A Multiorbital DMFT Analysis of Electron-Hole Asymmetry in the Dynamic Hubbard Model

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The Hubbard Model

$$H = -\sum_{i,j,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_{i} c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}$$

- restrict *i* and *j* to nearest neighbour lattice sites
- Pauli exclusion allows only two electrons per site
- *U* – double occupancy Coulomb repulsion
- t_{ij} – nearest-neighbour hopping

- single band model
- electron-hole symmetric

Double Occupancy and Orbital Relaxation

- The Hubbard model assumes a single orbital on each lattice site and an electron’s state is static regardless of occupancy.

- J. E. Hirsch, Phys. Rev. B **65**, 184502 (2002):

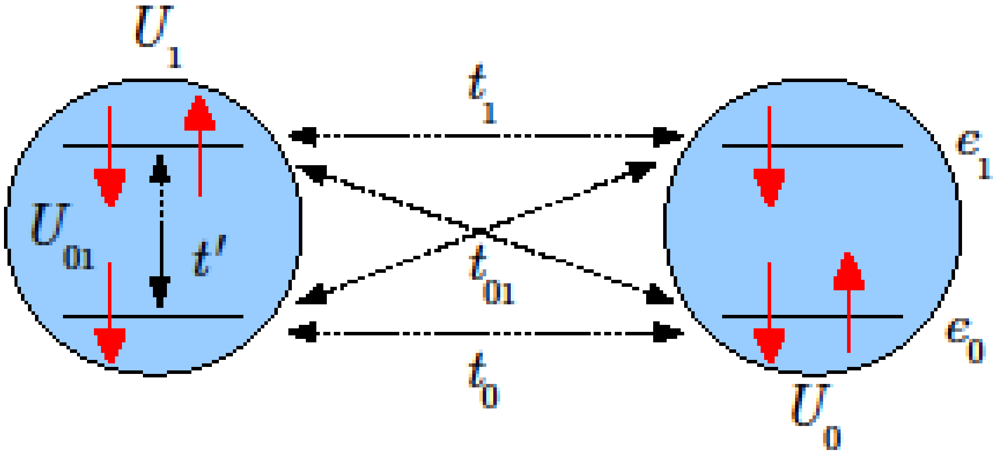
  The real electronic ground state includes higher-orbital contributions with weaker Coulomb repulsion which become especially important for strongly-correlated systems (large local Coulomb repulsion) at high filling

- Need to adjust the Hubbard model to capture the flexibility for electrons to change their state in response to changes in occupancy: dynamic Hubbard model

Dynamic Hubbard Model (DHM)

J. E. Hirsch, Phys. Rev. B **65**, 184502 (2002)

- Two non-degenerate orbitals: energies $\epsilon_0 < \epsilon_1$
- Three local Coulomb repulsions U_0, U_1, U_{01}
- Two intraband hopping parameters t_0, t_1
- Nonlocal hybridization (interband hopping) t_{01}
- Local interband hybridization t'



DHM Hamiltonian

$$H_{\mathrm{DHMe}} = H_{\mathrm{KE}} + H_{\mathrm{local}} + H_{\mathrm{hyb}}$$

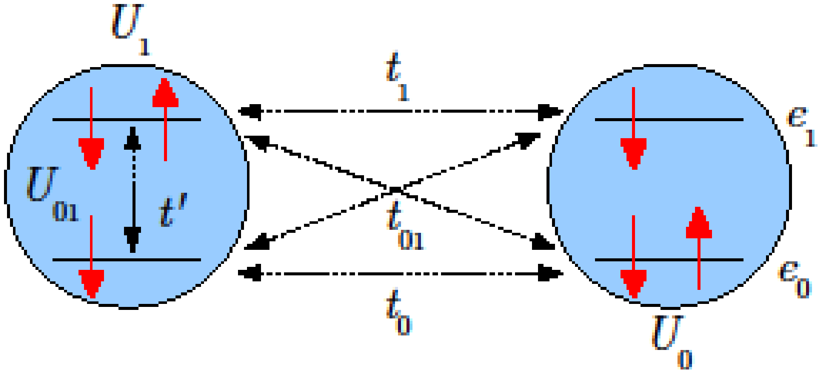
$$H_{\mathrm{KE}} = -\sum_{\langle ij\rangle\sigma}\Big[t_0(c^\dagger_{0i\sigma}c_{0j\sigma} + c^\dagger_{0j\sigma}c_{0i\sigma}) + t_1(c^\dagger_{1i\sigma}c_{1j\sigma} + c^\dagger_{1j\sigma}c_{1i\sigma})$$

$$+t_{01}(c^\dagger_{1i\sigma}c_{0j\sigma} + c^\dagger_{0j\sigma}c_{1i\sigma})\Big]$$

$$H_{\mathrm{local}} = U_0\sum_i n_{0i\uparrow}n_{0i\downarrow} + U_1\sum_i n_{1i\uparrow}n_{1i\downarrow} + U_{01}\sum_{i\sigma\sigma'} n_{0i\sigma}n_{1i\sigma'} + (\epsilon_0 - \mu)\sum_{i\sigma} n_{0\sigma}$$

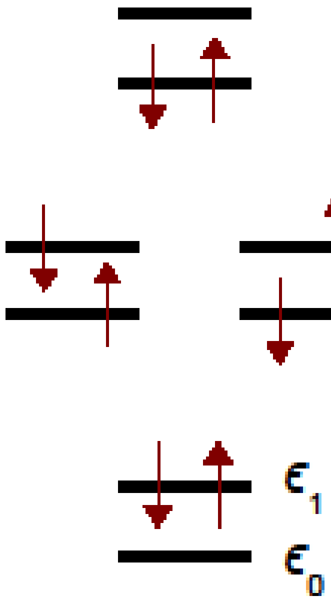
$$+ (\epsilon_1 - \mu)\sum_{i\sigma} n_{1\sigma}$$

$$H_{\mathrm{hyb}} = -t'\sum_{i\sigma}(c^\dagger_{0i\sigma}c_{1i\sigma} + c^\dagger_{1i\sigma}c_{0i\sigma})$$



Orbital Relaxation in the DHM

- Double occupancy energy-ordering conditions



$$E_2 = U_0 + 2\epsilon_0$$

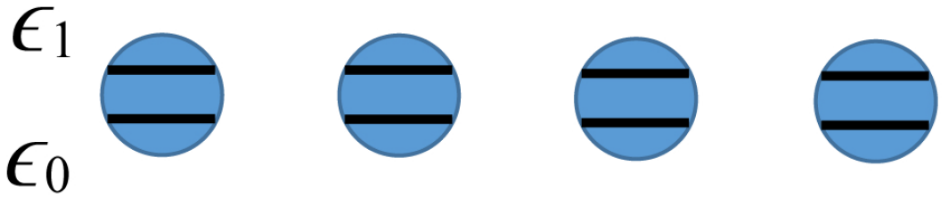
$$E_1 = U_{01} + \epsilon_0 + \epsilon_1$$

$$E_0 = U_1 + 2\epsilon_1$$

$$U_1 + 2\epsilon_1 < U_{01} + \epsilon_0 + \epsilon_1 < U_0 + 2\epsilon_0$$

Comparison: Four-Site Exact Diagonalization

- J. E. Hirsch, Phys. Rev. B **67**, 035103 (2003)



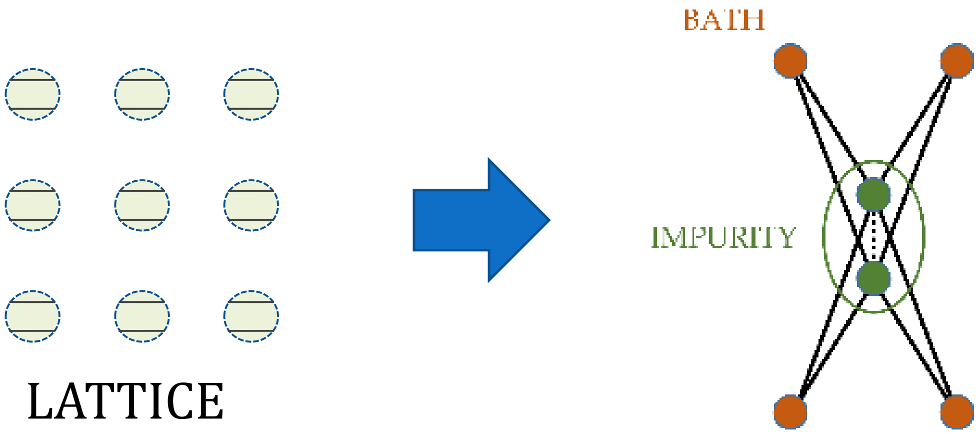
- Main result: electron-hole asymmetry in the Dynamic Hubbard Model

- fixed values of $t' = 0.2$, $t_{01} = 1.0 = t_0 = t_1$

Multiorbital Dynamical Mean Field Theory (MODMFT)

A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

- Maps an infinite-dimensional lattice model onto a local impurity model
- Solve the impurity model self-consistently for a set of effective mean field parameters which approximate the influence of the full lattice environment on a single site
- Retains the local dynamics of electronic occupancy of the impurity, yielding the Green's function and self energy of the system

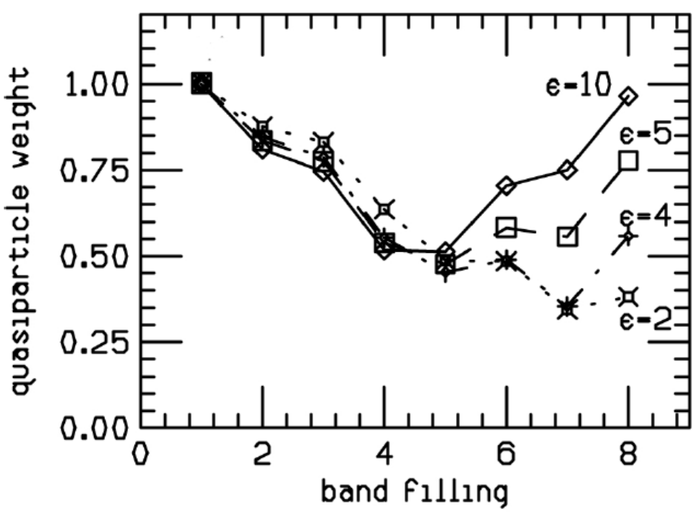


Result: Observed Asymmetry in Z

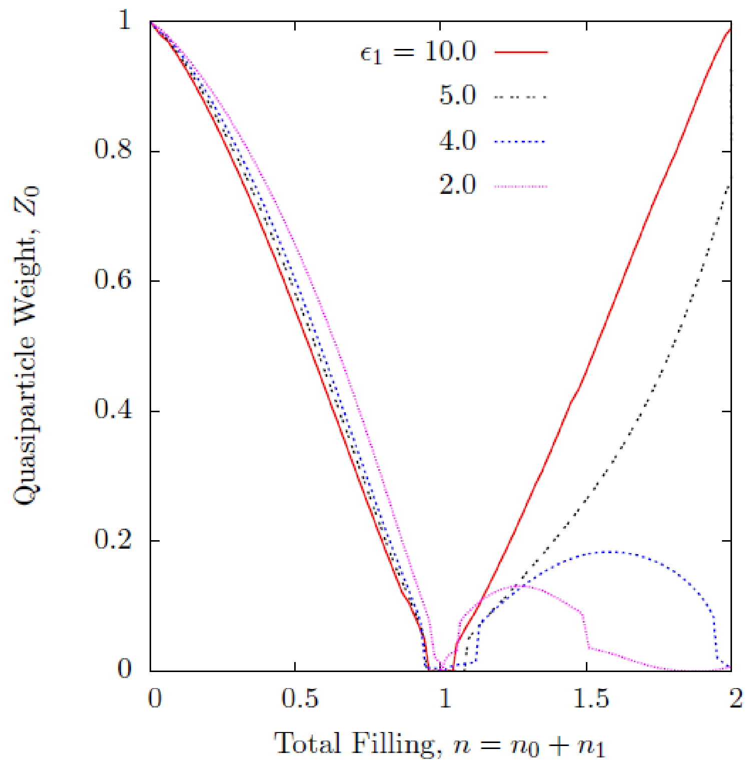
$U_0 = 10.0$, $U_{01} = 6.0$, $U_1 = 5.0$, $t_0 = t_1 = t_{01} = 1.0$, $t' = 0.2$

Quasiparticles become increasingly dressed with orbital relaxation.

Four Site ED



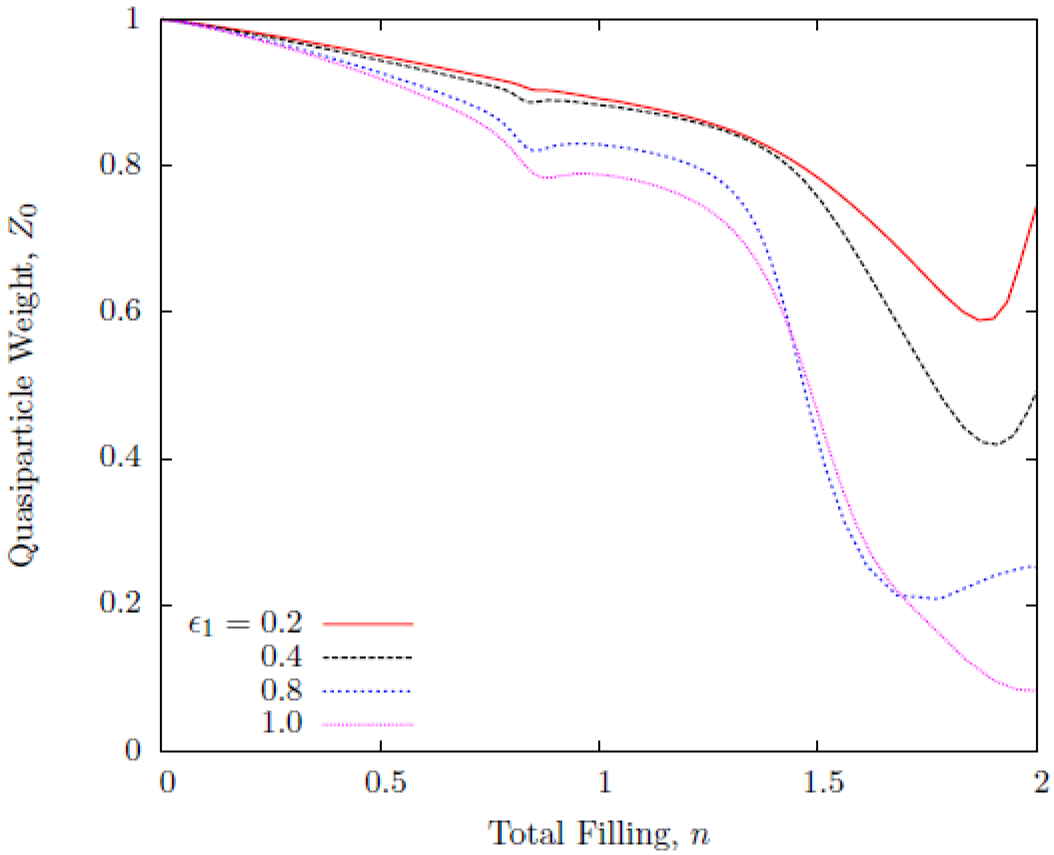
Bethe Lattice MODMFT



Or the Opposite Effect...

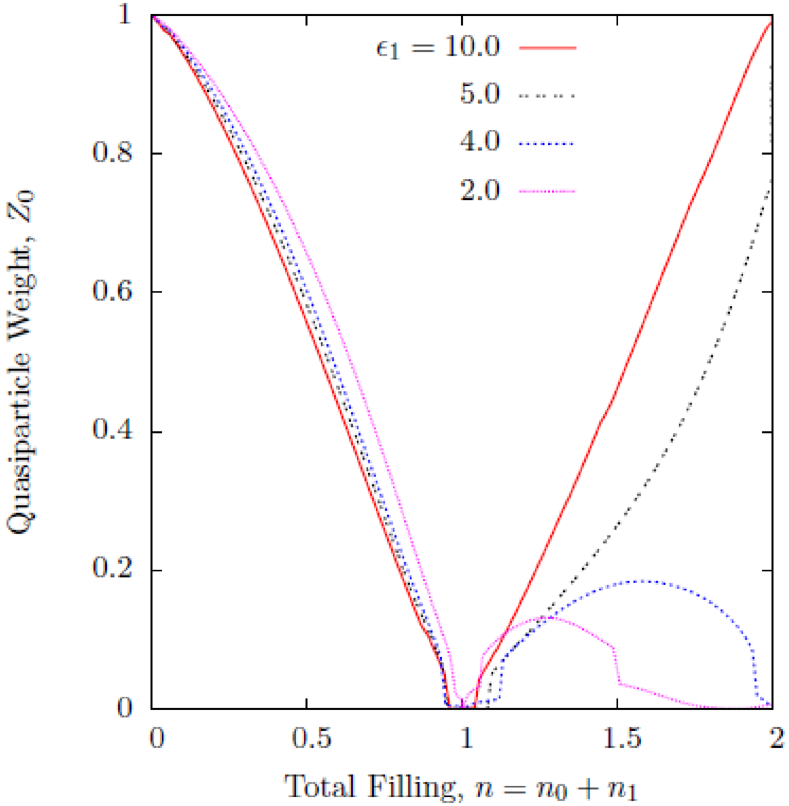
$U_0 = 3.0$, $U_{01} = 2.0$, $U_1 = 1.0$, $t_0 = t_1 = t_{01} = 1.0$, $t' = 0.2$

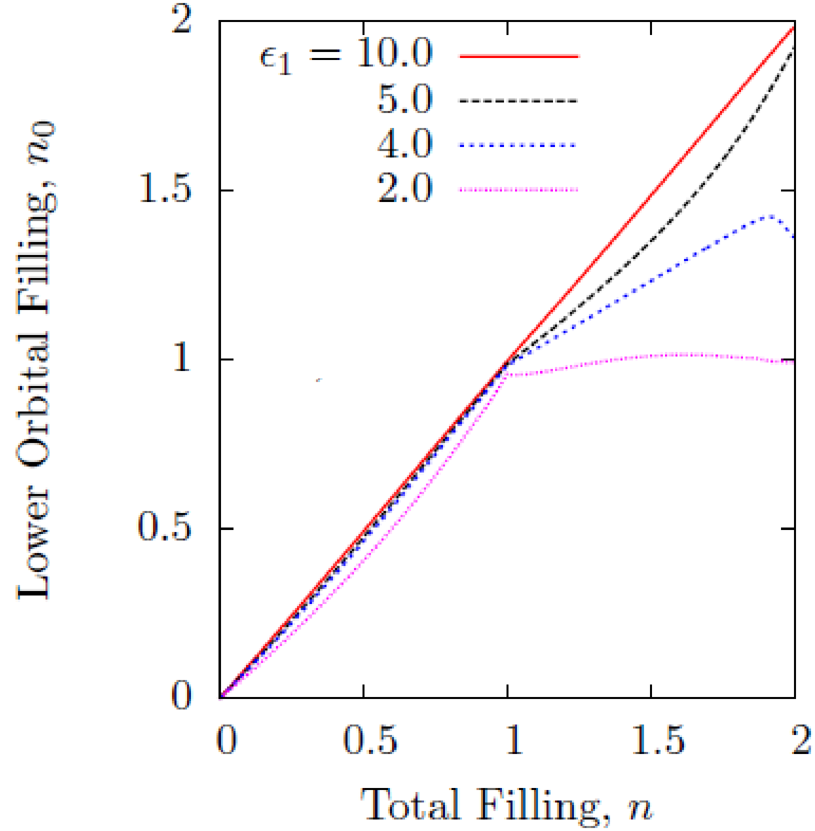
Quasiparticles can also *undress* with orbital relaxation.



The Influence of Mott Physics on Dressing (Not Evaluated in Hirsch's ED Study)

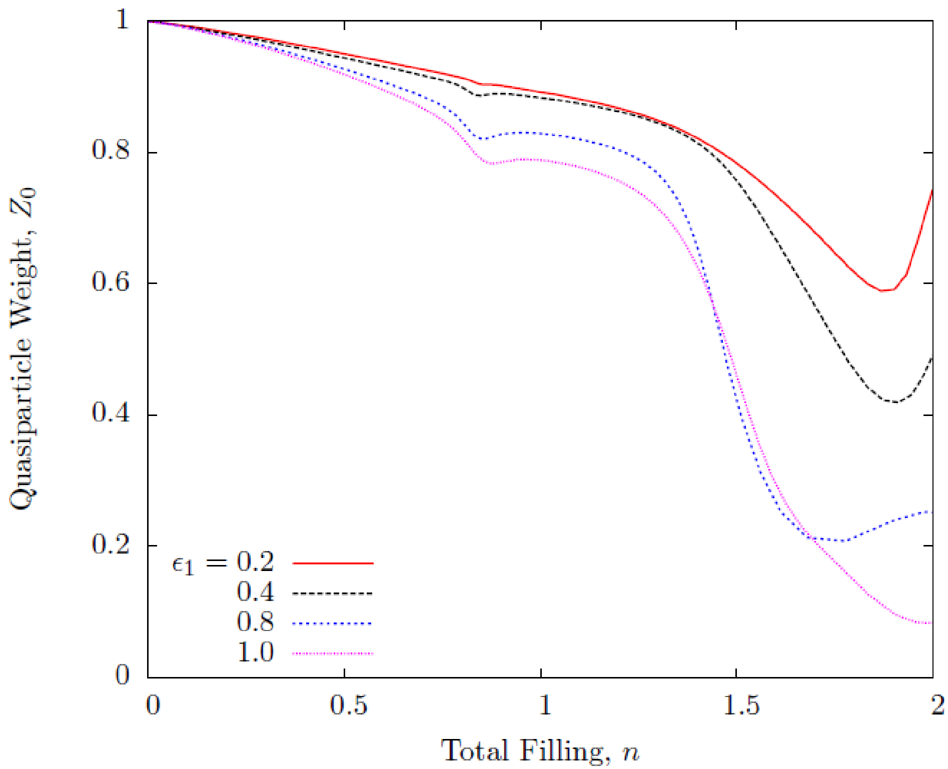
$U_0 = 10.0$, $U_{01} = 6.0$, $U_1 = 5.0$, $t_0 = t_1 = t_{01} = 1.0$, $t' = 0.2$

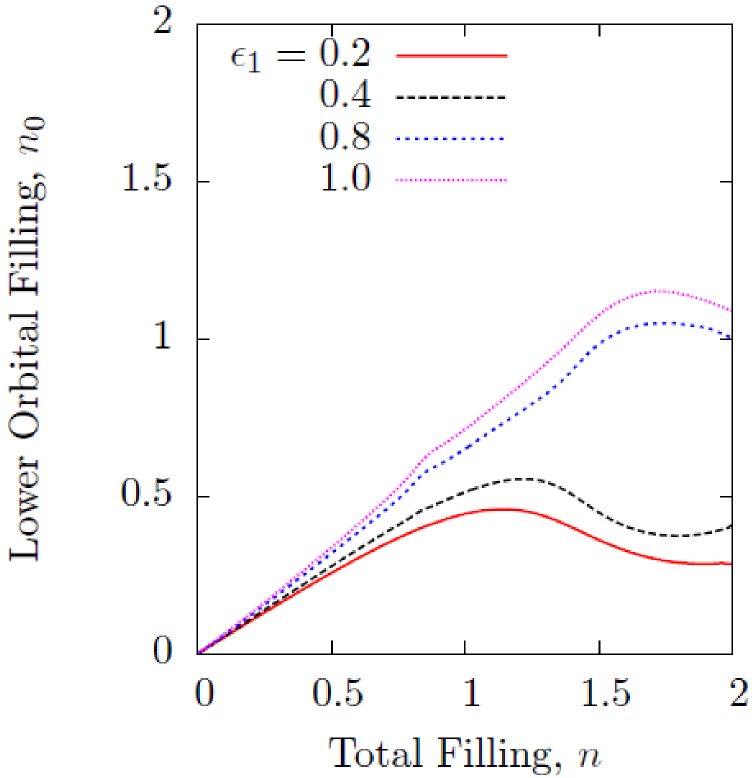




The Influence of Mott Physics on Undressing

$U_0 = 3.0, U_{01} = 2.0, U_1 = 1.0, t_0 = t_1 = t_{01} = 1.0, t' = 0.2$

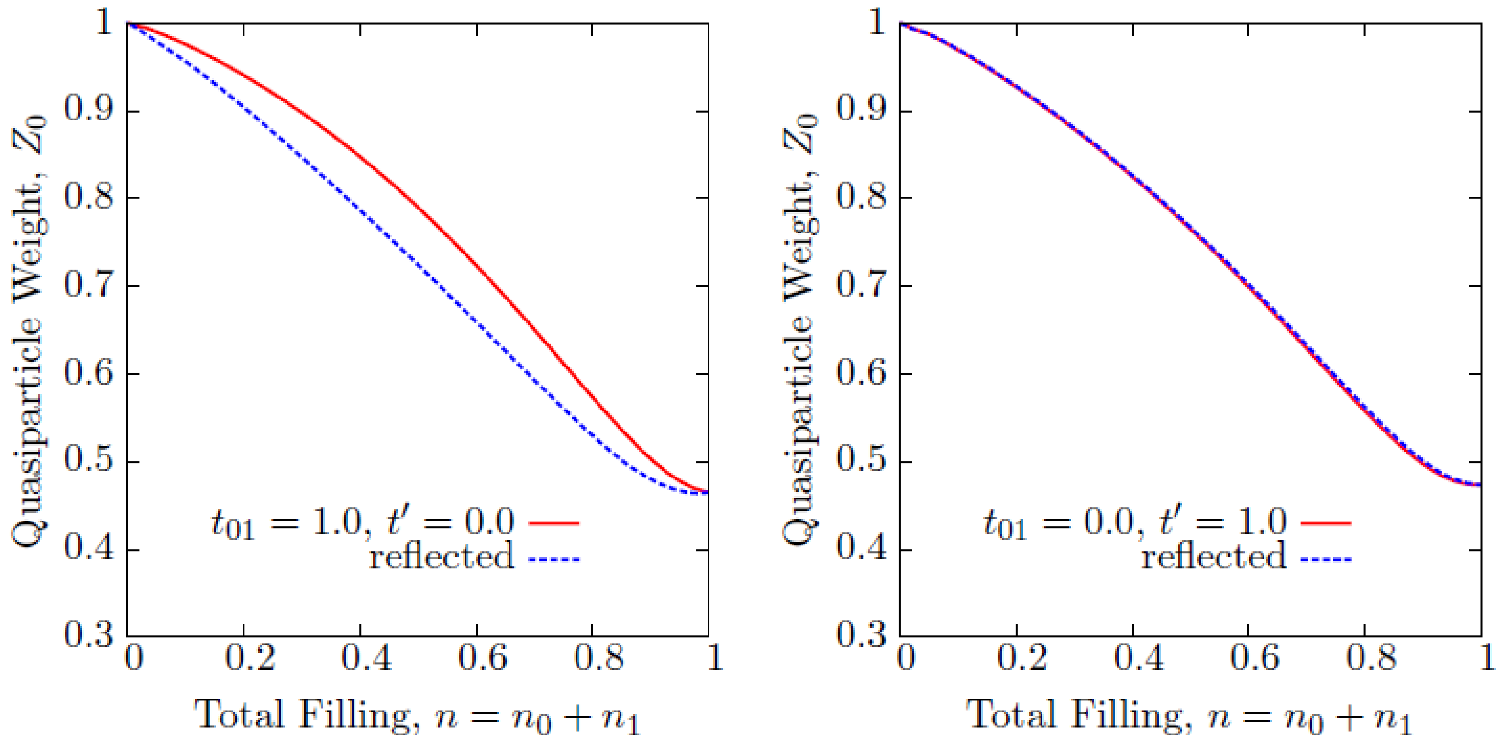




The Influence of Hybridization

- t_{01} is qualitatively more relevant to the physics of orbital relaxation than the (local) t' hybridization parameter. For example:

$U_0 = 3.0$, $U_{01} = 2.0$, $U_1 = 1.0$, $t_0 = t_1 = t_{01} = 1.0$, $t' = 0.2$, $\epsilon_1 = 10.0$



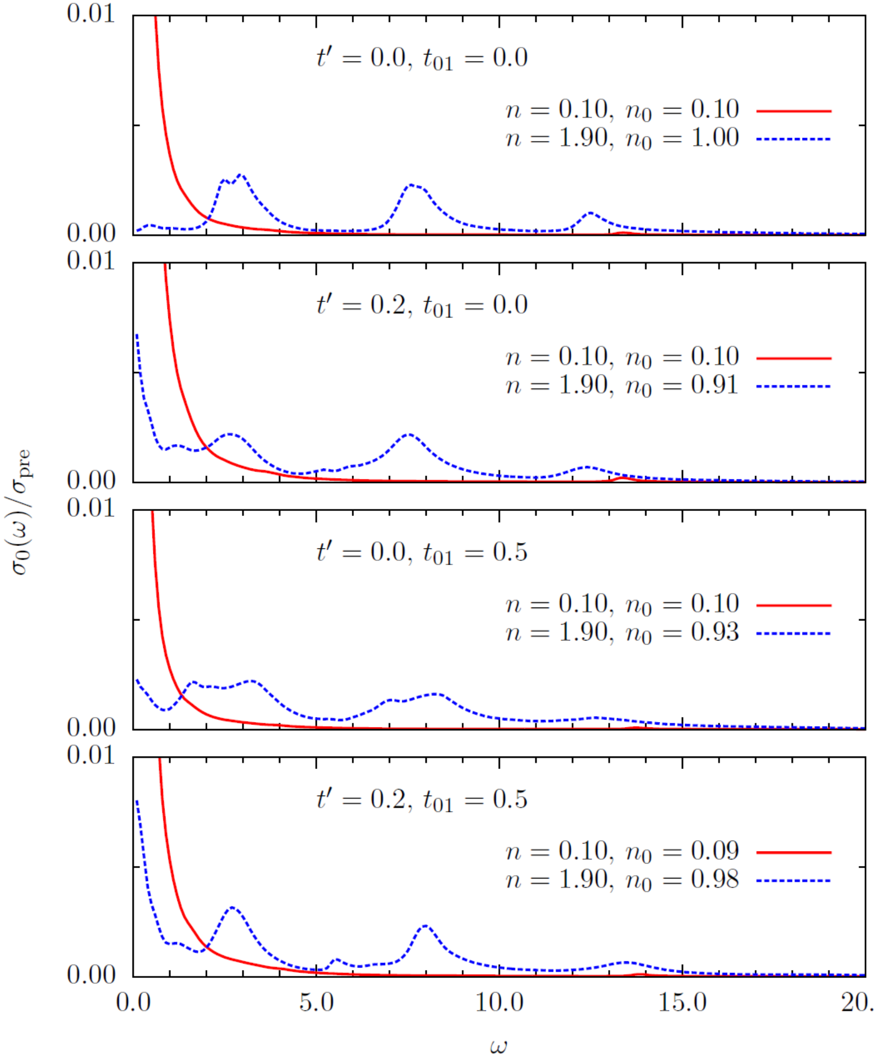
(a) Nonlocal hybridization. (b) Local hybridization.

Asymmetry Evidenced in Optical Conductivity Weight Transfer

$U_0 = 10.0$, $U_{01} = 5.0$, $U_1 = 0.5$,
$t_0 = t_1 = 1.0$, $\epsilon_1 = 4.0$, $\eta = 0.1$

- Hole regime shows transfer of low energy to higher energy features: electron-hole asymmetry

- Significant effect of hybridization on the low energy Drude region



Conclusions

- Confirmed Hirsch's four-site ED observation of electron-hole asymmetry in the dynamic Hubbard model
  - in the quasiparticle weight
  - in optical conductivity weight transfer
- Nonlocal hybridization is qualitatively more important than local hybridization
- Complicated dependence of orbital relaxation on the energy gap, hybridization values and Mott physics in the DHM

MODMFT Background

- MODMFT has been in use since the earliest years of DMFT studies
- Q. Si and G. Kotliar, Phys. Rev. Lett. **70**, 3143 (1993)
- Q. Si and G. Kotliar, Phys, Rev. B **48**, 13881 (1993)

- Benchmark: A. Liebsch and H. Ishida, J. Phys.-Condens. Mat. **24**, 053201 (2012)

- Several studies of two-orbital systems with local hybridization t'
- Few with nonlocal hybridization t_{01}
- Focus has been on orbital selective Mott transitions with Hund's coupling; none appear to address the dynamic Hubbard model