Effect of Particle-Hole Asymmetry on the Mott-Hubbard Metal-Insulator Transition

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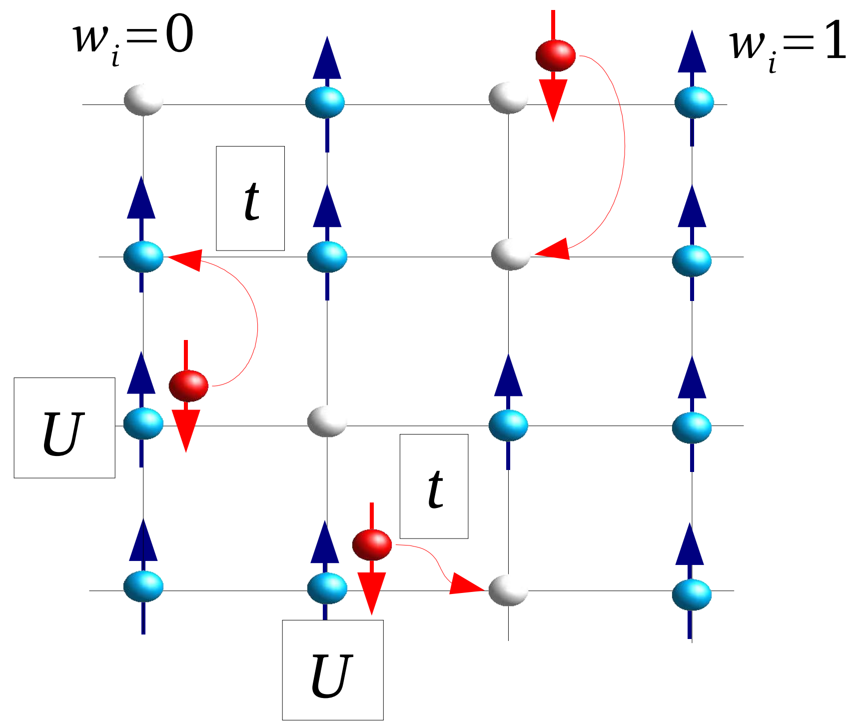
Mott-Hubbard metal-insulator transition (MIT)

- Local Coulomb repulsion U that forbids double occupancy, insulator when 1 particle per site
- Hubbard model: hard to describe both Fermi liquid and insulator phases with approximations
- Dynamical Mean Field Theory – progress, but:
- Numerics are very complicated and delicate
- Half filled single band model studied extensively
- What happens if particle-hole symmetry is broken?
- Most real materials generally do not have particle-hole symmetry

How to change the model?

- Modify the model so the MIT occurs when particle-hole symmetry is removed
- Falicov-Kimball model
- Binary alloy picture
- Ta_xN – example, MIT occurs for x=0.6
- Model has MIT for a wide range of fillings $0 < w_1 < 1$
- Numerics are under excellent control



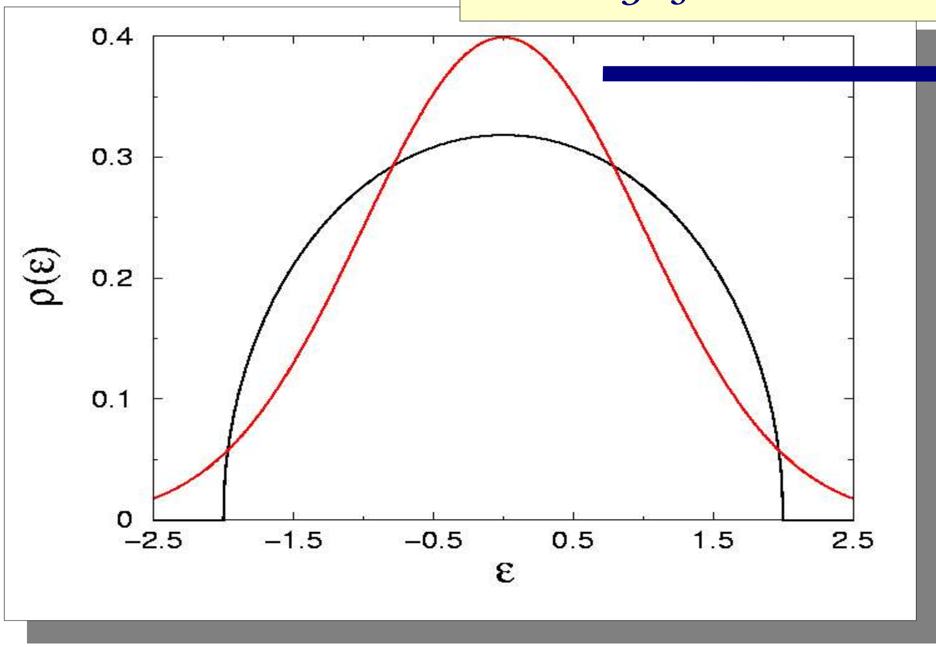
$$H = -t \sum_{\langle i,j \rangle} c_i^+ c_j + U \sum_i w_i c_i^+ c_i$$

$w_1 = \langle w_i \rangle$ - average filling

$\rho_e = 1 - w_1$ - fix total number of particles

Algorithm - DMFT

Feed in noninteracting density of states



Converge $\Sigma(\omega)$

Hilbert transformation:

$$G(\omega)=\int d\epsilon\,\rho(\epsilon)\frac{1}{\omega+\mu-\Sigma(\omega)-\epsilon+i\delta}$$

Dyson's equation:

$$G_0(\omega)=\left[G(\omega)^{-1}+\Sigma(\omega)^{-1}\right]^{-1}$$

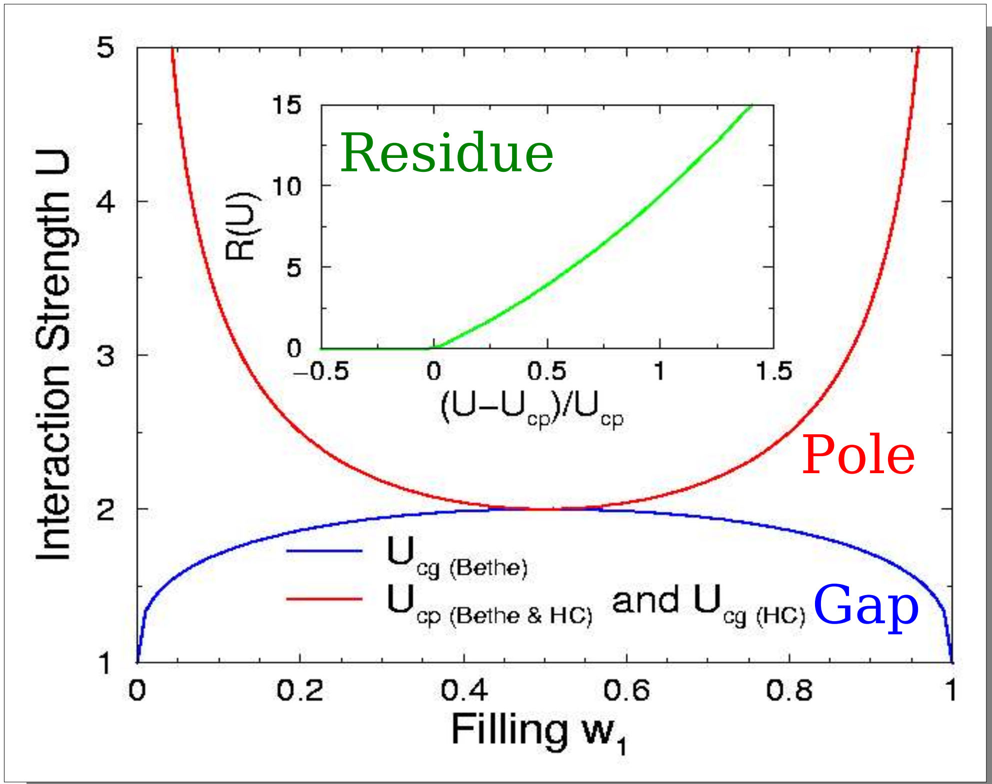
Exact impurity solution:

$$G(\omega)=(1-w_1)G_0(\omega)+w_1\frac{1}{G_0(\omega)^{-1}-U}$$

- Model can be solved in infinite dimensions, self-energy is local – DMFT, two lattices in infinite dimensions
- Hypercubic (HC) – infinite bandwidth
- Bethe – finite bandwidth
- Bethe lattice also allows analytical solution for the Green's function

MIT and Pole, are they related?

- At half filling self-energy develops a pole at MIT
- HC – pole and 'pseudogap' occur at the same *U*
- Bethe – pole and gap occur at *different U's away from half-filling*
- Residue of the pole is universal on both lattices



The scenarios for the MIT on HC and Bethe lattices are NOT the same

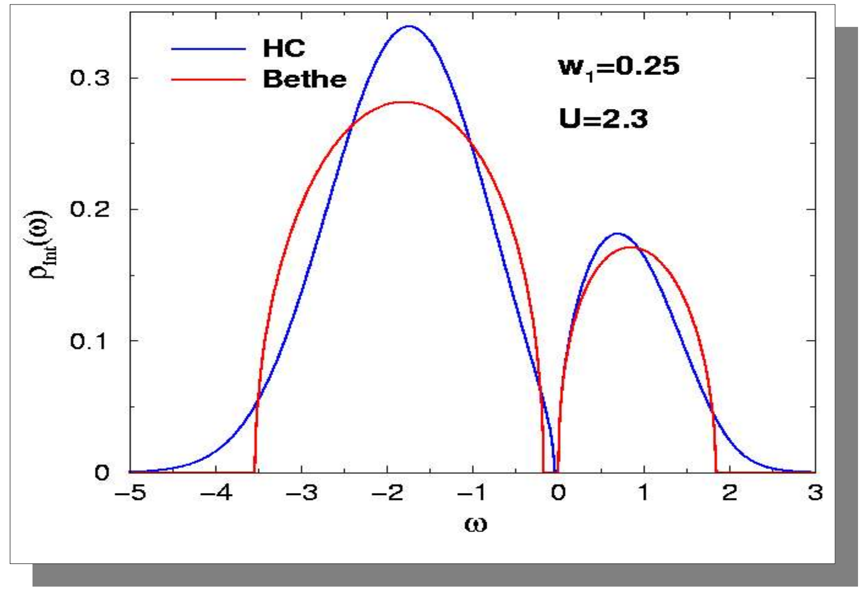
$$U_{c(pole)}=\frac{1}{\sqrt{w_1(1-w_1)}}$$

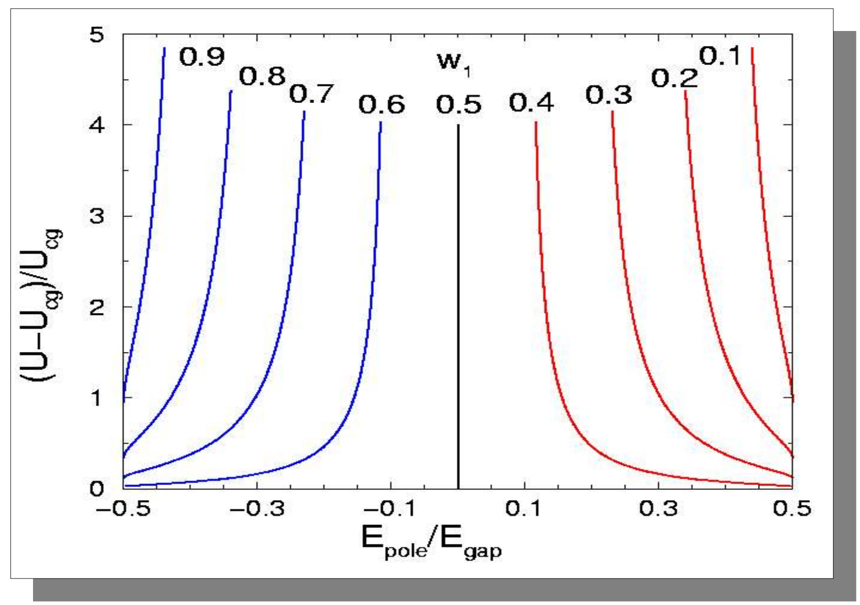
$$U_{c(gap)}=\sqrt{1+3w_1^{1/3}(1-w_1)^{1/3}[(1-w_1)^{1/3}+w_1^{1/3}]}$$

Pole and Gap

relative interaction strength vs. relative location of the pole

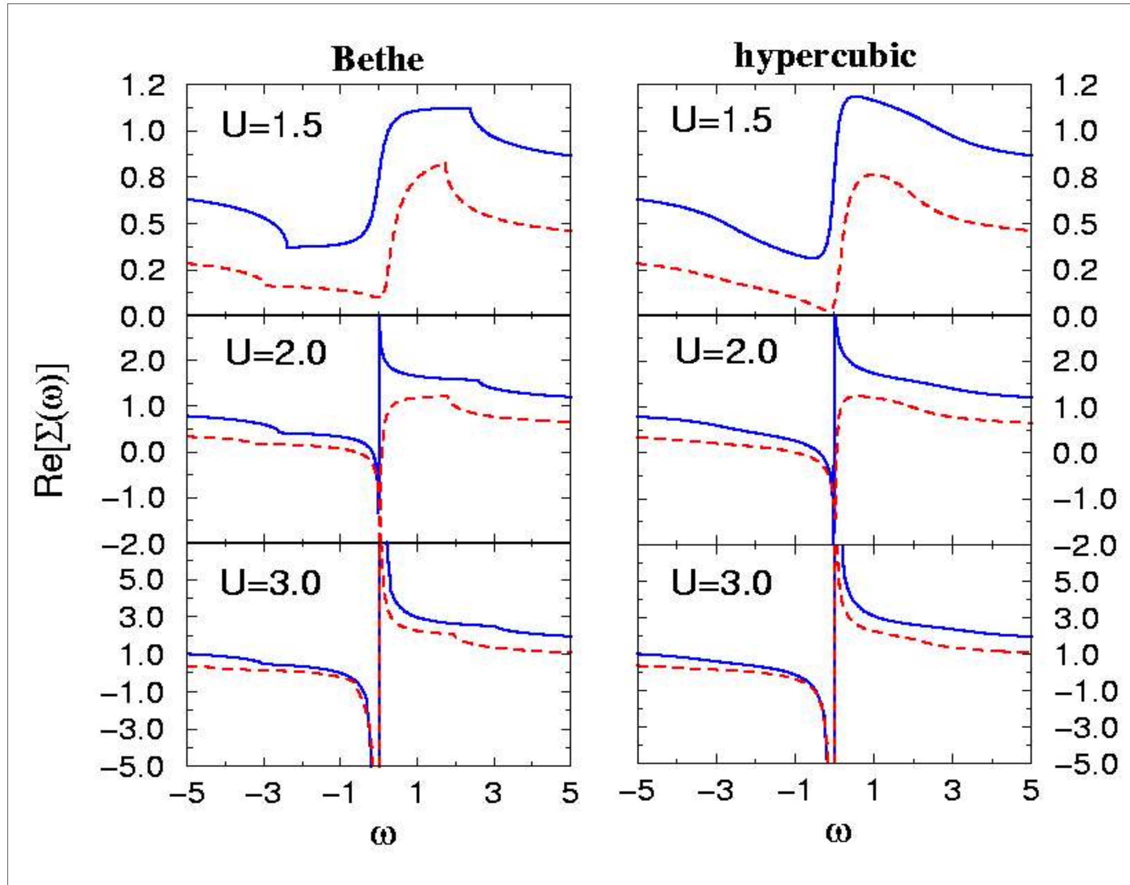
- Bethe – well defined gap
- Half filling – pole in the middle of the gap
- Away form half filling – pole appears at a band edge and drifts closer to the center
- No smooth transition from half filled to particle-hole asymmetric case
- HC – no well defined gap, $\rho_{int}(\omega)=0$ at a single point ('pseudo-gap')
- 3-d cubic calculations in local approximation show scenario similar to Bethe lattice

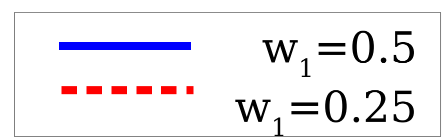




Evolution of the self-energy

- Compare real part of self-energy on HC and Bethe
- Top panel – $U<U_{c(pole,gap)}$
- Middle panel – on the Bethe lattice – there exists a phase where gap is opened but there is no pole yet
- Bottom panel – $U>U_{c(pole,gap)}$





Transport calculations do not show any differences between a correlated insulator with or without a pole

Conclusions

- The scenarios of the MIT on the Bethe and hyper-cubic lattices are different
- Development of the pole and MIT are unrelated away from half filling on the Bethe lattice
- Although it might be tempting to use residue of the pole as an “order parameter” for the MIT, it fails to describe the process off of half filling on lattices with finite bandwidth
- No obvious difference in properties of an insulator with or without a pole in the self-energy