Title: Physics of the Disorder-Induced Zero Bias Anomaly in Strongly-Correlated Systems

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Abstract:

Effects of Strong Correlations on the Disorder-Induced Zero Bias Anomaly

April 23, 2009

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NSERC (Canada)
CFI/OIT

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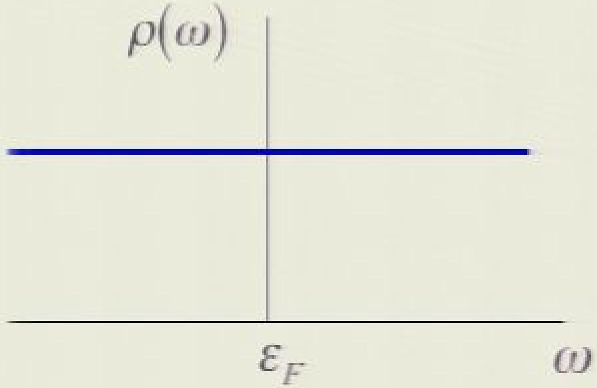
SHARCNET
HPCVL

Overview

- **Broad Goal:** Understand the role of disorder in strongly-correlated materials.
  - Many strongly-correlated materials (high temperature superconductors) have their electronic properties tuned by chemical doping. e.g. $La_{2-x}Sr_xCuO_4$
  - This introduces disorder.
  - Effects of disorder are poorly understood, often ignored.

- **Goal for this talk:** Understand the disorder-induced zero-bias anomaly (ZBA) in the Anderson-Hubbard model.

Disorder-induced ZBA in conventional materials:



Disorder or Interactions:
DOS at Fermi energy is qualitatively unchanged from clean noninteracting limit.

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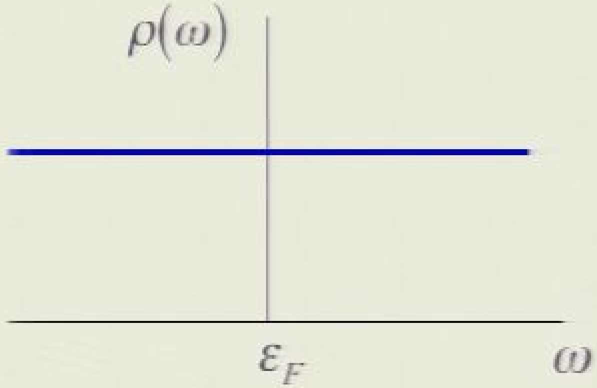

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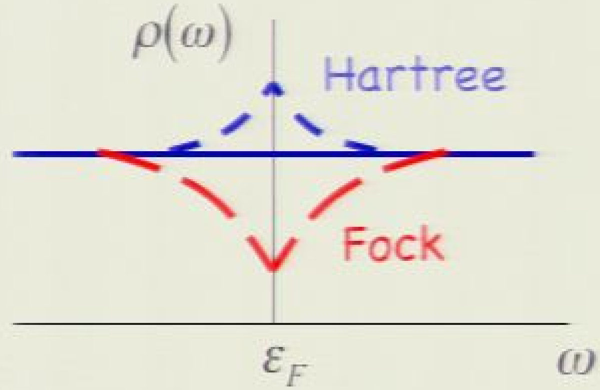

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DOS at Fermi energy has a correction. (Altshuler & Aronov)

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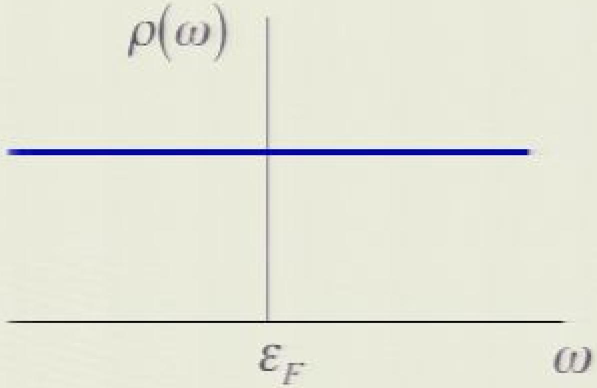

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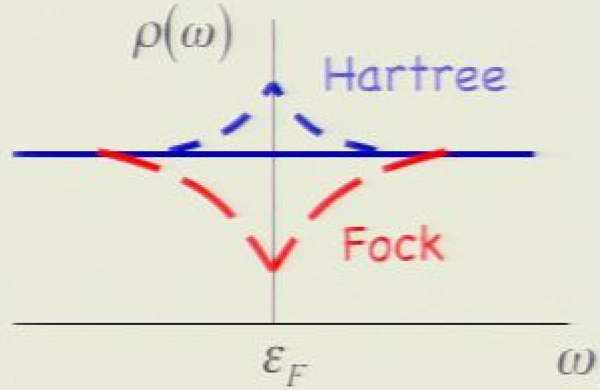

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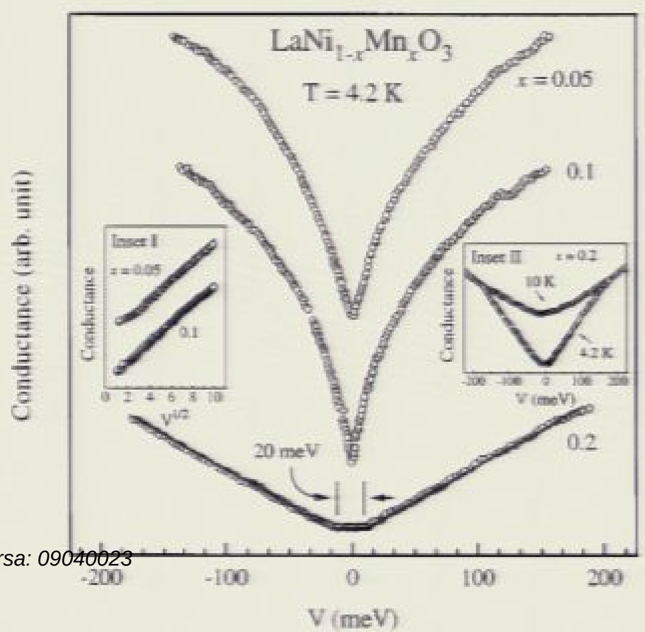

- Sarma et al, PRL 80, 4004 (1998)
- Ino et al, PRB 69, 195116 (2004)
- Kim et al, PRB 73, 235109 (2006)
- Nakatsuji et al, PRL 93, 146401 (2004)
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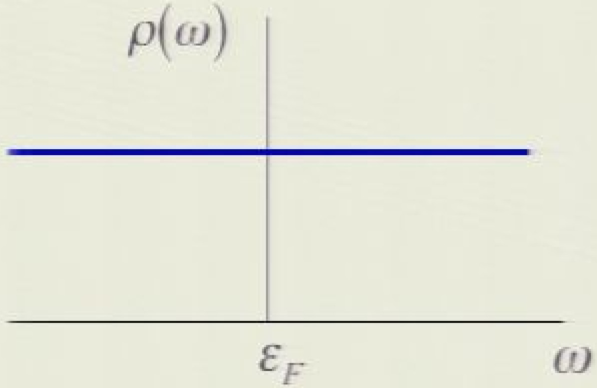

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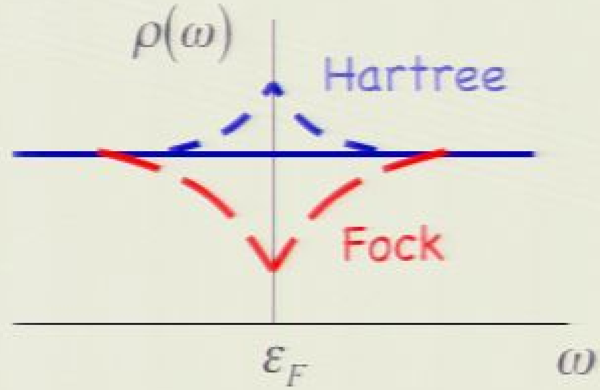

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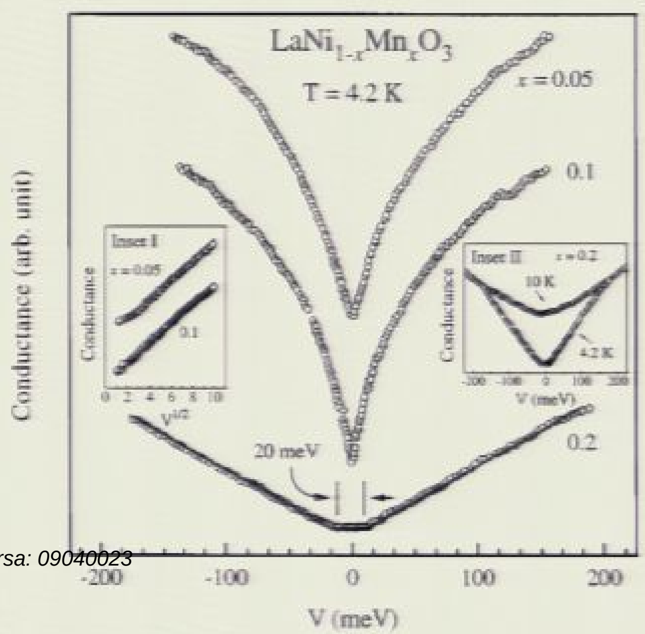

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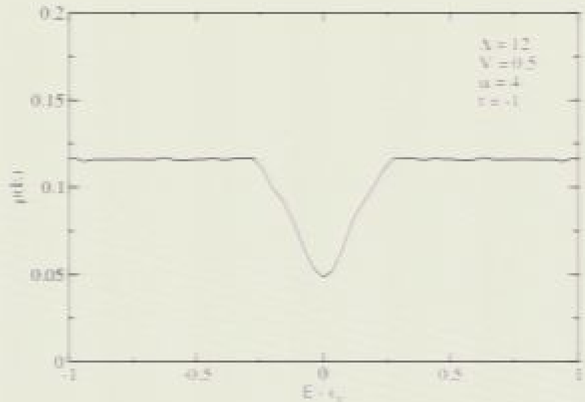
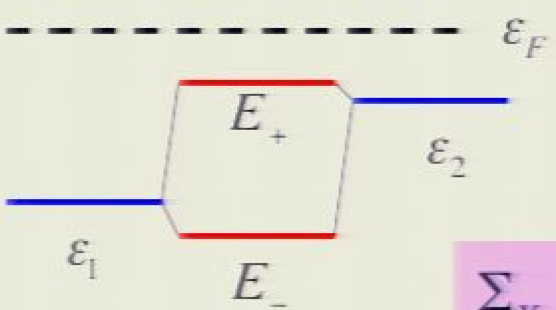
Is there novel physics associated with the ZBA in strongly-correlated materials?

Simple Explanation: Level Repulsion

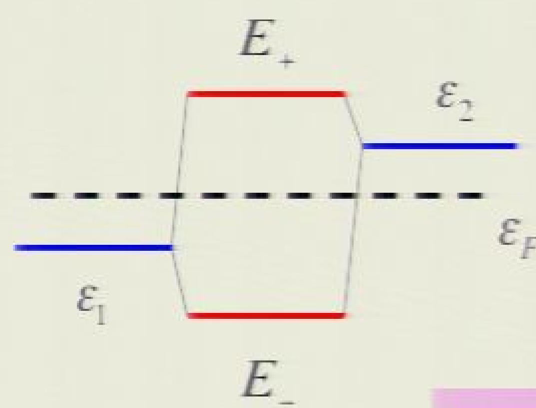
$$H = \begin{bmatrix} \varepsilon_1 & -t + \Sigma_X \\ -t + \Sigma_X & \varepsilon_2 \end{bmatrix}$$

where $\varepsilon_i \in \left[-\frac{\Delta}{2}, \frac{\Delta}{2}\right]$ and $\Sigma_X = -V\langle c_1^{+} c_2 \rangle$





$\Sigma_X = 0$



$\Sigma_X < 0$

ZBA comes from level repulsion between states on either side of the Fermi energy.

Anderson-Hubbard Model

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i}\left(\varepsilon_i n_i + U n_{i\uparrow} n_{i\downarrow}\right)$$

where $\varepsilon_i \in \left[-\frac{\Delta}{2},\frac{\Delta}{2}\right]$

Anderson-Hubbard Model
atomic limit:

$$H = -t \sum_{\langle i,j\rangle \sigma} c^{+}_{i\sigma} c_{j\sigma} + \sum_i \left(\varepsilon_i n_i + U n_{i\uparrow} n_{i\downarrow} \right)$$

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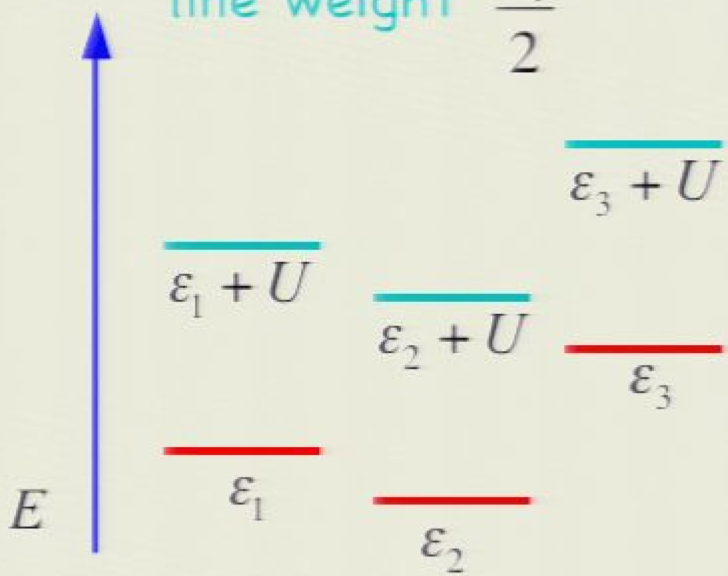
line weight $\frac{n_i}{2}$



line weight $1 - \frac{n_i}{2}$

Anderson-Hubbard Model atomic limit:

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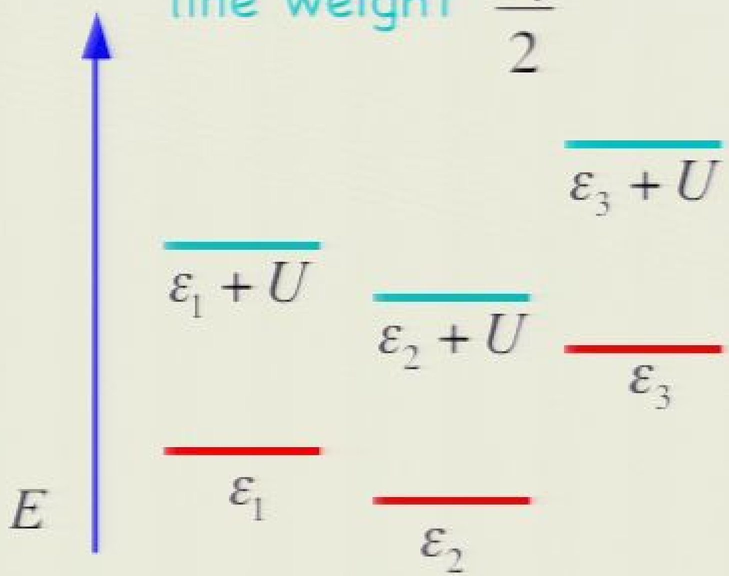

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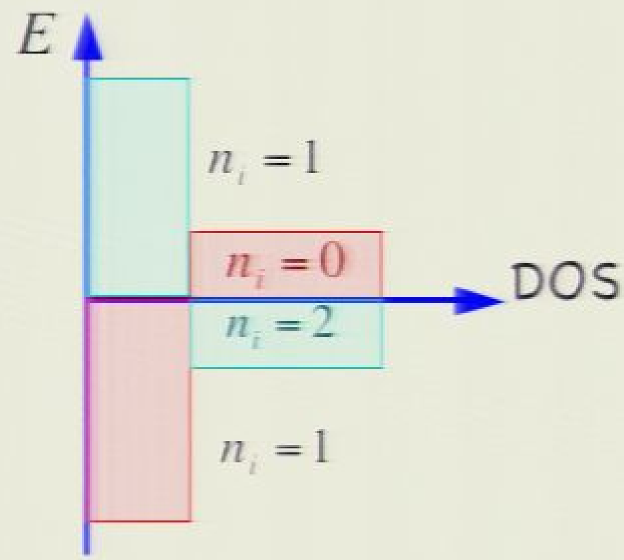

What happens away from atomic limit?

Other Results for the Anderson-Hubbard Model

Different approaches find different results

Hartree-Fock:

Milanovic, PRL **63**, 82 (1989)
Tusch, PRB **48**, 14843 (1993)
Heidarian, PRL **93**, 126401 (2004)
Fazileh, PRL **96**, 046410 (2006)
...and many others

Effective Medium DMFT

Ulmke, PRB (1995)
Laad, PRB **64**, 195114 (2001)
Byczuk, PRB **94**, 056404 (2005)
Balzer, Physica B **359-61**, 768(2005)
Lombardo, PRB **74**, 085116 (2006)
Dobrosavljevic, PRL **78**, 3943 (1997)
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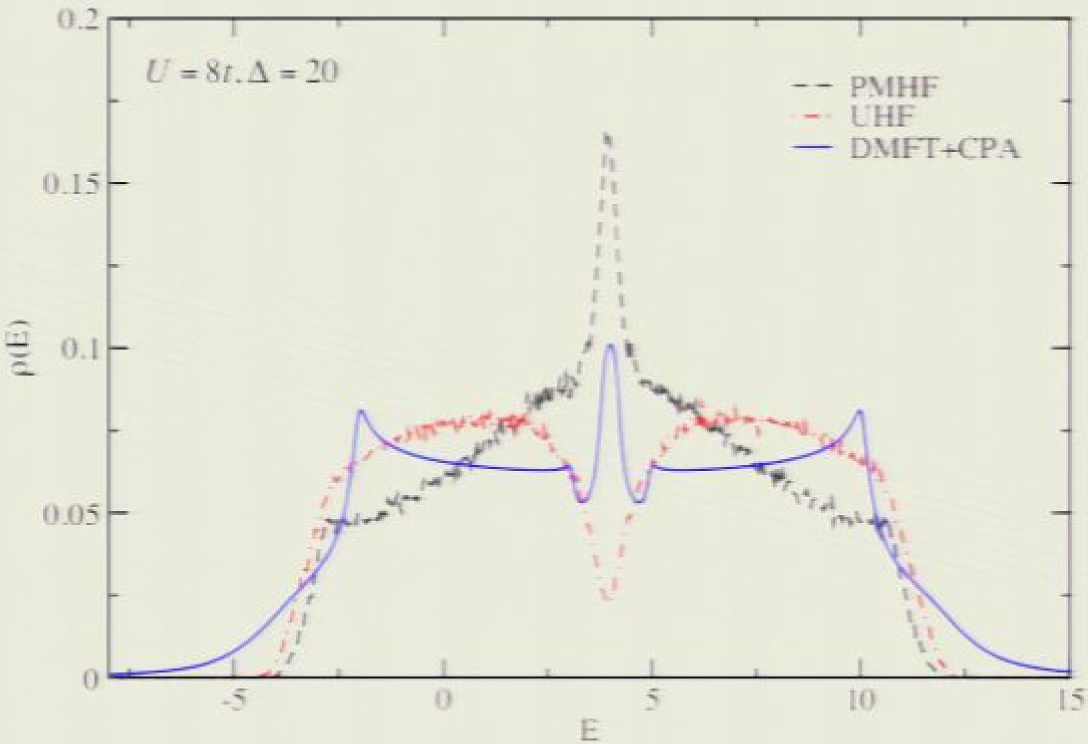
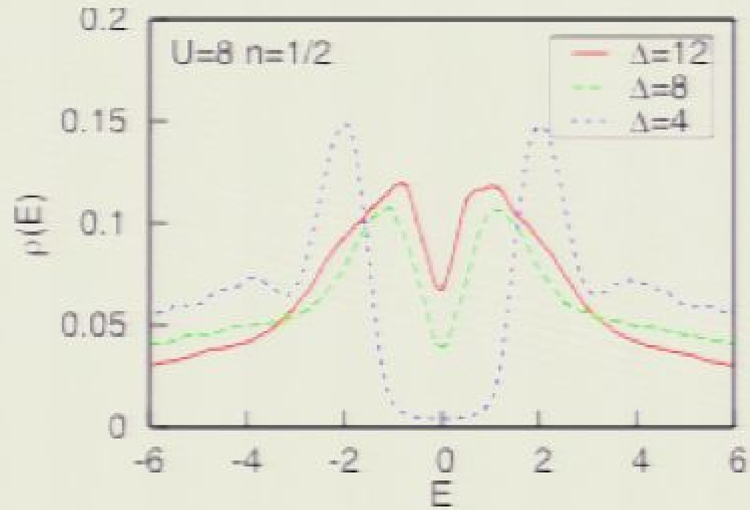


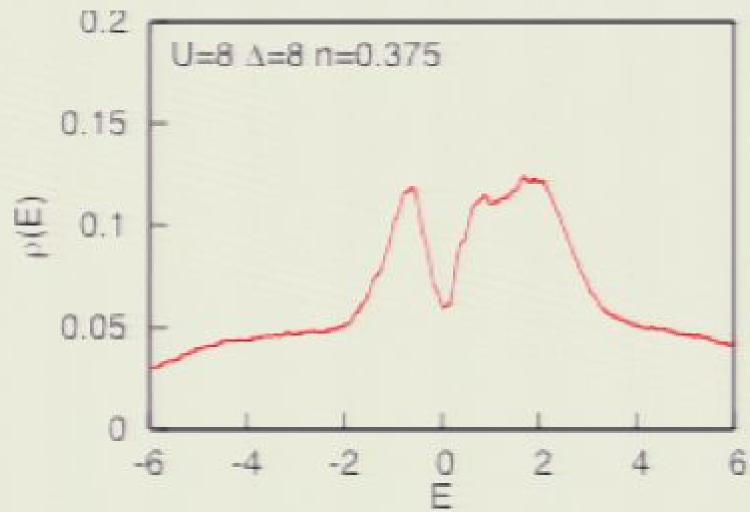
Challenge: Correctly include disorder and strong correlations.

Exact Results for the Anderson-Hubbard Model



$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{+} c_{j\sigma} + \sum_i \left(\varepsilon_i n_i + U n_{i\uparrow} n_{i\downarrow} \right)$$

where $\varepsilon_i \in \left[-\frac{\Delta}{2}, \frac{\Delta}{2} \right]$



- Lanczos
- N=12 sites
- 1000 disorder configuration

AHM has a -ve ZBA even though exchange self-energy vanishes!

c.f. Chiesa et al, PRL 101, 086401 (2008)

Origin of the ZBA

Approach:

- Use exact results for small clusters. Lanczos method gives the full Green's function $G_{ij\sigma}(\omega)$

- Use the Green's function to extract local and nonlocal inelastic self-energies.

- Use these self-energies in an approximate expression for the density of states. This allows us to examine the effect of each piece of the self-energy separately.

- Note: the goal is not to calculate the DOS (this comes directly from Lanczos) but to separate the different contributions to the DOS.

Origin of the ZBA

Inelastic self-energy from ED for each disorder configuration:

$$\Sigma_{ij\sigma}(\omega) = \left[\mathbf{G}_0(\omega)^{-1} - \mathbf{G}(\omega)^{-1}\right]_{ij\sigma}$$

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Inelastic self-energy from ED for each disorder configuration:

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It is always possible to write:

$$G_{ii\sigma}(\omega) = \frac{1}{\omega - \varepsilon_i - \Sigma_{ii\sigma}(\omega) - \Lambda_{i\sigma}(\omega)}$$

Local Self-Energy. => Splits local spectrum into LHO/UHO

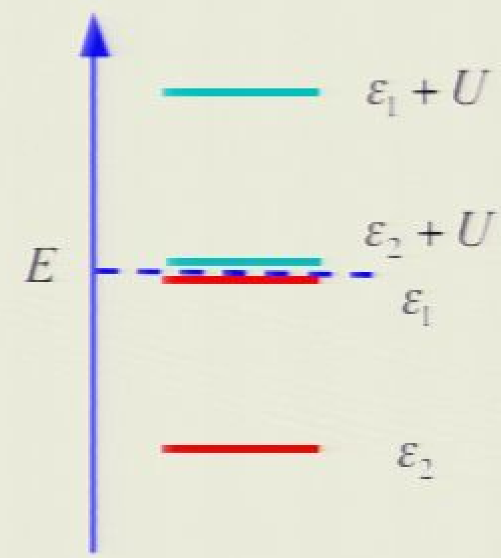
Hybridization function. => Level repulsion.

$$\Lambda_{i\sigma}(\omega) = \omega - \varepsilon_i - \Sigma_{ii\sigma}(\omega) - \frac{1}{G_{ii\sigma}(\omega)}$$

Density of States (large disorder):

$$\rho(E) = \frac{1}{\Delta}\left[\frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E} + \frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E-U}\right]$$

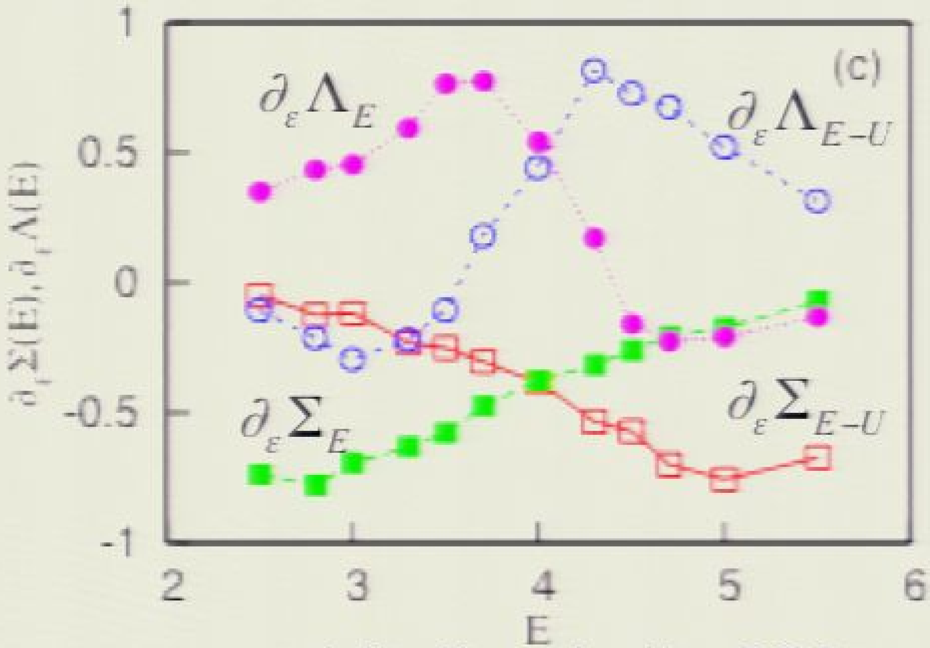
- Two types of sites have spectral weight at E (LHO and UHO).
- DOS depends on derivatives of self-energy and hybridization function.



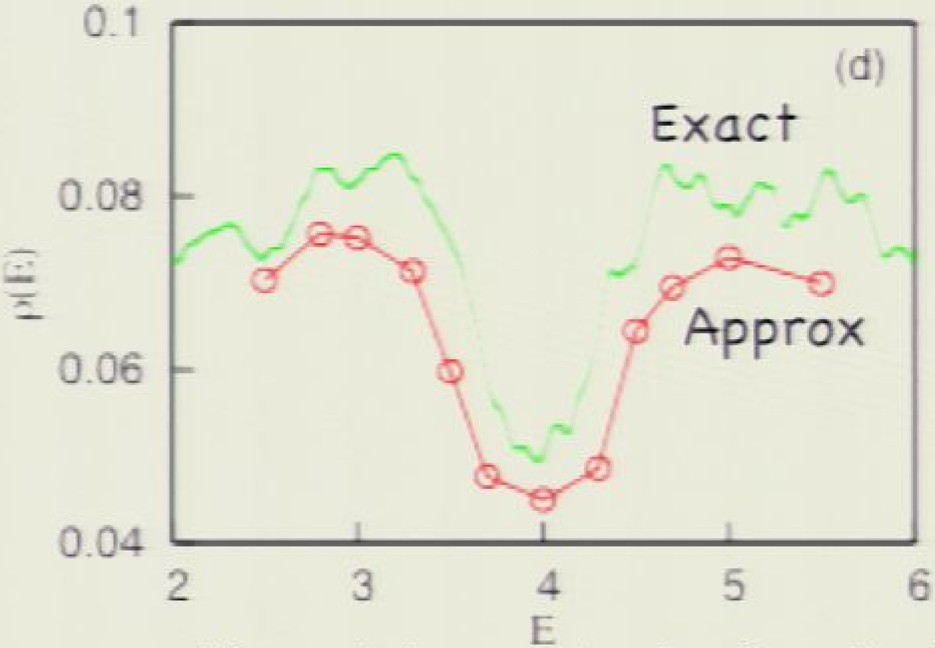
Can distinguish local and nonlocal self-energy contributions to the DOS

Comparing local and nonlocal contributions to the DOS

$$\rho(E) = \frac{1}{\Delta}\left[\frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E} + \frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E-U}\right]$$



contributions to the DOS



self-consistency check of method

Conclusion: ZBA comes from nonlocal self-energy.

BUT: Nonlocal SE vanishes in HF => higher order correlations

Nonlocal self-energy has a continued fraction form:

$$\Sigma_{ij\sigma}(\omega) = \cfrac{-tU^2 p_{ij}}{(\omega - \varepsilon_i - Uh_{i\bar{\sigma}})(\omega - \varepsilon_j - Uh_{j\bar{\sigma}}) + \cfrac{O(t^2)}{\omega - \ldots}}$$

$$\boxed{h_{i\bar{\sigma}} = 1 - n_{i\bar{\sigma}}}$$

Depends on fluctuations via the correlation function p_{ij},

$$p_{ij} = \langle n_{i\bar{\sigma}} n_{j\bar{\sigma}} \rangle - \langle n_{i\bar{\sigma}} \rangle \langle n_{j\bar{\sigma}} \rangle + \langle S_{i+} S_{j-} \rangle - \langle D_i^+ D_j \rangle$$

where $D_i = c_{i\uparrow} c_{i\downarrow}$

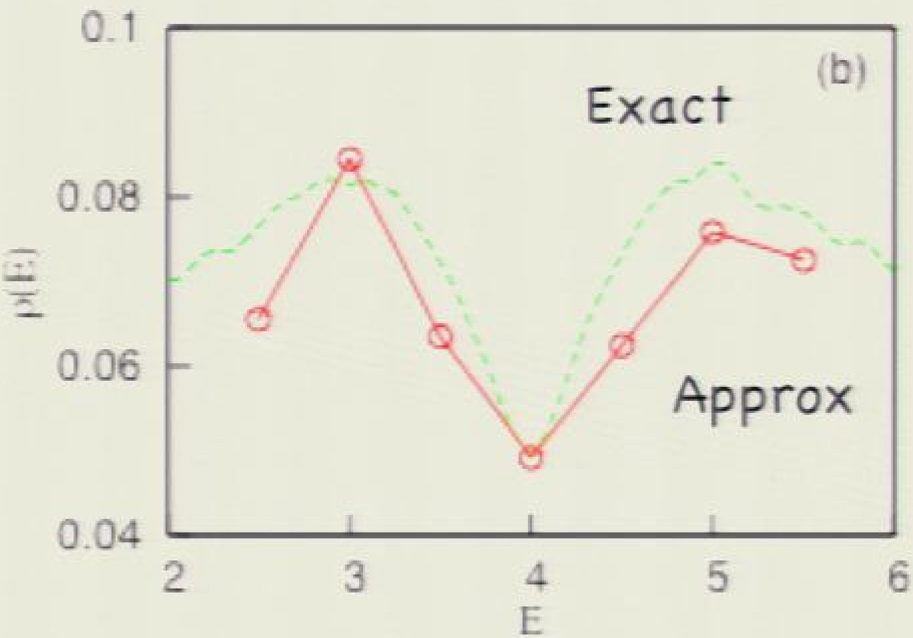
small

Song et al, http://arxiv.org/abs/0808.3356

DOS Using Approximate Nonlocal Self-Energy

$$\rho(E) = \frac{1}{\Delta}\left[\left.\frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E)+\partial_\varepsilon \Lambda_\varepsilon(E)}\right|_{\varepsilon=E} + \left.\frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E)+\partial_\varepsilon \Lambda_\varepsilon(E)}\right|_{\varepsilon=E-U}\right]$$

$$\Lambda_{i\sigma}(\omega) = \sum_{j,k}\left[t-\Sigma_{ij\sigma}(\omega)\right]G^{i}_{jk}(\omega)\left[t-\Sigma_{ki\sigma}(\omega)\right]$$



Charge and Spin Fluctuations both contribute to ZBA

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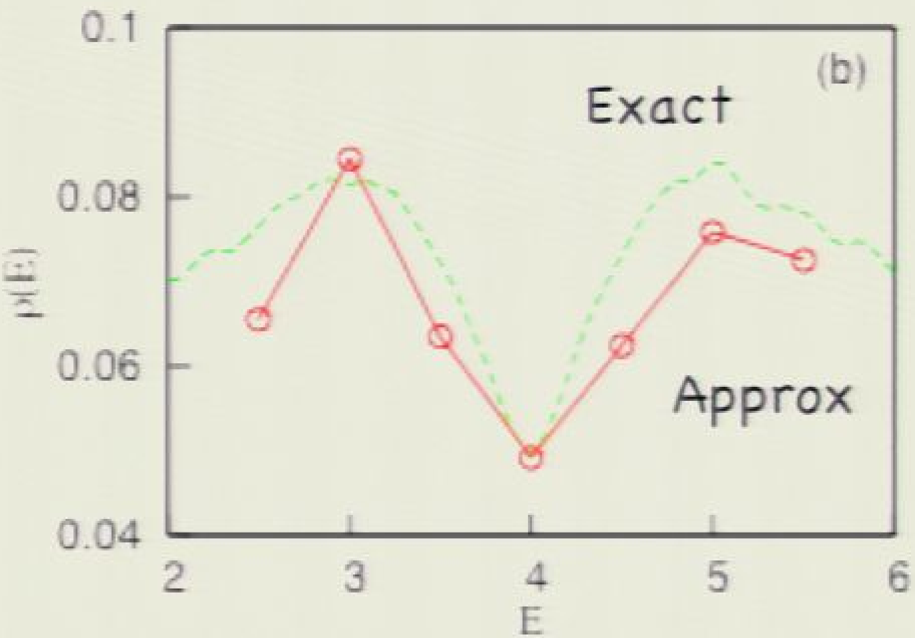

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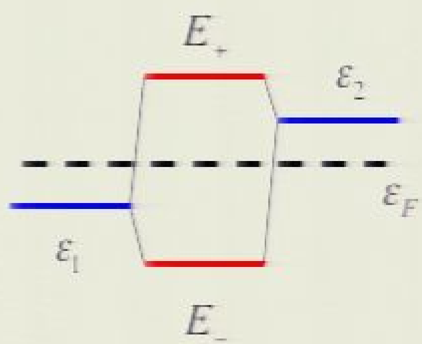
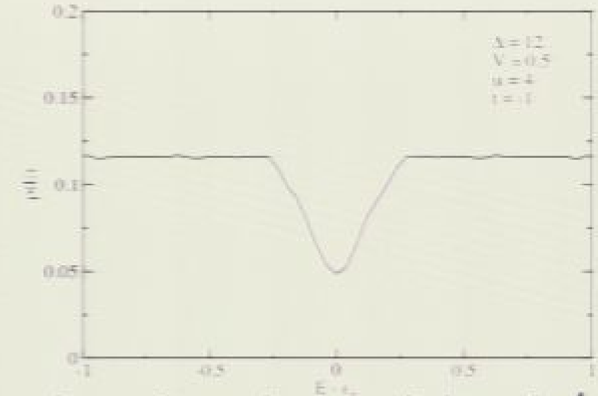
Asymmetry in the DOS

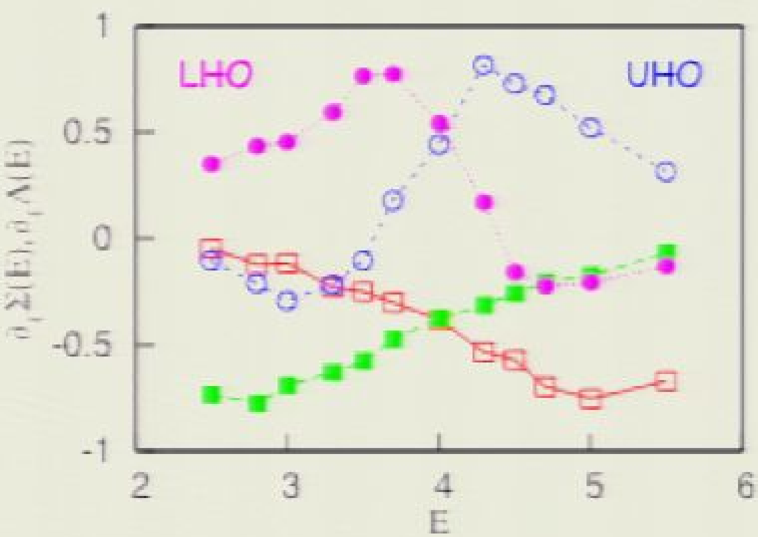




Recall: 2-site example. Level repulsion b/w states on opposite sites of Fermi energy.

$\varepsilon_1 < \varepsilon_F < \varepsilon_2$

Anderson Hubbard model: ZBA is asymmetric w/in each band.



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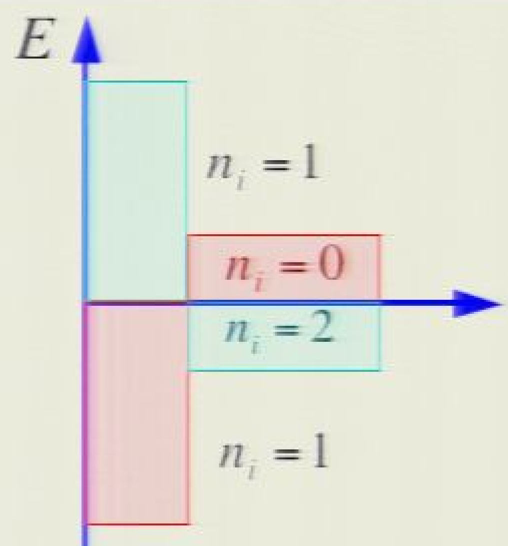

atomic-limit DOS

$\varepsilon_1 < \varepsilon_F < \varepsilon_2 + U ?$

DOS Using Approximate Nonlocal Self-Energy

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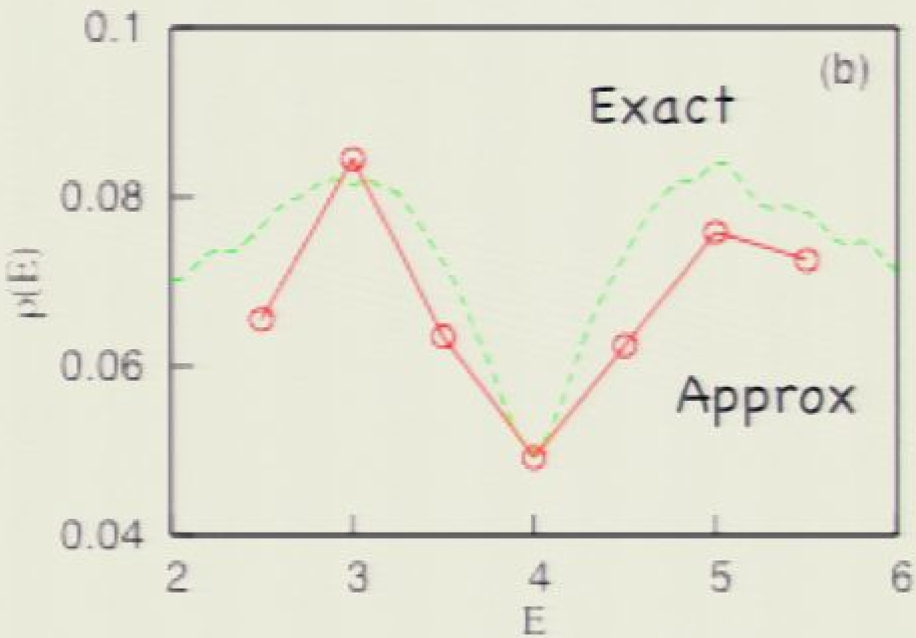

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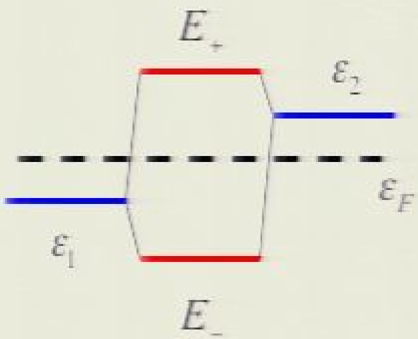

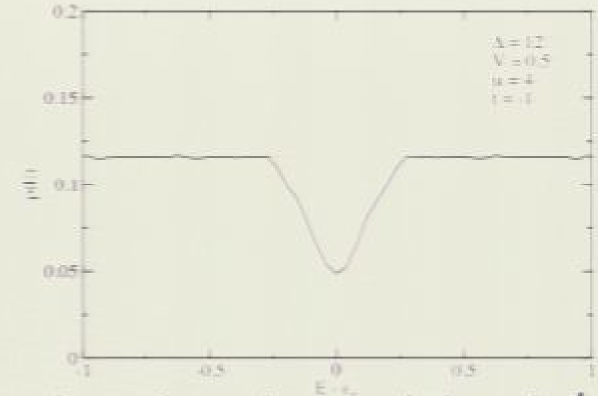

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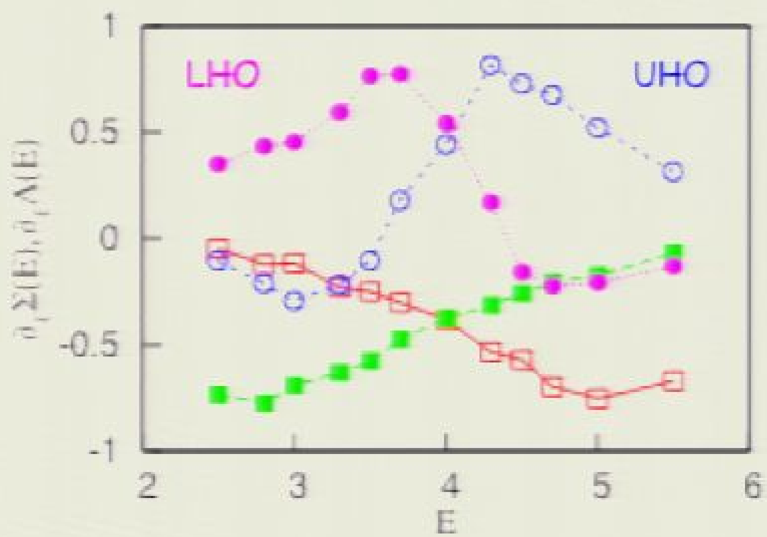

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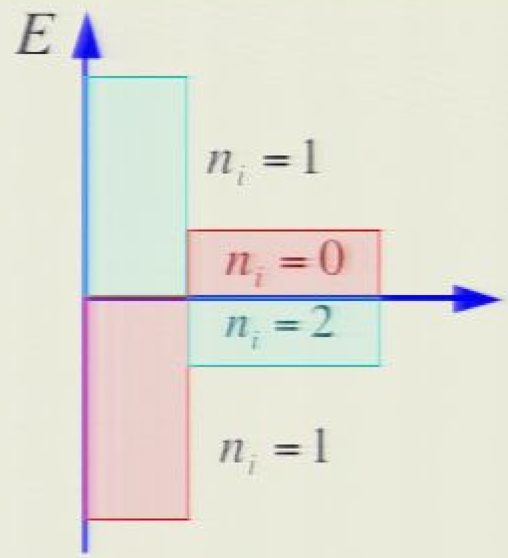

atomic-limit DOS

$\varepsilon_1 < \varepsilon_F < \varepsilon_2 + U?$

Results for two sites:

$$\rho(E) = \frac{1}{\Delta}\left[\left.\frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\right|_{\varepsilon=E} + \left.\frac{1}{1+\partial_\varepsilon\Sigma_\varepsilon(E)+\partial_\varepsilon\Lambda_\varepsilon(E)}\right|_{\varepsilon=E-U}\right]$$

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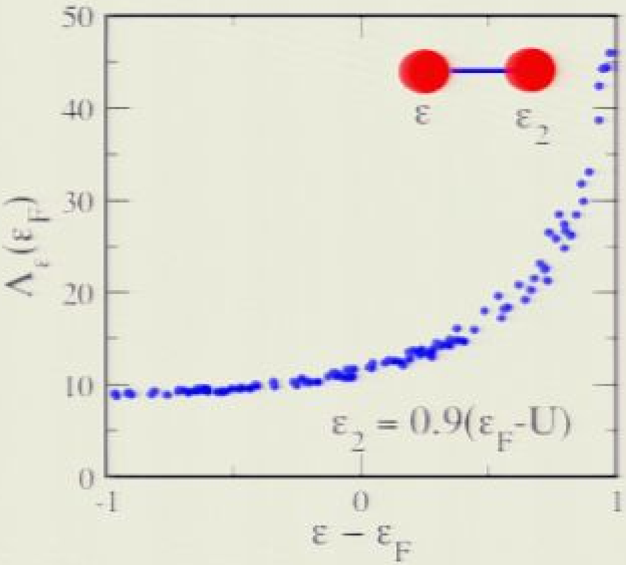
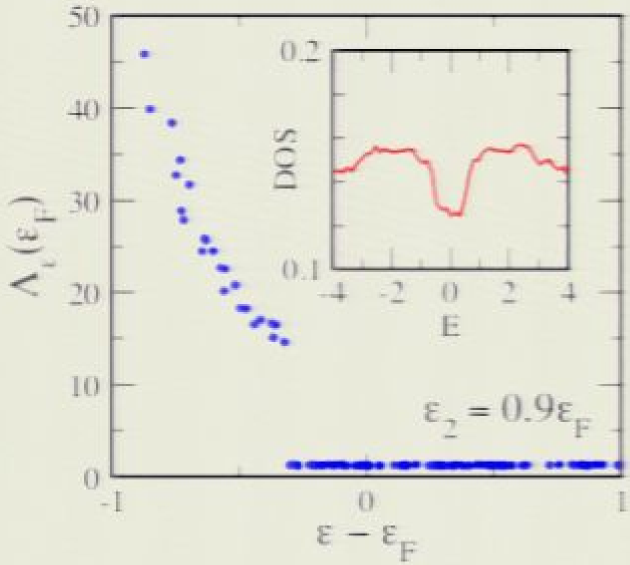
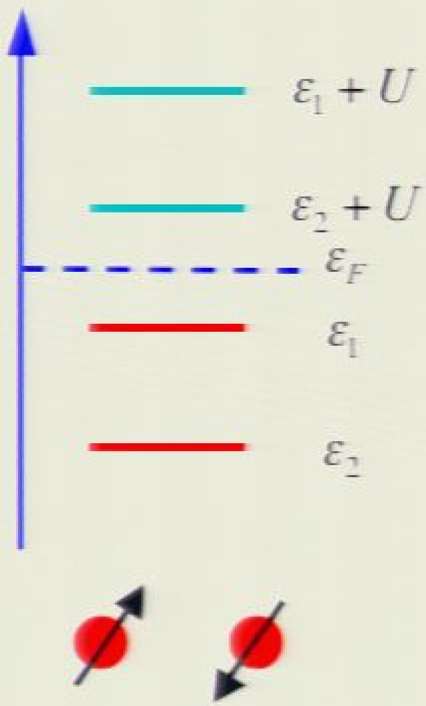


$\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\big|_{\varepsilon=\varepsilon_F} > 0$



$\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\big|_{\varepsilon=\varepsilon_F} = 0$



ZBA comes from level repulsion between UHO and LHO of singly-occupied sites

Conclusions

- What's special about ZBA in the Anderson-Hubbard model?
  - Can't be understood (even qualitatively) at level of Hartree-Fock theory.

- Where does the ZBA come from in the Anderson-Hubbard model?
  - ZBA comes from the nonlocal self-energy involving dynamical charge and spin fluctuations.
  - Level repulsion between LHO and UHO of singly-occupied sites!
  - Behaviour is very non-mean-field.

Results for two sites:

$$\rho(E) = \frac{1}{\Delta}\left[\left.\frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E) + \partial_\varepsilon \Lambda_\varepsilon(E)}\right|_{\varepsilon=E} - \left.\frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E) + \partial_\varepsilon \Lambda_\varepsilon(E)}\right|_{\varepsilon=E-U} \right]$$

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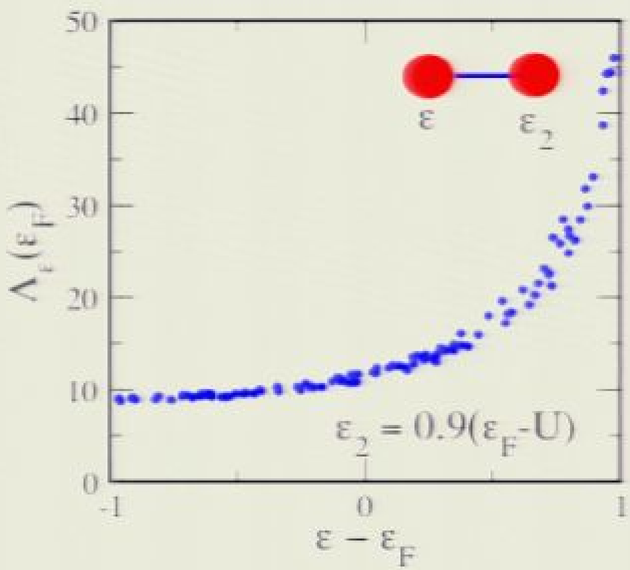
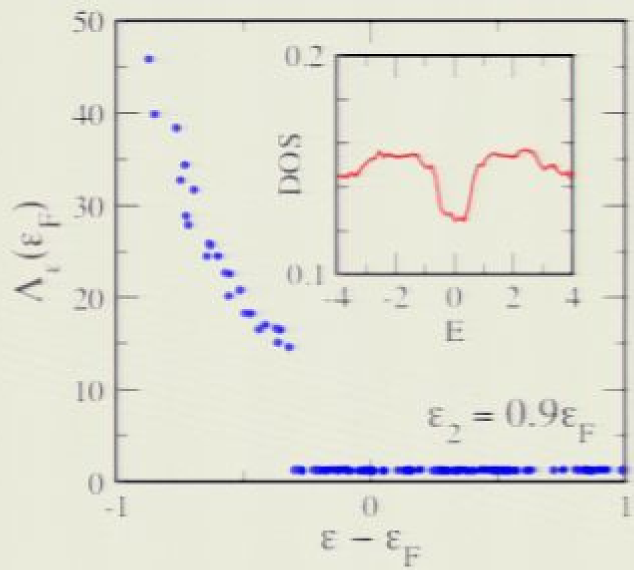
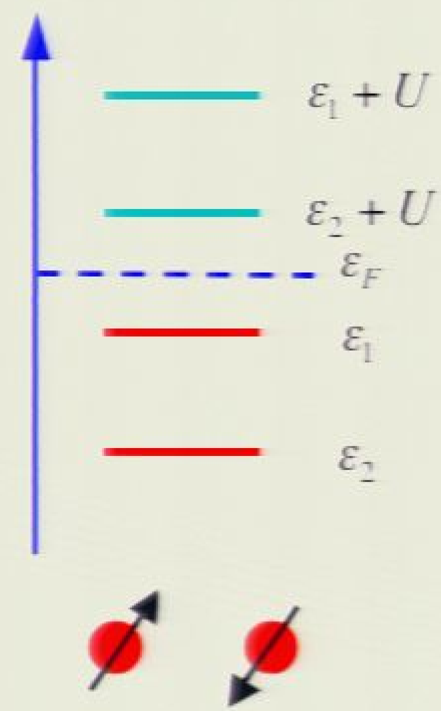




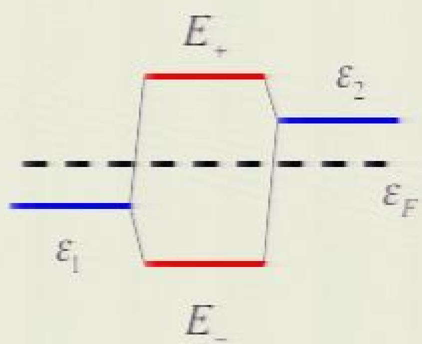


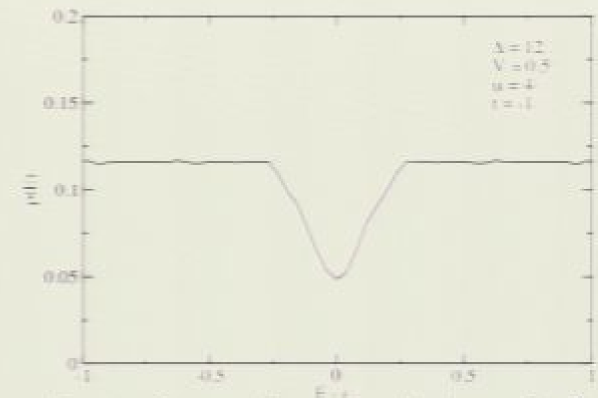
$$\left.\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\right|_{\varepsilon=\varepsilon_F} > 0$$

$$\left.\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\right|_{\varepsilon=\varepsilon_F} = 0$$

ZBA comes from level repulsion between UHO and LHO of singly-occupied sites

Asymmetry in the DOS

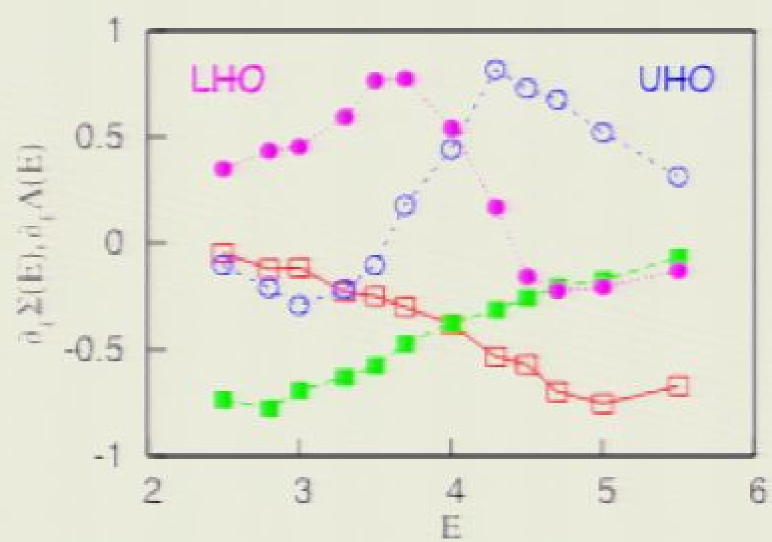




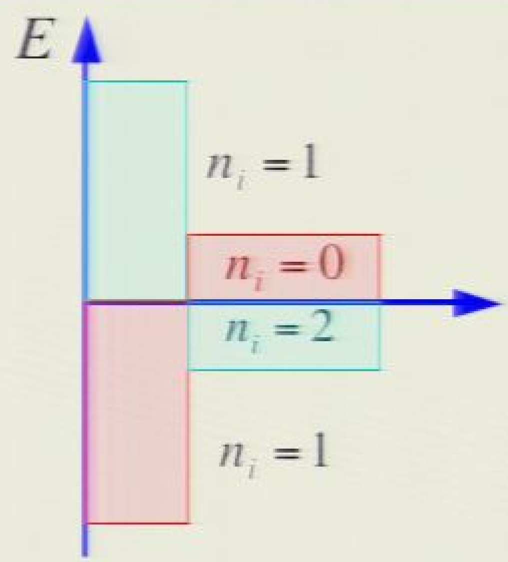
Recall: 2-site example. Level repulsion b/w states on opposite sites of Fermi energy.

$\varepsilon_1 < \varepsilon_F < \varepsilon_2$

Anderson Hubbard model: ZBA is asymmetric w/in each band.



$$\Sigma_{ij\sigma} \sim \langle n_{i\bar{\sigma}} n_{j\bar{\sigma}} \rangle - \langle n_{i\bar{\sigma}} \rangle \langle n_{j\bar{\sigma}} \rangle + \langle S_{i+} S_{j-} \rangle$$

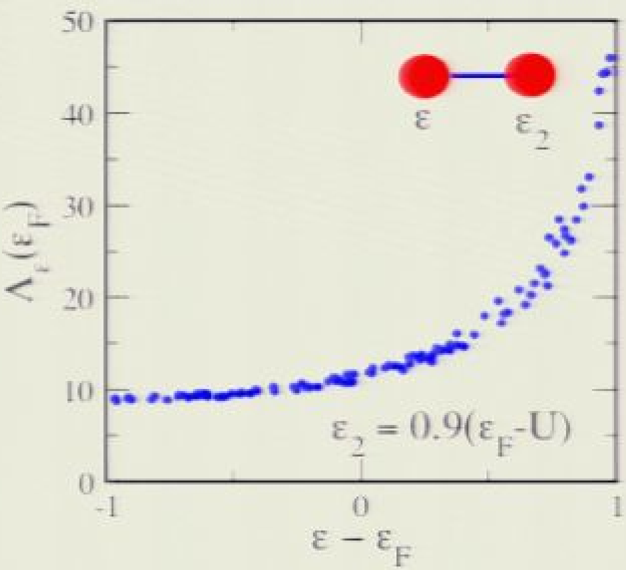


atomic-limit DOS

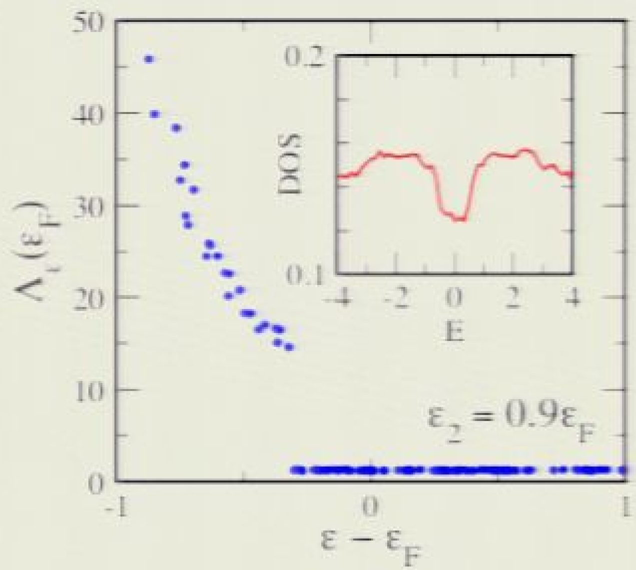
$\varepsilon_1 < \varepsilon_F < \varepsilon_2 + U?$

Results for two sites:

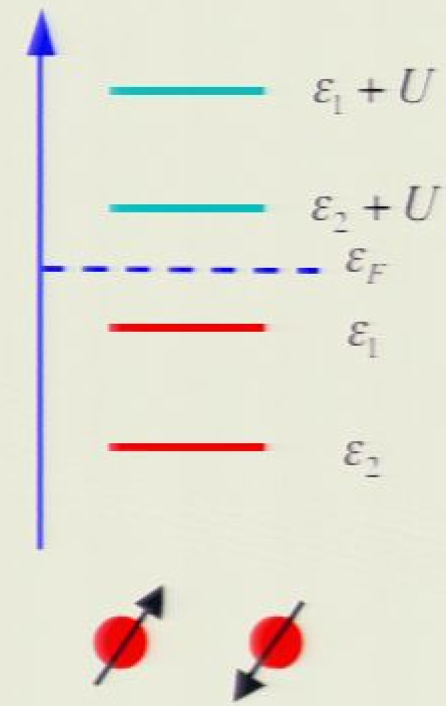
$$\rho(E) = \frac{1}{\Delta}\left[\frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E) + \partial_\varepsilon \Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E} - \frac{1}{1+\partial_\varepsilon \Sigma_\varepsilon(E) + \partial_\varepsilon \Lambda_\varepsilon(E)}\bigg|_{\varepsilon=E-U} \right]$$



$$\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\Big|_{\varepsilon=\varepsilon_F} > 0$$



$$\partial_\varepsilon \Lambda_\varepsilon(\varepsilon_F)\Big|_{\varepsilon=\varepsilon_F} = 0$$



ZBA comes from level repulsion between UHO and LHO of singly-occupied sites