DMRG overview

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1 Introduction

Suppose we are to find the single-particle Green function of a condensed matter system. The standard procedure is to find the irreducible self-energy Σ by Feynman diagram resummation (although there are subtleties concerning the well-definedness and uniqueness of Feynman diagram resummation techniques [1]). In strongly correlated systems, deciding diagrams with most contributions is generally hard, and brutal-force resummation proves intractable.

If, however, it is found that the self-energy (or two-particle vertex, or similar "n-particle self-energy diagrams") is highly local, then in principle, it can be replicated in a *few-body* model: suppose, for example, that $\Sigma_{\boldsymbol{ij}}$ is only important when $|\boldsymbol{i}-\boldsymbol{j}| \leq n$, then we can just choose a cluster of sites satisfying the $|\boldsymbol{i}-\boldsymbol{j}| \leq n$ condition, and integrate out the rest of electron modes, and in the resulting few-body model, $\Sigma_{\boldsymbol{ij}}$ is exactly the same as in the original model. The main obstacle now is to decide the parameters in this new few-body model, which can be solved by adopting a self-consistent scheme: $\Sigma_{\boldsymbol{ij}}$, together with the free part of the original model, decides the one-particle Green function, which then can be used to fit the parameters in the few-body model, and then the few-body model can be solved to update the self-energy.

It can be seen that diagrammatically speaking, this idea is also a resummation strategy, though here we pick up diagrams according to their locality, and *all* diagrams, as long as they are local enough and fit in the ansatz of the form of the few-body model, are included when we solve the few-body model. This can also be seen as a mean-field approach, just like many other self-consistent Feynman diagram resummation strategies. Since the parameters in the few-body model may contain time explicitly, we may say what we are doing is a *dynamic* mean-field theory.

This report reviews

2 DMFT for the Hubbard model

We map the

The single-site model can be instantiated by replacing $\mathcal{G}$ by a bath of non-interactive electrons, and we get an Anderson impurity model. TODO: whether this is actually done in real calculation

This approximation is exact in an infinite lattice [2].

For Hubbard model, the interaction term in the few-body problem is exactly $Un_\uparrow n_\downarrow$, because it is strictly local and is not corrected when electrons on other sites are integrated out. For models with nearest-neighbor interaction, this is no longer exact, because now integrating out other electron modes means screening of the interaction. An even more important fact about models with repulsion between electrons from different sites is the interaction term cannot appear in a single-site model. To solve the above problems, a possible way is to use a Hubbard-Stratonovich transformation and use an auxiliary boson field to introduce the interaction. The resulting single-site model is in an itinerant electron bath and a bosonic bath [3].

Unfortunately, in some scenarios the original single-site DMFT is bound to fail. This is exemplified in phrase transition, in which long-wavelength behaviors are highly important, and a strictly local Σ cannot be the case. A possible direction of improvement is to use a few-body dual Hamiltonian – essentially a many-body impurity model – involving a larger cluster of states [4, 5]. The main problem of this approach is the speed: the impurity model concerning a large impurity cluster has to be solved with high accuracy, and this is demanding for existing solvers [6, 7]. Improvement can also be made by relaxing the strict locality condition for the self-energy, which leads to the dynamic vertex approximation approach introduced in the next section.

3 Going beyond DMFT: the DΓA

In the dynamic vertex approximation (DΓA), we assume that Σ is not local, but the 2-particle vertex Γ is local. The spatial-varying self-energy can then be calculated from Γ by TODO

4 DMFT in *ab initio* calculation

5 Conclusion

References

[1] O. Gunnarsson et al. "Breakdown of Traditional Many-Body Theories for Correlated Electrons". In: *Phys. Rev. Lett.* 119 (5 Aug. 2017), p. 056402. DOI: 10.1103/PhysRevLett.119.056402. URL: https://link.aps.org/doi/10.1103/PhysRevLett.119.056402.

[2] Antoine Georges and Gabriel Kotliar. "Hubbard model in infinite dimensions". In: *Phys. Rev. B* 45 (12 Mar. 1992), pp. 6479–6483. DOI: 10.1103/PhysRevB.45.6479. URL: https://link.aps.org/doi/10.1103/PhysRevB.45.6479.

[3] Ping Sun and Gabriel Kotliar. "Extended dynamical mean-field theory and $\mathrmGW$ method". In: *Phys. Rev. B* 66.8 (Aug. 2002), p. 085120. DOI: 10.1103/PhysRevB.66.085120. URL: https://link.aps.org/doi/10.1103/PhysRevB.66.085120.

[4] Gabriel Kotliar et al. "Cellular dynamical mean field approach to strongly correlated systems". In: *Physical review letters* 87.18 (2001). Publisher: APS, p. 186401.

[5] Hyowon Park, Kristjan Haule, and Gabriel Kotliar. "Cluster dynamical mean field theory of the Mott transition". In: *Physical review letters* 101.18 (2008). Publisher: APS, p. 186403.

[6] Michael Potthoff. "Cluster Extensions of Dynamical Mean-Field Theory". In: *DMFT: From Infinite Dimensions to Real Materials*. 2018, p. 20. URL: https://www.cond-mat.de/events/correl18/manuscripts/potthoff.pdf.

[7] Emanuel Gull et al. "Continuous-time Monte Carlo methods for quantum impurity models". In: *Rev. Mod. Phys.* 83.2 (May 2011). Publisher: American Physical Society, pp. 349–404. DOI: 10.1103/RevModPhys.83.349. URL: https://link.aps.org/doi/10.1103/RevModPhys.83.349.