Dual-fermion approach to interacting disordered fermion systems

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Models

- Anderson-Hubbard model:

\[ \mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ \mathcal{P}(\epsilon_i) = \Theta(D/2 - |\epsilon_i|)/D \]

- U=0: Anderson disorder model
- D=0: Hubbard model
- Freeze the hopping of spin-down electron: AFK model

- Anderson-Falicov-Kimball (AFK) model

\[ \mathcal{H} = -t \sum_{\langle ij \rangle} c_{i}^\dagger c_{j} - \sum_{i} \epsilon_i n_{i}^c + U \sum_i n_{i}^c n_{i}^f \]

Relevant parameter U~W: strongly correlated system, non-perturbative in nature
D~U: treat interaction and disorder on equal footing
How to solve these models?? --> numerical method
Numerical methods

- Local approximation: DMFT+CPA
  - DMFT (dynamical mean-field theory): interacting system (D=0)
  - CPA (coherent potential approximation): disorder system (U=0)

- Non-local approximation
  - Cluster DMFT, such as DCA (dynamical cluster approximation)
  - Expansion on DMFT solution, such as DΓA (dynamical vertex approximation), DF (Dual fermion)

A great success
Best for the local physics, e.g. Mott physics
Missing non-local physics, e.g. d-wave superconductivity

A. Georges et al., RMP 68, 13 (1996)

Th. Maier et al., RMP 77, 1027 (2005).

A. Toschi, et al., PRB 75, 045118 (2007)

A. N. Rubtsov et al., PRB 77, 33101 (2008)
Dual-fermion method

A. N. Rubtsov et al., PRB 77, 33101 (2008)
H. Terletska et al, PRB 87, 134208 (2013)

DF mapping:
\[ G_{d0} = G_{lat} - G_{imp} \]
\[ V \approx F \]

Real fermion

- local and long length-scales
- strongly-correlated

Dual fermion

- intermediate length-scale
- weakly-correlated
Contributions to the full vertex $F$

- Disorder

- Interaction

- Mixed

\[ \text{crossing symmetry} \]
Contributions to the full vertex $F$

- Disorder
- Interaction
- Mixed

Crossing symmetry

$F$
Construct DF self-energy diagrams

- Crossing-symmetrized vertex

\[
V \quad = \quad \quad + \quad \quad +
\]

- Schwinger-Dyson equation

\[
\Sigma \quad = \quad \quad + \quad \quad +
\]

- Remove non-physical diagrams
Numerical results for 1D AFK model

- DMFT+CPA results are temperature independent
- DF results gain a rich temperature dependence by including the non-local correlations
Correction due to DF

- DMFT+CPA are good for small and large U limits
- DF has the largest correction when U~W=1
- Disorder will shift peak location to larger U
- Correction increases when decreasing temperature
Phase-diagram for 2D AFK model

\[ \text{Im} \delta G = \text{Im} G_{\text{loc}}(3i\pi T) - \text{Im} G_{\text{loc}}(i\pi T) \]

determined by the slope of \( \text{Im} G \)

- \( >0 \): metal-like
- \( <0 \): insulator-like

\[ \text{Im} \delta G < 0 \]

\[ \text{Im} \delta G > 0 \]
Phase-diagram for 2D AFK model

\[ \text{Im} \, \delta G = \text{Im} G_{\text{loc}}(3i\pi T) - \text{Im} G_{\text{loc}}(i\pi T) \]

- >0: metal-like
- <0: insulator-like

\[ \Gamma \chi_0 \phi = \lambda \phi \]

- Detect charge-density-wave (CDW) instability
- Closer to 1, more susceptible to CDW ordering

Metal-bad-metal crossover is driven by CDW correlations. But, no signature of Anderson localization.
Phase-diagram for 2D AFK model

- Vertex contribution included
- Show signature of the Anderson localization
- Anderson localization line connects continuously to the CDW metal-bad-metal crossover line
Conclusion


- We have generalized the dual fermion formalism for the interacting disorder system
- Numerical results for the Anderson-Falicov-Kimball model show a pronounced improvement by including non-local contributions from DF
- Application on the Anderson-Hubbard model is in progress

Thank you!