Oral Exam Topic
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Quantum Lattice Models

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1 Introduction

Simple models are an indispensable tool for the theorist. Nature presents us with extremely complicated systems with $\sim 10^{23}$ particles, each behaving in a manner that depends on all of the others. How can one begin to understand the behavior on the scale of human experience when there is no way to calculate analytically or numerically? We need to be clever and reduce the problem to its essential elements (and not further).

Many interesting problems for the condensed matter theorist involve the behavior of electrons in a crystal lattice. A large part of the behavior of materials, in particular, metals, semiconductors, and band insulators have been well explained. The BCS theory for superconductors gives a good picture for the "low T_c" superconductors. However, there are still many unexplained phenomena in materials like the "high T_c" superconductors and the Heavy Fermion Materials. These systems have strongly correlated electrons, and so many of the usual techniques (like ignoring correlations) do not adequately describe the physics.

So, in order to approach the problem, we make a simple model. Each electron can only be located on a site of a lattice. Each lattice site can represent the ions of the solid, and the electron will be localized to that atom. Even with this simplification, we can still only solve the models exactly only for special cases such as in one or two dimensions, infinite dimensions, non-interacting limits, etc.

2 Quantum Lattice Models

Each site of the lattice can be occupied (by electrons, for example). and so we can write a Hamiltonian for the system using creation and annihilation operators on the sites. One example of such a model is the well known Hubbard Model, with the Hamiltonian:

$$\mathcal{H}_{HM} = -t \sum_{<i,j>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

Where $c^\dagger_{i\sigma}$ creates an electron with spin σ on site i and $n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$. The first term, the hopping term, allows for the "hopping" of an electron from site i to a neighboring site j (the angle bracket $< i, j >$ indicates nearest neighbors). If $U > 0$, there is a short range repulsion of electrons. There is an energy cost for two electrons to occupy the same site. That electrons only "see each other" if they are occupying the same site is justified by fact that the electrons are screened in the real solid, and the interaction decays exponentially.

Another term may be added to the Hubbard Model that favors the occupation of one sub-lattice. This model is referred to as the Ionic Hubbard Model (IHM):

$$\mathcal{H} = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \Delta \sum_i (-1)^i n_i \tag{2}$$

At half filling, when $U - \Delta >> t$, the ground state will be the same as the Hubbard Model at large U, namely a Mott Insulator with anti-ferromagnetic ordering. At $\Delta - U >> t$, however, there will be double occupancy on all of the sites favored by Δ, and the ground state will be a band insulator. It has been shown by Batista and Aligia [3] that in one dimension, the IHM has a distinct "bond ordered" phase in between. However, the methods employed in [3] for the IHM in one dimension do not extend well to higher dimensions, which leads us to explore another technique.

3 Linked Cluster Expansions

We want to calculate an extensive property P on a lattice $\mathcal{L}$ with N sites. For example, P might be the ground state energy, spin-spin correlations, dimer-dimer correlations, etc.. The key idea is to express P as a sum over all distinct clusters c

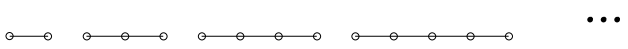
$$\frac{P(\mathcal{L})}{N} = \sum_c L(\mathcal{L}, c) * W(c) \tag{3}$$

where $L(\mathcal{L}, c)$ is the lattice constant and

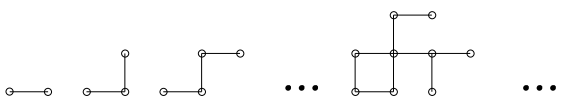
$$W(c) = P(c) - \sum_{g \subset c}{}' W(g) \tag{4}$$

is the weight of the cluster, $P(c)$ is the series expansion for the property defined on the finite cluster c, and $g \subset c$ means that g is a linked cluster that can be embedded into c.

So, to implement the expansion ([1],[2]), we must first identify the number of relevant connected real-space clusters. Then, for each cluster, we construct the perturbation expansion for the extensive quantity (energy, correlation function) under consideration. Then finally, the results for the various clusters are then combined using "subgraph subtraction" to get the quantity per site on the infinite lattice. Identifying the finite number of relevant connected real-space clusters in one dimension is trivial:



In two or higher dimensions, one needs to generate a list of real space clusters:



Since most of the embeddings will give the same weight calculation as other embeddings. We can save a lot of computation by performing a weight calculation on only one of a set of embeddings with the same topology. For this, we can use our list of embeddings to generate a list of topologies, and a lattice constant for each topology.

Once we have the list of topologies, we can then construct a power series for the quantities on a finite cluster.

We begin by writing our Hamiltonian as

$$\mathcal{H} = \mathcal{H}_0 + \lambda \mathcal{H}_1 \tag{5}$$

And expand our energy and wave function as a power series in λ

$$E = \langle \mathcal{H} \rangle = \sum_i E_i \lambda^i \tag{6}$$

$$|\Psi(\lambda)\rangle = |0\rangle + \sum_i \lambda^i \sum_m a_{i,m} |m\rangle \tag{7}$$

Which we can iteratively solve to find the coefficients.

The results for the clusters are now combined via "subgraph subtraction" to get the weight of the cluster $W(c)$.

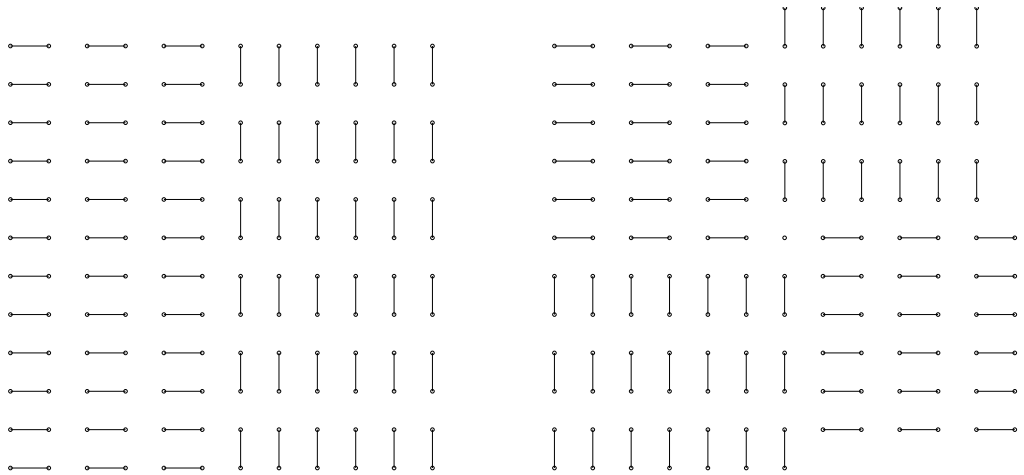
$$W(c) = P(c) - \sum_{g \subset c}{}' W(g) \tag{8}$$

This property allows for an excellent check of the algorithm. When the graphs are subtracted, the weight $W(c)$ should only contribute at an appropriate order. If it doesn't, then there is a problem in the weight calculation.

4 Projects

With this technique we are able to study many interesting problems in condensed matter theory. The techniques used to show that the IHM has a bond ordered phase between the band and Mott insulators do not work in higher dimensions. With linked cluster expansions, I would like to study the IHM in two dimensions to possibly establish the existence of a bond ordered phase. We can calculate the ground state energy, local moment, spin-spin correlation $\langle \vec{S}_i \cdot \vec{S}_j \rangle$, and dimer-dimer correlations $\langle \vec{S}_i \cdot \vec{S}_{i+1} \cdot \vec{S}_j \cdot \vec{S}_{j+1} \rangle$.

Other interesting problems involve studying the energy cost of a domain wall and a vortex:



There is interest ([4],[5]) in the quantum critical point between a Néel ordered and bond ordered phase where these vortex excitations, which carry spin 1/2 , may be deconfined.

5 Conclusion

Quantum Lattice Models are simple models that lead to extremely rich behaviors. By applying techniques such as linked cluster expansions combined with modern computers we will be able to explore aspects of these models that are as of yet still not well understood.

References

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