Extended Dynamical Mean Field Theory and Model GW Method

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OUTLINE

P. Sun & G. Kotliar, Phys. Rev. B 66, 85120 (2002)

1. E-DMFT + GW

2. QMC Implementation of E-DMFT via Hubbard-Stratonovich Auxiliary Field

3. Application I : E-DMFT of 3D U-V Model
   - Density Instability and Phase Diagram
   - Energy-Dependent U

4. Application II : E-DMFT + GW of 1D U-V Model

5. Conclusion

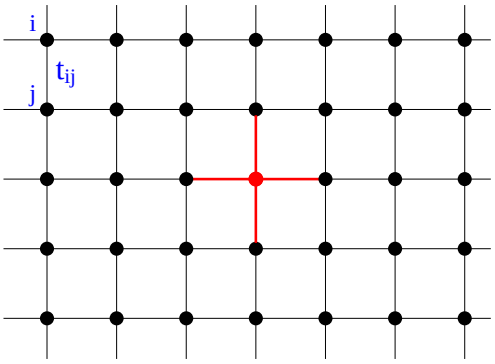
DMFT of Hubbard Model

- W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)
- A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

- Hamiltonian:

$$H = -\frac{1}{2}\sum_{ij,\sigma}\left(t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}\right) + U\sum_{i} : n_{i\uparrow} :: n_{i\downarrow} :$$

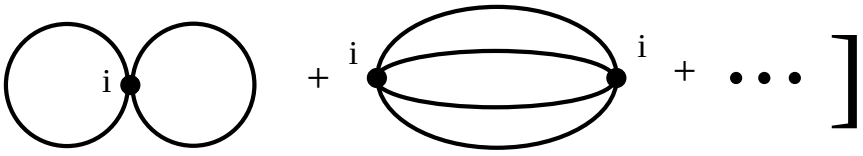
- Cavity Construction:



$$t_{ij} \propto 1/z^{||i-j||/2}$$

- Baym-Kadanoff Functional

$$\Gamma = \text{Tr}\ln G - \text{Tr}[\mathcal{G}_0^{-1} - G^{-1}]G + \Phi[G]$$

$\Phi = \sum_i$ []

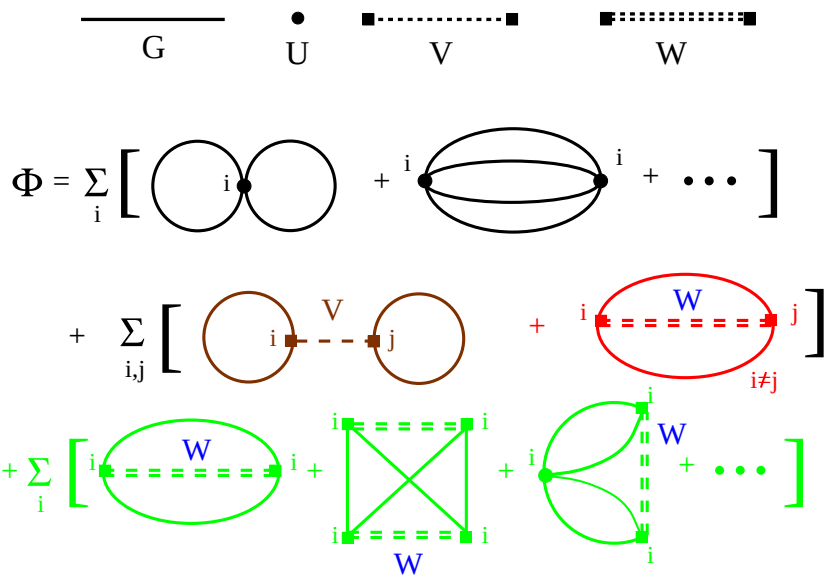
E-DMFT + GW

- Motivation
  - Model Calculation: Non-Local Interaction
  - Electron Structure: Energy-Dependent U

- Baym-Kadanoff Functional

$$\Gamma = \mathrm{Tr}\ln G - \mathrm{Tr}\ln[\mathcal{G}_0^{-1} - G^{-1}]G$$

$$-\frac{1}{2}\mathrm{Tr}\ln W + \frac{1}{2}\mathrm{Tr}\ln[\mathcal{W}_0^{-1} - W^{-1}]W + \Phi[G, W]$$



- E-DMFT + GW:
  - E-DMFT: Local, Non-Perturbative, Numerically Expensive
  - GW: Non-Local, Perturbative, Numerically Cheap
    Lars Hedin, Phys. Rev. **139**, A796 (1965)

EXTENDED - DMFT

- G. Kotliar and S.Y. Savrasov, *Model Hamiltonians and First Principles Electronic Structure Calculations* in *New Theoretical Approaches to Strongly Correlated Systems*, Ed. A.M. Tsvelik, Kluwer Academic Publishers (2001)
- R. Chitra and G. Kotliar, Phys. Rev. Lett. **84**, 3678 (2000).
- Q. Si and J. L. Smith, Phys. Rev. Lett. **77**, 3391 (1996); J. L. Smith and Q. Si, Phys. Rev. B **61**, 5184 (2000).
- S. Sachdev and J. Ye, Phys. Rev. Lett. **70** 3339 (1993); O. Parcollet and A. Georges, Phys. Rev. B **59**, 5341 (1999).

- Model Hamiltonian:

$$H = -\frac{1}{2}\sum_{ij,\sigma}\left(t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}\right) - \mu\sum_{i} n_i$$

$$+U\sum_{i} : n_{i\uparrow} :: n_{i\downarrow} : + \frac{1}{2}\sum_{i\neq j} : n_i : V_{ij} : n_j :$$

- Effective DMFT Action:

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\sigma} c^{\dagger}_{0\sigma}(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_{0\sigma}(\tau')$$

$$+U\int_0^\beta : n_{0\uparrow}(\tau) :: n_{0\downarrow}(\tau) :$$

$$+\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' : n_0(\tau) : \mathcal{W}_0(\tau-\tau') : n_0(\tau') :$$

Fermion & Boson Baths

- Cavity Method:

$$\mathcal{G}_0^{-1}(\tau-\tau') = -\partial_\tau + \mu - \sum_{ij} t_{0i} t_{0j} G^{(0)}_{ij}(\tau-\tau')$$

$$\mathcal{W}_0(\tau-\tau') = \sum_{ij} V_{0i} V_{0j} \chi^{(0)}_{ij}(\tau-\tau')$$

$$\left[\quad \chi^{(0)}_{ij}(\tau-\tau') \stackrel{\text{def}}{=} -\langle n_i(\tau) n_j(\tau') \rangle_0 \quad \right]$$

- Dyson Equations – General:

$$[G(k,ip_n)]^{-1} = ip_n + \mu - t_k - \Sigma(k, ip_n)$$

$$[\chi(k,i\omega_n)]^{-1} = -V_k + [P(k, i\omega_n)]^{-1}$$

- Dyson Equations – Local:

$$G^{\text{loc}}(ip_n) = \left[\mathcal{G}_0^{-1}(ip_n) - \Sigma(ip_n)\right]^{-1} \equiv \sum_k G(k, ip_n)$$

$$\chi^{\text{loc}}(i\omega_n) = \left[-\mathcal{W}_0(i\omega_n) + [P(i\omega_n)]^{-1}\right]^{-1} \equiv \sum_k \chi(k, i\omega_n)$$

Hubbard-Stratonovich Auxiliary Field

- Auxiliary Field
  - Decoupling Complicated Interactions, QMC
  - Broken Symmetry, Generalized Landau-Ginzberg

    Semiclassical Limit: S. Pankov, G. Kotliar, and Y. Motome, Phys. Rev. B **66**, 45117 (2002)

- Precaution: Positive-Definite Matrix

$$\tilde{V}_{ij} = \lambda\delta_{ij} - V_{ij}$$

- Effective Action

$$S = \int_0^\beta d\tau \{ \sum_{i,\sigma} [c^\dagger_{i,\sigma}(\tau)\partial_\tau c_{i,\sigma}(\tau) - \mu_i n_{i,\sigma}(\tau)]$$

$$-\frac{1}{2}\sum_{ij,\sigma} t_{ij}[c^\dagger_{i,\sigma}(\tau)c_{j,\sigma}(\tau) + \text{ h.c.}]$$

$$+(U+\lambda)\sum_i [n_{i,\uparrow}(\tau) - \frac{1}{2}][n_{i,\downarrow}(\tau) - \frac{1}{2}]$$

$$+\frac{1}{2}\sum_{i,j}\phi_i(\tau)\tilde{V}^{-1}_{ij}\phi_j(\tau) - \sum_i \phi_i(\tau)[n_i(\tau) - 1]\}$$

Solving DMFT: Anderson Impurity Model

A. Georges and G. Kotliar, Phys. Rev. **B** 45, 6479 (1992)

- General Anderson Impurity Model: Electron Bath and Phonon Bath

$$\mathcal{H} = \sum_{l\sigma} \epsilon_l a^\dagger_{l\sigma} a_{l\sigma} + \sum_{l\sigma} V_l^{\rm el} (a^\dagger_{l\sigma} c_{0\sigma} + c^\dagger_{0\sigma} a_{l\sigma})$$

$$+\epsilon_d \sum_\sigma c^\dagger_{0\sigma} c_{0\sigma} + U c^\dagger_{0\uparrow} c_{0\uparrow} c^\dagger_{0\downarrow} c_{0\downarrow}$$

$$+\frac{1}{2}\sum_m (P_m^2 + \omega_m^2 \phi_m^2) + \sum_m V_m^{\rm ph} \phi_m \phi_0$$

$$+\phi_0 (c^\dagger_{0\uparrow} c_{0\uparrow} + c^\dagger_{0\downarrow} c_{0\downarrow})$$

- QMC Impurity Solver:
  - Fermion: Quantum Monte Carlo (QMC) Simulation Hirsch-Fye [Phys. Rev. Lett. **56**, 2521 (1986)]
  - Boson: [Motome and Kotliar, Phys. Rev. B **62**, 12800 (2000)]

$$\exp\left[-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \phi(\tau) \mathcal{W}_0^{-1}(\tau - \tau') \phi(\tau')\right]$$

Application–3D U-V Model: Density Instability

1. What is the Difference between DMFT and E-DMFT, PHYSICALLY ?

   E-DMFT incorporates the Response Functions into the method which serves as the Bosonic Self-Consistent Bath.

2. Example: Density Instability

   (a) Electron Density Green's Function:

$$\chi(k, i\omega_n) = -\frac{P(i\omega_n)}{1 - V_k P(i\omega_n)}$$

   (b) Instability:

$$V_k P(i\omega_n) = 1$$

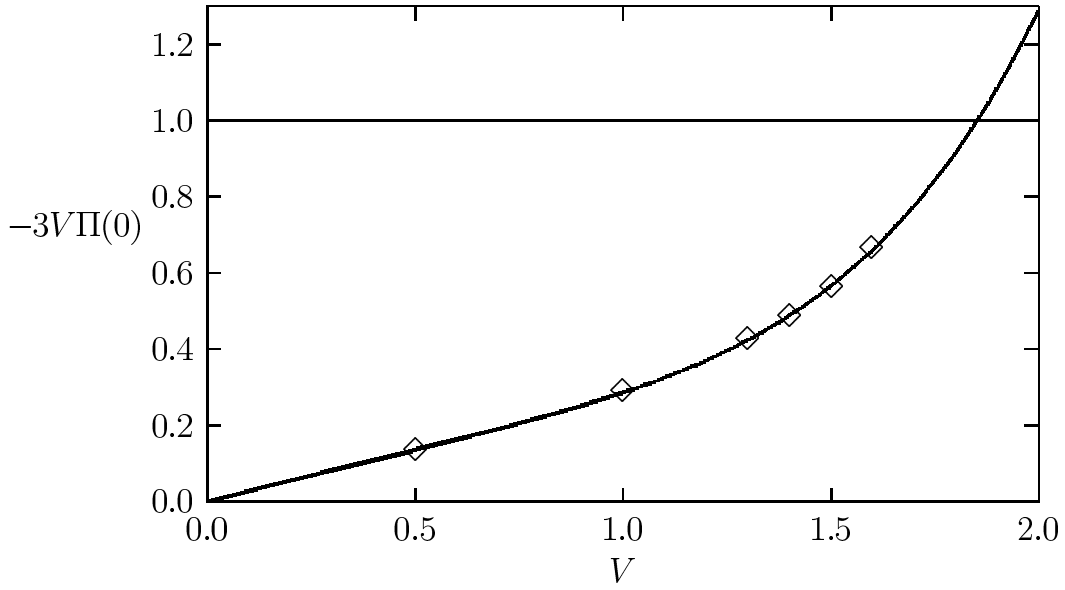
   (c) Nearest-Neighbor Density-Density Interaction:

$$V_{ij} = \frac{1}{2} V(\delta_{i,j-1} + \delta_{i,j+1}) \Rightarrow V_k = V \sum_i \cos k_i$$

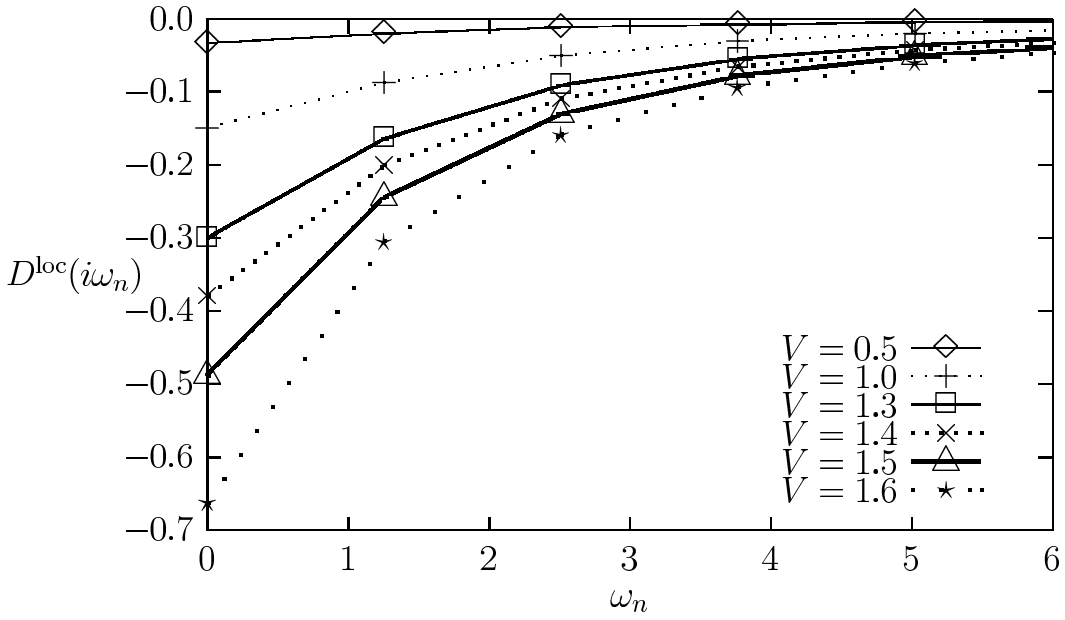
   Since $P(i\omega_n) < 0$ approaches zero monototically as frequency increases, instability appears first at $k = (\pi, \pi, \pi)$ (CDW) and $\omega_n = 0$ (static) when

$$V_c = \frac{1}{P(0)d}$$

3. Rescaled Phonon Self Energy at $U = 3.0$, $\beta = 5.0$

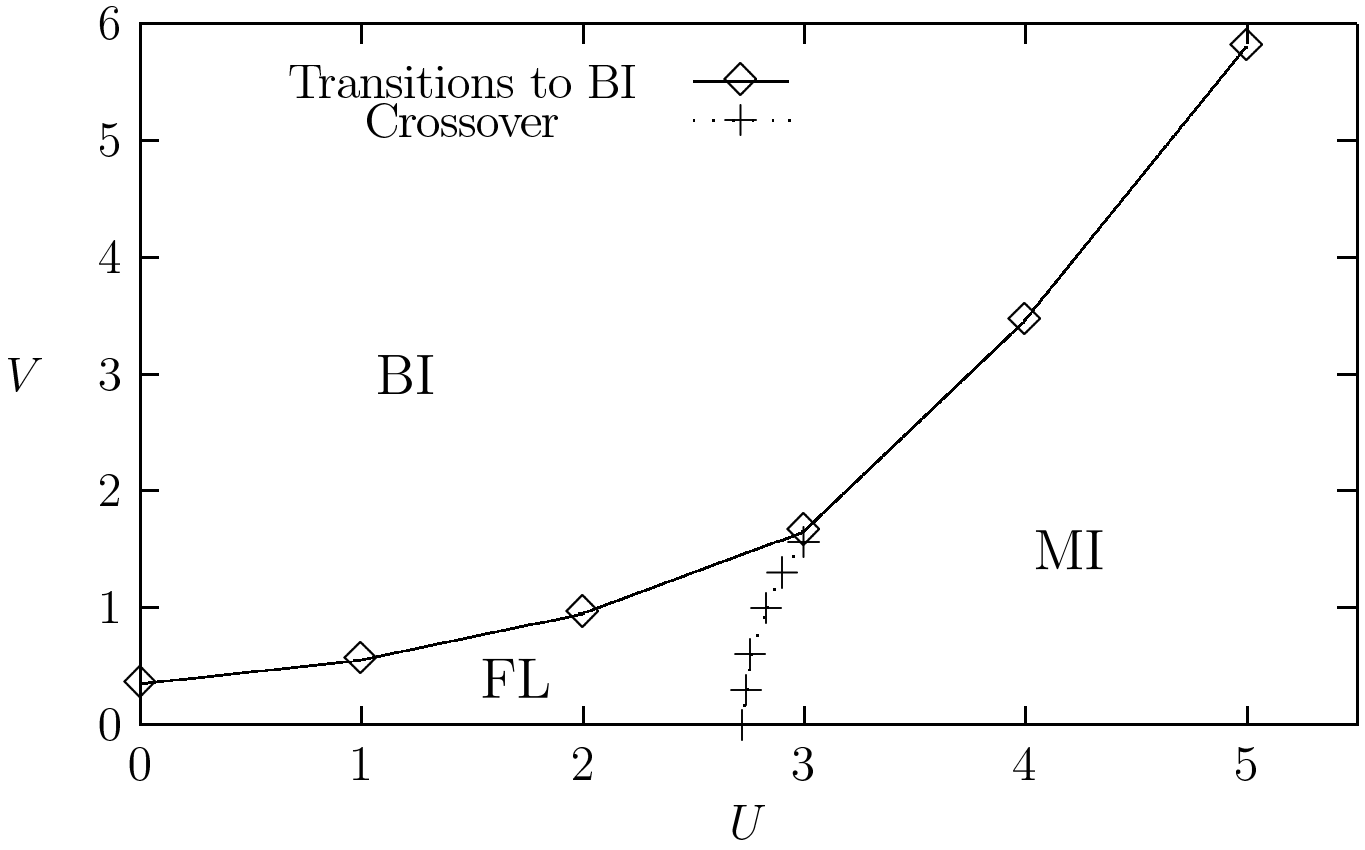


4. The Local Phonon Green's Function at $U = 3.0$, $\beta = 5.0$



Application–3D U-V Model: Phase Diagram at $\beta = 5.0$

BI: Band Insulator
MI: Mott Insulator
FL: Fermi Liquid

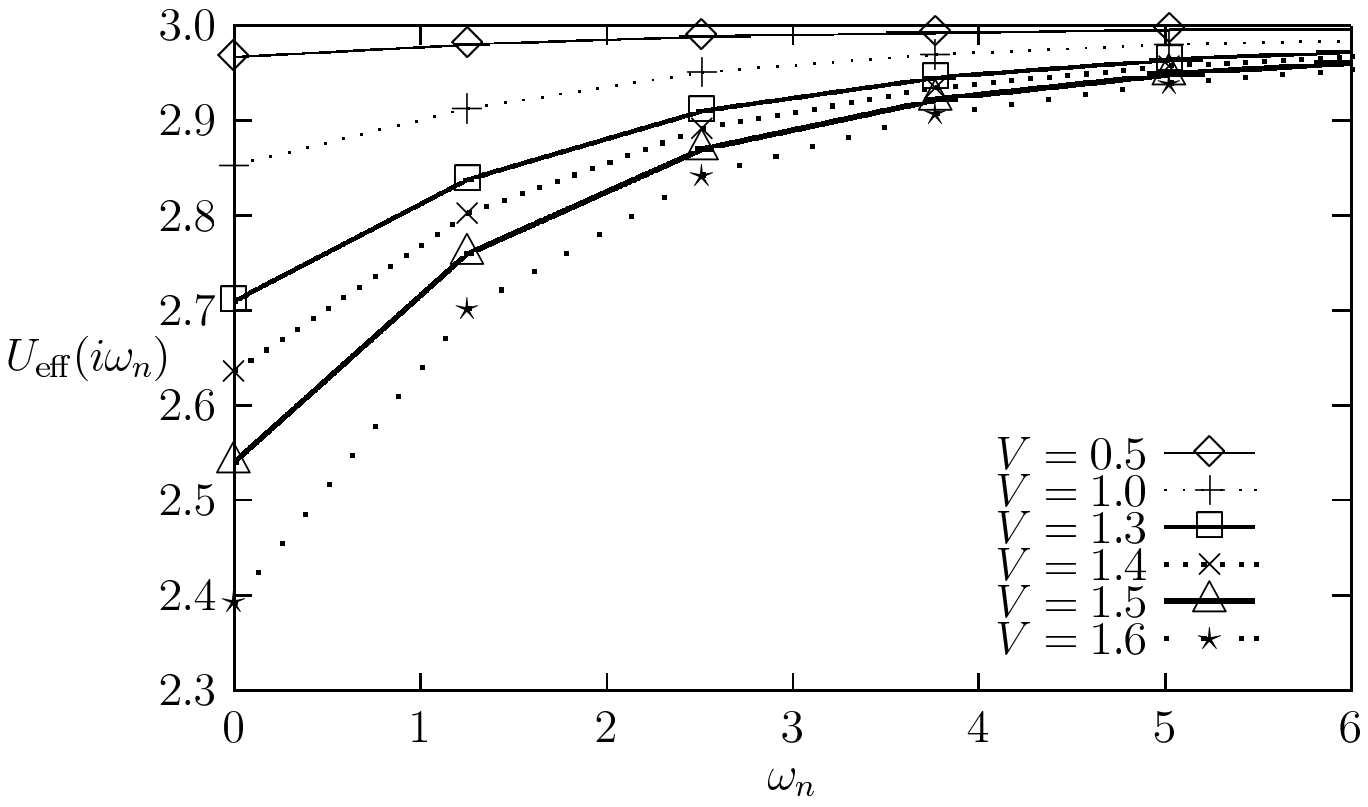


Energy Dependent U

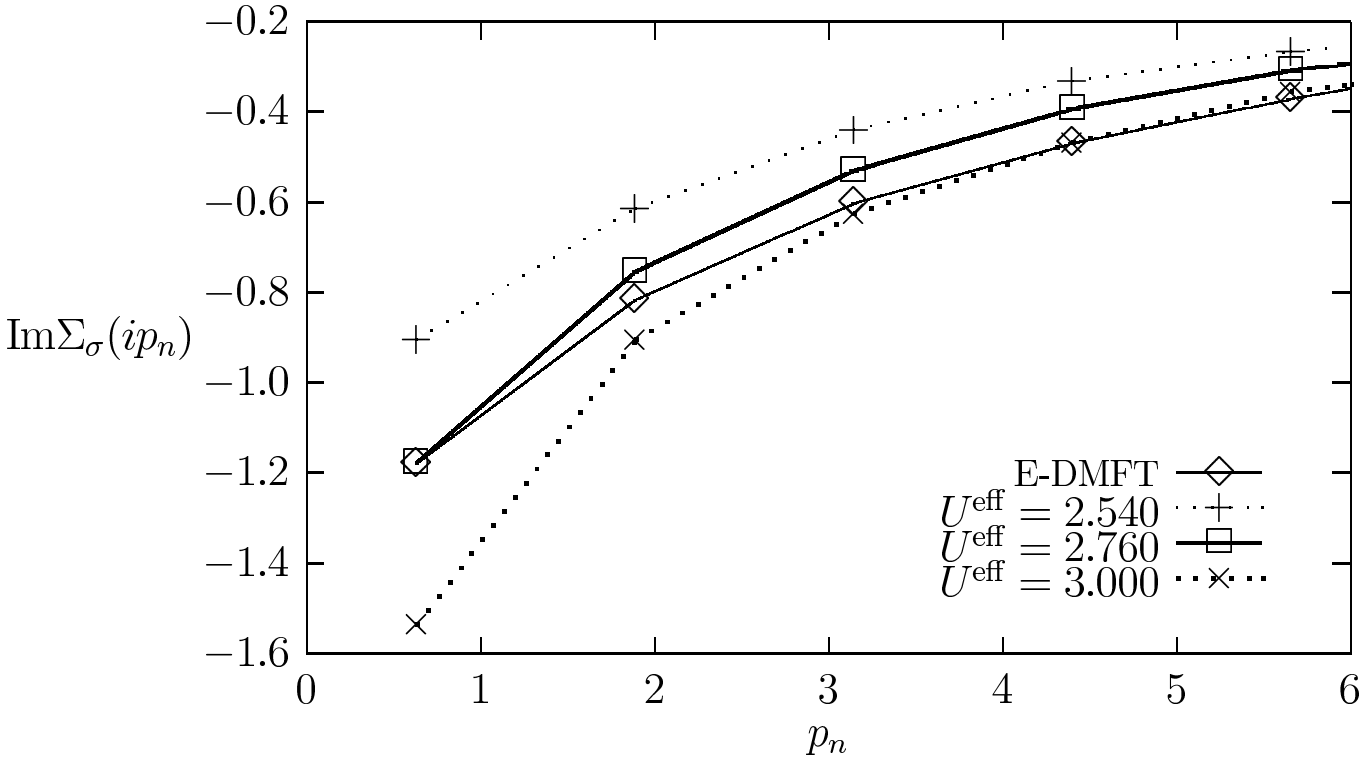
- Energy Dependent U:

$$U_{\text{eff}}(i\omega_n) \stackrel{\text{def}}{=} U + \mathcal{W}_0(i\omega_n)$$

- U_{eff} at $U = 3.0$, $\beta = 5.0$



- Self Energy for $U = 3.0$, $V = 1.5$, $\beta = 5.0$



- What We Learn:

  An energy dependent U result in non-trivial effects which CAN NOT be reproduced by a single effective constant U

Application II: E-DMFT + GW on 1D Band Insulator

- E-DMFT Combined with GW Method
  - GW + E-DMFT
    To incorporate more accurate SPATIAL correlations into E-DMFT
  - What is New in 1D?

(A) Interaction Vertices

(B) Generilized GW Self–Energies

- Reasons to choose 1D Band Insulator:
  - Exactly Soluble: Compare to DMRG
    S.S. Kancharla and C. Bolech, Phys. Rev. B **64**, 85119 (2001)
  - Band Insulator: Eliminate Temperature Effects
  - Correlation: Non-Trivial
  - Pure E-DMFT Not Enough
  - 1D: Worst Case For Mean Field Theories

- The 1D Extended Hubbard Model:

$$H = -t \sum_{i,\sigma} \left(c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \text{h.c.} \right) - \mu \sum_{i} (-1)^{i} n_i$$

$$+U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)$$

$$+V \sum_{i} \left(n_i - 1 \right) \left(n_{i+1} - 1 \right)$$

- Single Electron Green's Function ($\mu_A = -\mu_B = \mu$):

$$\begin{bmatrix} G^{\text{AA}}_{\sigma} & G^{\text{AB}}_{\sigma} \\ G^{\text{BA}}_{\sigma} & G^{\text{BB}}_{\sigma} \end{bmatrix}^{-1} (k, ip_n) =$$

$$\begin{bmatrix} ip_n + \mu_{\text{A}} & te^{-ik/2} \cos\frac{k}{2} \\ te^{ik/2} \cos\frac{k}{2} & ip_n + \mu_{\text{B}} \end{bmatrix} - \begin{bmatrix} \Sigma^{\text{AA}}_{\sigma} & 0 \\ 0 & \Sigma^{\text{BB}}_{\sigma} \end{bmatrix} (ip_n)$$

- Auxiliary Phonon Green's Function:

$$\begin{bmatrix} D^{\mathrm{AA}} & D^{\mathrm{AB}} \\ D^{\mathrm{BA}} & D^{\mathrm{BB}} \end{bmatrix}^{-1}(k, i\omega_n) =$$

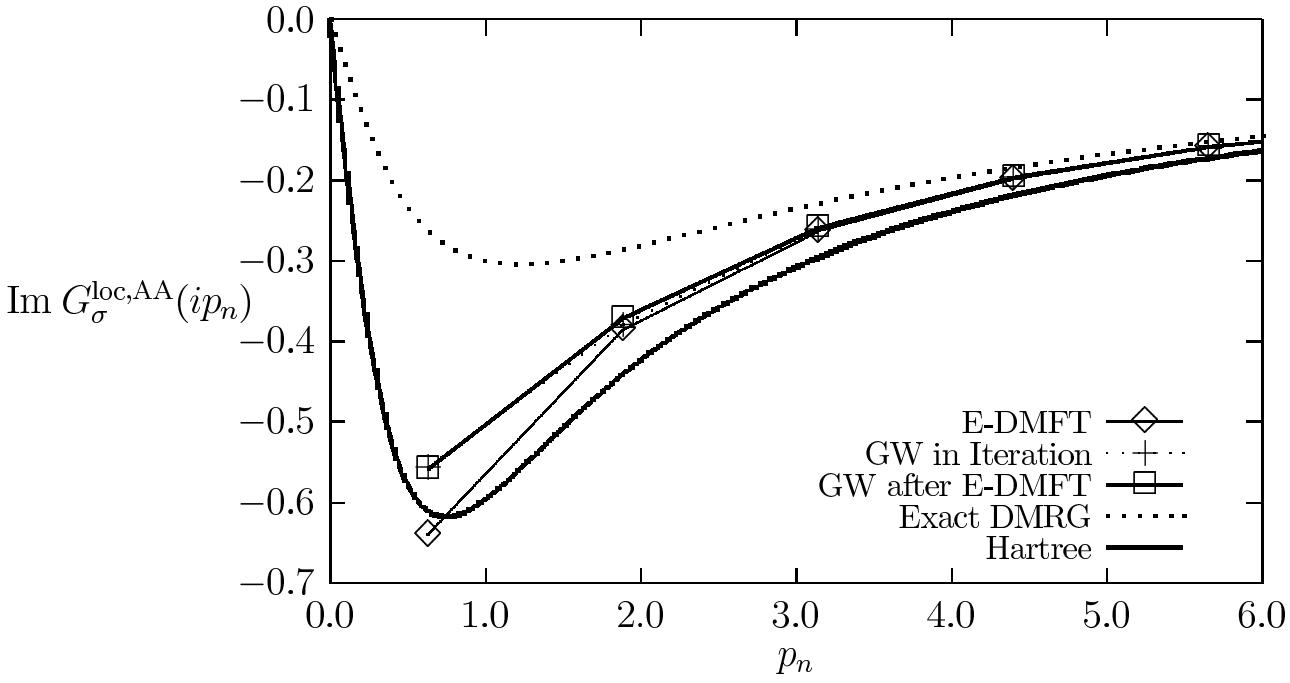
$$\begin{bmatrix} -\lambda & 2Ve^{-ik/2}\cos\frac{k}{2} \\ 2Ve^{ik/2}\cos\frac{k}{2} & -\lambda \end{bmatrix}^{-1} - \begin{bmatrix} \Pi^{\mathrm{AA}} & 0 \\ 0 & \Pi^{\mathrm{BB}} \end{bmatrix}(i\omega_n)$$

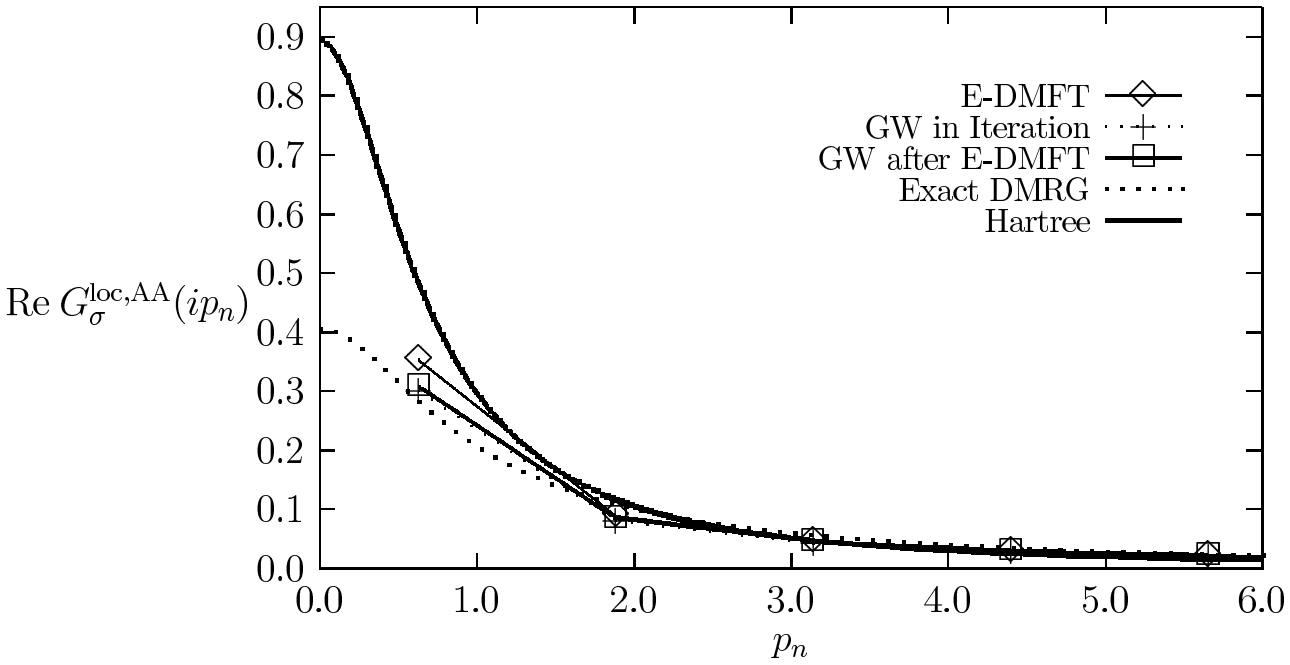
- Electron Density Green's Function:

$$\begin{bmatrix} \chi^{\mathrm{AA}} & \chi^{\mathrm{AB}} \\ \chi^{\mathrm{BA}} & \chi^{\mathrm{BB}} \end{bmatrix}^{-1}(k, i\omega_n) =$$

$$\begin{bmatrix} \lambda & -2Ve^{-ik/2}\cos\frac{k}{2} \\ -2Ve^{ik/2}\cos\frac{k}{2} & \lambda \end{bmatrix} + \begin{bmatrix} \Pi^{\mathrm{AA}} & 0 \\ 0 & \Pi^{\mathrm{BB}} \end{bmatrix}^{-1}(i\omega_n)$$

- Single Particle Green's Function





Conclusion

- E-DMFT + GW: Methodology and Implementation
- Applications
  - Phase Transition
  - Energy-Dependent U
  - E-DMFT + GW on 1D Band Insulator
- On-Going Work
  - Periodic Anderson Model
  - 2D & 3D Coulomb Gas