Master Thesis: Cluster-Perturbation Theory for fermion-boson problems

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1 Background

An iconic model in strongly correlated electrons is the Hubbard model describing itinerant, but strongly correlated, electrons, as well as its variants for various multi-orbital models. In the case of integer filling (half filling for the one-orbital case) and strong onsite repulsion, charge fluctuations are suppressed, and physics is dominated by the spin (and potential orbital) degrees of freedom. Neglecting charge fluctuations then leads to simpler, but still usually not exactly solvable models, like the t-J and Kugel-Khomskii models.

The simplest of these, the t-J model, boils down to a Heisenberg model at half filling. Even though the Néel state ($\uparrow, \downarrow, \uparrow, \dots$) is not the true ground state, it is a decent approximation for dimensions higher than one. This can most easily be exploited if spins are expressed in terms of bosons: While the transformation can still be made exact, terms with more than two bosons are typically neglected, and this is an approximation. For a nice discussion, see e.g. Ref. [1]. However, this only becomes a problem at high boson densities, i.e., when the magnetic background starts to loose too much of its ordered pattern.

A variety of approaches are based on such transformations, e.g., the self-consistent Born approximation (SCBA) allows us to obtain the spectral density of a hole moving in an antiferromagnetic (AFM) background by taking into account some classes of diagrams describing a fermion coupling to bosons. For an introduction, see Ref. [2, 3]; for applications to orbital models see Refs. [4–6]. The most important of the approximations may be the "non-crossing approximation", where bosons created last need to be annihilated first. In the AFM spin t-J model on the square lattice, the lowest-order diagrams violating this restriction drop out by symmetry [7], but their importance in general is hard to gauge.

More recently, an alternative approach termed "variational approximation" has been introduced, where states with a few bosons close to the hole are included in the equation of motion for a charge carrier. It has been applied to spin [8, 9], orbital [10] and spin-orbital models [11].

In the theses, cluster-perturbation theory [12, 13] and possibly the variational cluster approach [14] (quite different from the "variational approximation" mentioned in the previous paragraph) are to be used for the same problem. Both have been applied extensively to "Hubbard-like" models, i.e., the original models including charge fluctuations [10, 15, 16], but cannot easily be extended to spin models [17]. We do thus not have access to the large-J limit of t-J-like models. However, both approaches are valid for boson problems [18–20], and have been applied to electron-phonon models [21]. They are thus expected to work for spin models transformed into bosonic models, at least in the regime with few bosons, i.e. in the robustly ordered state.

2 Goals and Methods

In this Master's thesis, the spectral density for one (or a few) charge carrier (hole or electron) in t-J models is to be studied using cluster-perturbation theory, where the description of the AFM background is to be reformulated from spins into bosons.

If possible, the approach is to be extended to the variational cluster approach. An aim is here also to find out how suitable the variational cluster approach is for such problems.

Finally, connections to the "variational Ansatz" based on equations of motion [8–11] are to be clarified. While both approaches appear at first to be conceptually distinct, the physical limitations inherent in both are equivalent: There must not be too many bosons, and these must be located close to the charge carrier (and to each other).

2.2 Work program

- Understand cluster-perturbation theory and the Holstein-Primakoff transformation
- Implement square-lattice t-J model with spins transformed into bosons. Existing code can be extended, or new code developed. Test and evaluate spectral density.
- Go to triangular lattice, where the non-crossing approximation of the SCBA is likely to be more of an issue.
- Other examples can be investigated, e.g., honeycomb model or multi-orbital models.
- Variational Cluster Approach
  - Check whether there are at this point major red flags that make it appear unsuitable and unrealistic. If so, extend previous point and go to following one.
  - Implement optimization of grand potential, e.g. w.r.t. boson number.
  - Gauge limits of the approach.
- Elucidate connections to equations-of-motion based approach.

3 Bibliography

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