamic limit.

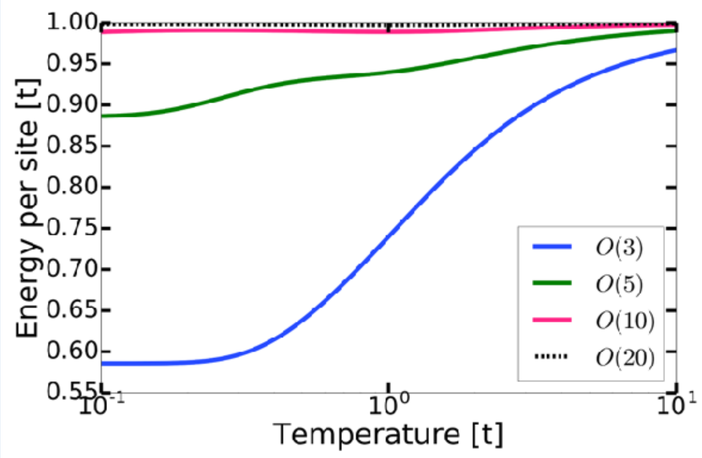
Research Questions

- How can we systematically eliminate effects in lattice models due to finite sizes using *cluster expansion* techniques?
- Do we expect conducting/insulating/magnetic properties to survive as we take $N \to \infty$, where *N* is the system size?

Quantum: Non-Interacting Hubbard Model



$$H = -t \sum_{<i,j>} C^{+}_{i\sigma} C_{j\sigma} \cdot$$



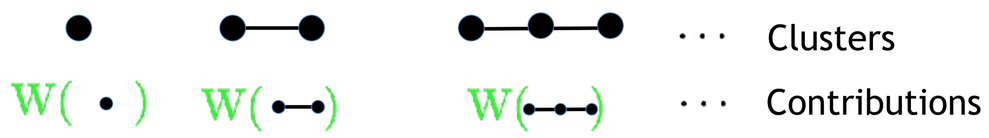
$$- \mu \sum_i (n_{i\uparrow} - n_{i\downarrow})$$

As *N* increases, we see a convergence to the chemical potential value (μ), which is expected in the thermodynamic limit.

(Here $t = 1, \mu = 1$)

Method: Numerical Linked-Cluster Expansion in 1D

Identify all the clusters that can be embedded in a chain:



$$W(m) = E(m) - \sum_{n \subset m} L(n) W(n)$$

$$O(m) = \sum_{n=1}^{m} W(n)$$

m, n : Cluster Sizes
L : Multiplicity
E : Total Energy
O : Apprx. to Energy in Macro. Limit

References and Acknowledgements

A short introduction to numerical linked-cluster expansions, B Tang, E Khatami, M Rigol, Computer Physics Communications 184 (3), 557-564

Thermodynamics of strongly interacting fermions in two-dimensional optical lattices, E Khatami, M Rigol, Physical Review A 84 (5), 053611

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