Distributional exact diagonalization for quantum impurity problems

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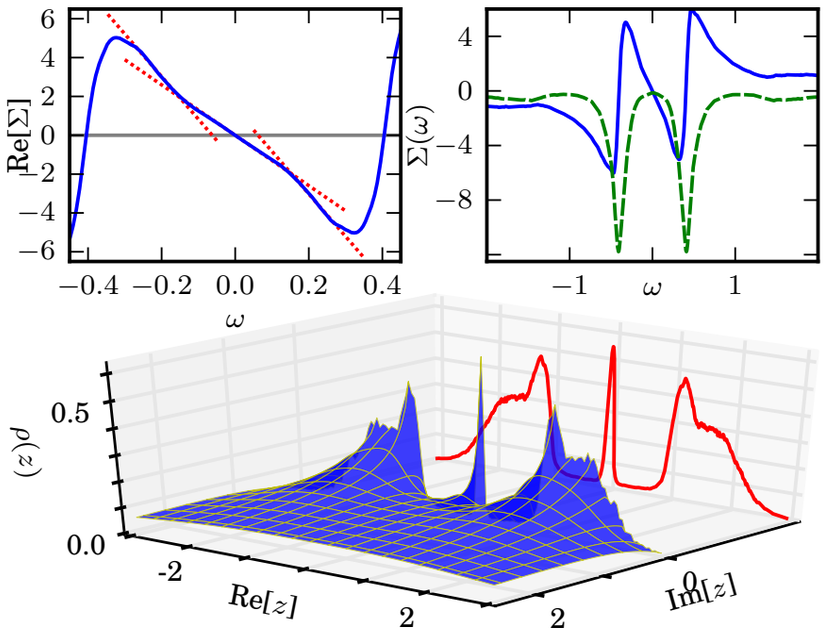

with Hugo U.R. Strand

arXiv:1201.6160v1

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The problem:

We have:

$$S = -\int d\tau d\tau' \sum_\sigma c_\sigma^\dagger(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') \qquad (1)$$

$$-\mu \int d\tau \sum_\sigma c_\sigma^\dagger(\tau) c_\sigma(\tau) + U \int d\tau c_\uparrow^\dagger(\tau) c_\downarrow^\dagger(\tau) c_\downarrow(\tau) c_\uparrow(\tau)\,,$$

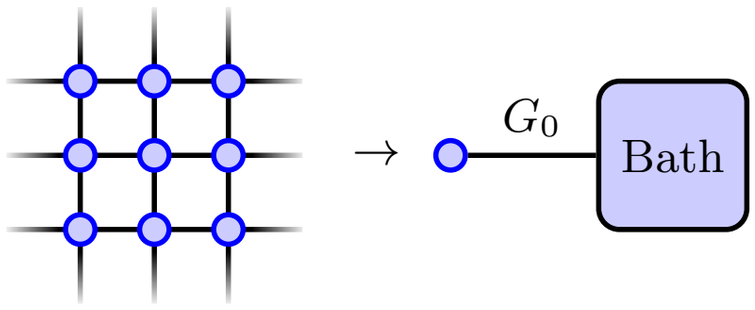
We want:

$$G_\sigma(\tau - \tau') = -\langle T c_\sigma(\tau) c_\sigma^\dagger(\tau') \rangle_S$$

Or equivalently:

$$\Sigma(z) - \mu = G_0(z)^{-1} - G(z)^{-1}$$

For example in Dynamical mean field theory

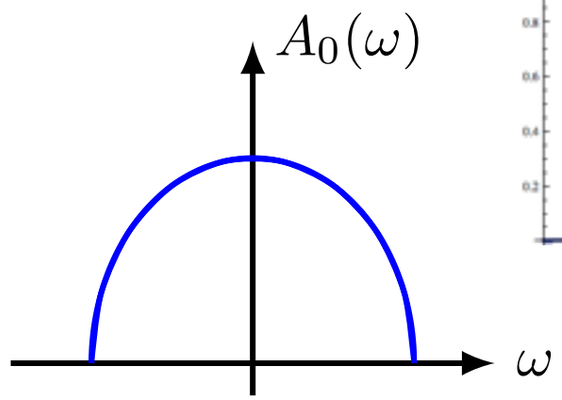


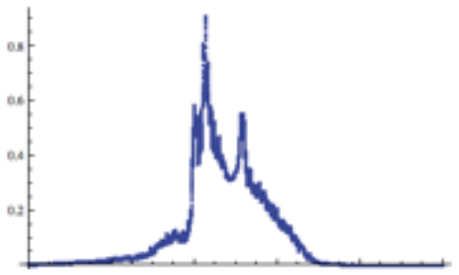
New (very good) method for calculating self energy

Distribution of poles

$$G_0(z) = \int \frac{d\omega}{2\pi} \frac{A_0(w)}{z-\omega}$$

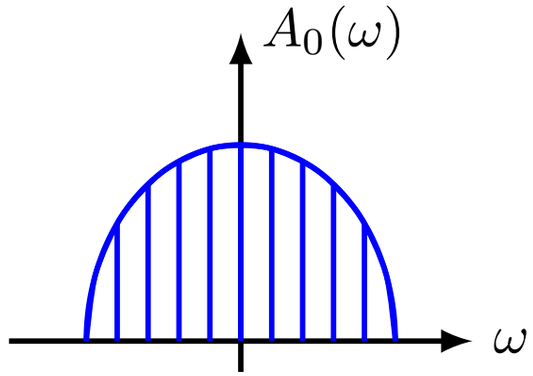
$$A_0(\omega) = -2ImG_0(\omega + i\delta)$$





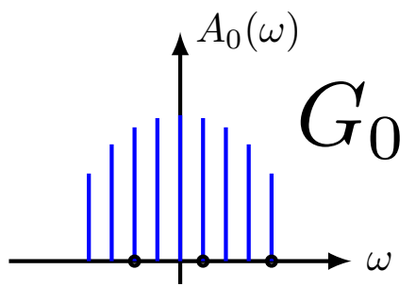
The non-interacting Green's function is well represented by a very large number of poles:

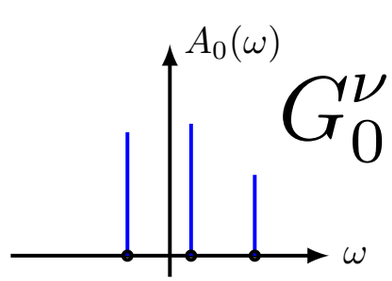
$$G_0(z) \approx \sum_{i=1}^{M} \frac{\tilde{a}_i}{z-b_i}$$



Divide the poles into small groups of n=5,6, or 7 or so poles:

$$G_0(z) = \frac{1}{N}\sum_{\nu=1}^{N}\sum_{j=1}^{n} \frac{a_j^\nu}{z-b_j^\nu} = \frac{1}{N}\sum_{\nu} G_0^\nu(z)$$

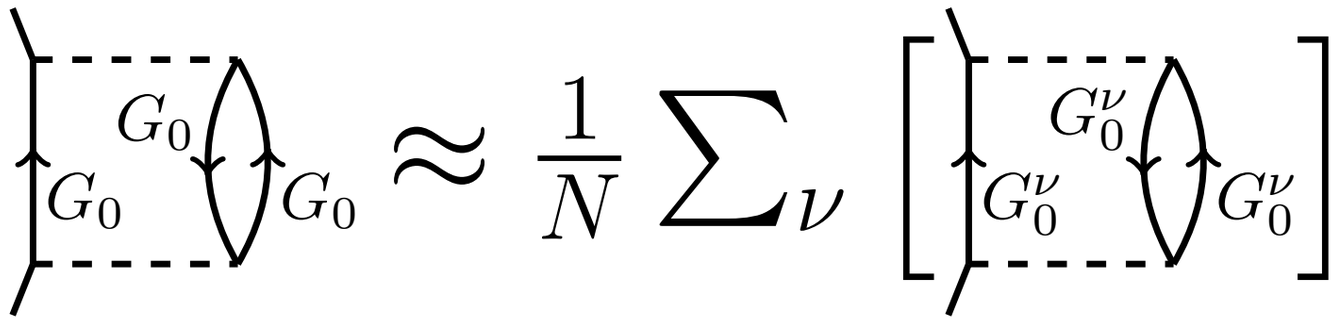




The approximation:

Replace intergroup correlations by intragroup correlations

Ex:



$$\Sigma^{(2)}(z) = \frac{U^2}{\beta^2} \sum_{z_p, z_q} G_0(z_p) G_0(z_q) G_0(z_p + z_q - z) =$$

$$= \frac{U^2}{\beta^2} \sum_{z_p, z_q} \frac{1}{N^3} \sum_{\nu,\sigma,\tau} G_0^\nu(z_p) G_0^\sigma(z_q) G_0^\tau(z_p + z_q - z)$$

$$\approx \frac{1}{N} \frac{U^2}{\beta^2} \sum_{z_p, z_q} \sum_\nu G_0^\nu(z_p) G_0^\nu(z_q) G_0^\nu(z_p + z_q - z) =$$

$$= \frac{1}{N} \sum_\nu \Sigma^{(2),\nu}(z) \,.$$

Thus: $$\Sigma \approx \frac{1}{N} \sum_\nu \Sigma^\nu$$

To all orders

Σ^ν is the exact self energy of G_0^ν with interaction U

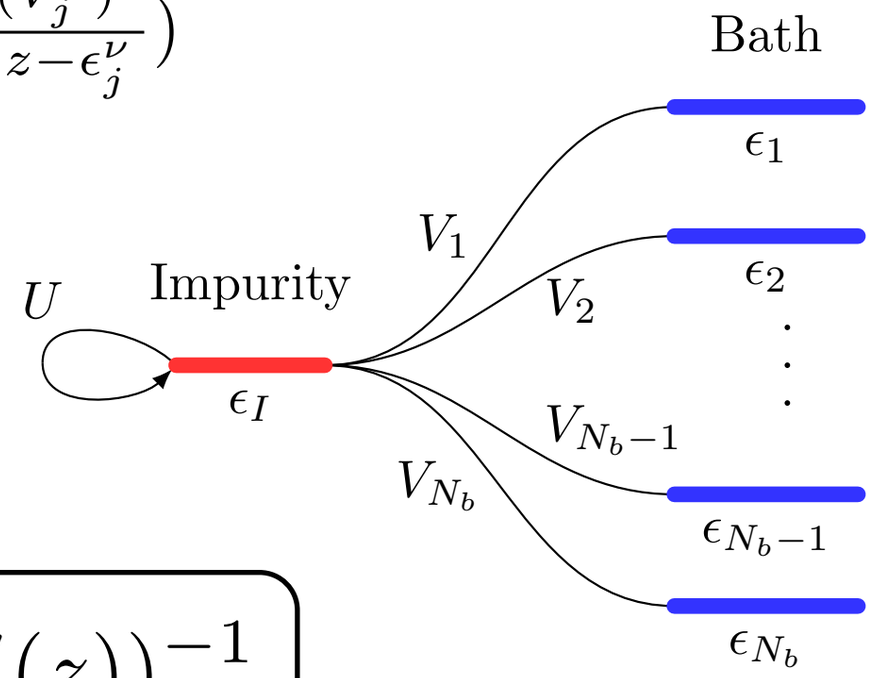
$$G_0^\nu = \sum_{j=1}^{n} \frac{a_j^\nu}{z - b_j^\nu}$$

Map to Anderson model

$$G_0^\nu = 1/(z - \epsilon_0^\nu - \sum_{j=1}^{n-1} \frac{(V_j^\nu)^2}{z - \epsilon_j^\nu})$$

$$H_0 = \epsilon_0^\nu \sum_\sigma c_\sigma^\dagger c_\sigma + \sum_{\sigma,j=1}^{n-1} [V_j^\nu (c_\sigma^\dagger c_{j\sigma} + h.c.) + \epsilon_j^\nu c_{j\sigma}^\dagger c_{j\sigma}]$$

$$H = H_0 + \mu \sum_\sigma c_\sigma^\dagger c_\sigma + U c_\uparrow^\dagger c_\downarrow^\dagger c_\downarrow c_\uparrow$$



$$\Sigma^\nu(z) - \mu = (G_0^\nu(z))^{-1} - (G^\nu(z))^{-1}$$

This step is done by Exact diagonalization
(same as in standard ED-DMFT formalism)

Caffarel and Krauth, PRL 1994

Sample average:

$$\Sigma \approx \frac{1}{N} \sum_\nu \Sigma^\nu$$

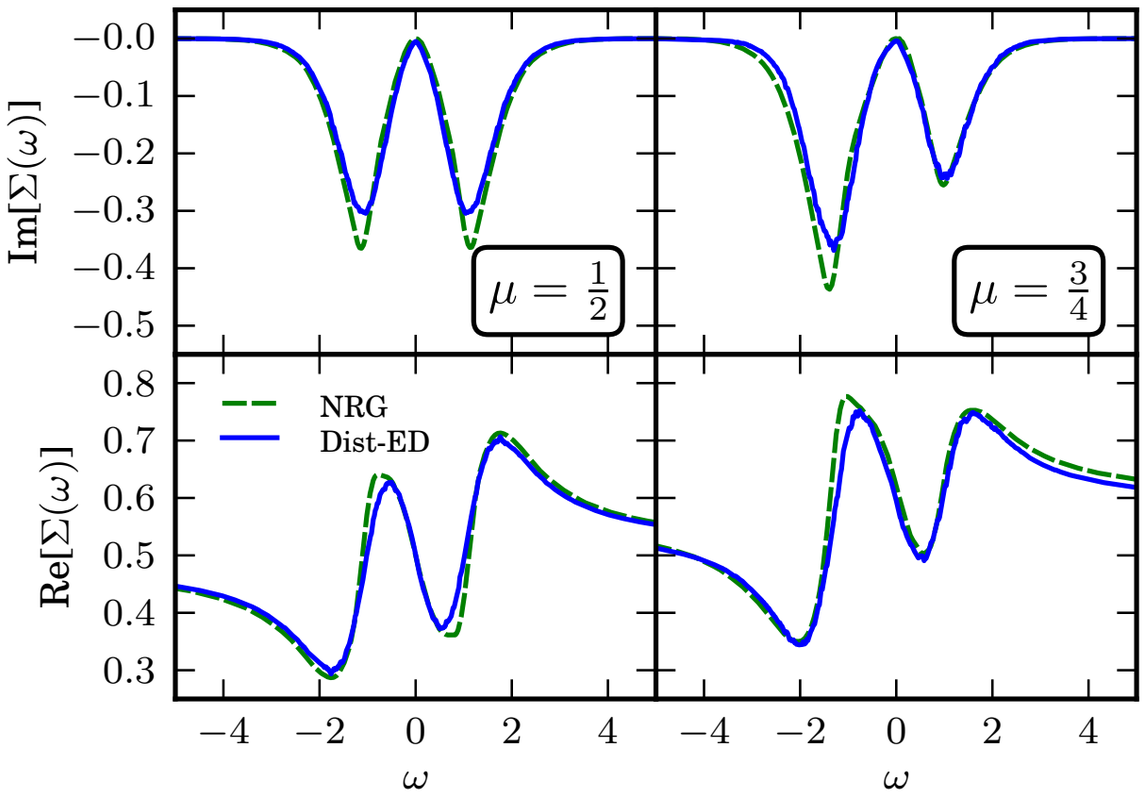
DMFT,
Semicircular DOS
n=6

It works surprisingly well

No free parameters

Self energies compared to Numerical renormalization group:

$2 \cdot 10^4$ samples



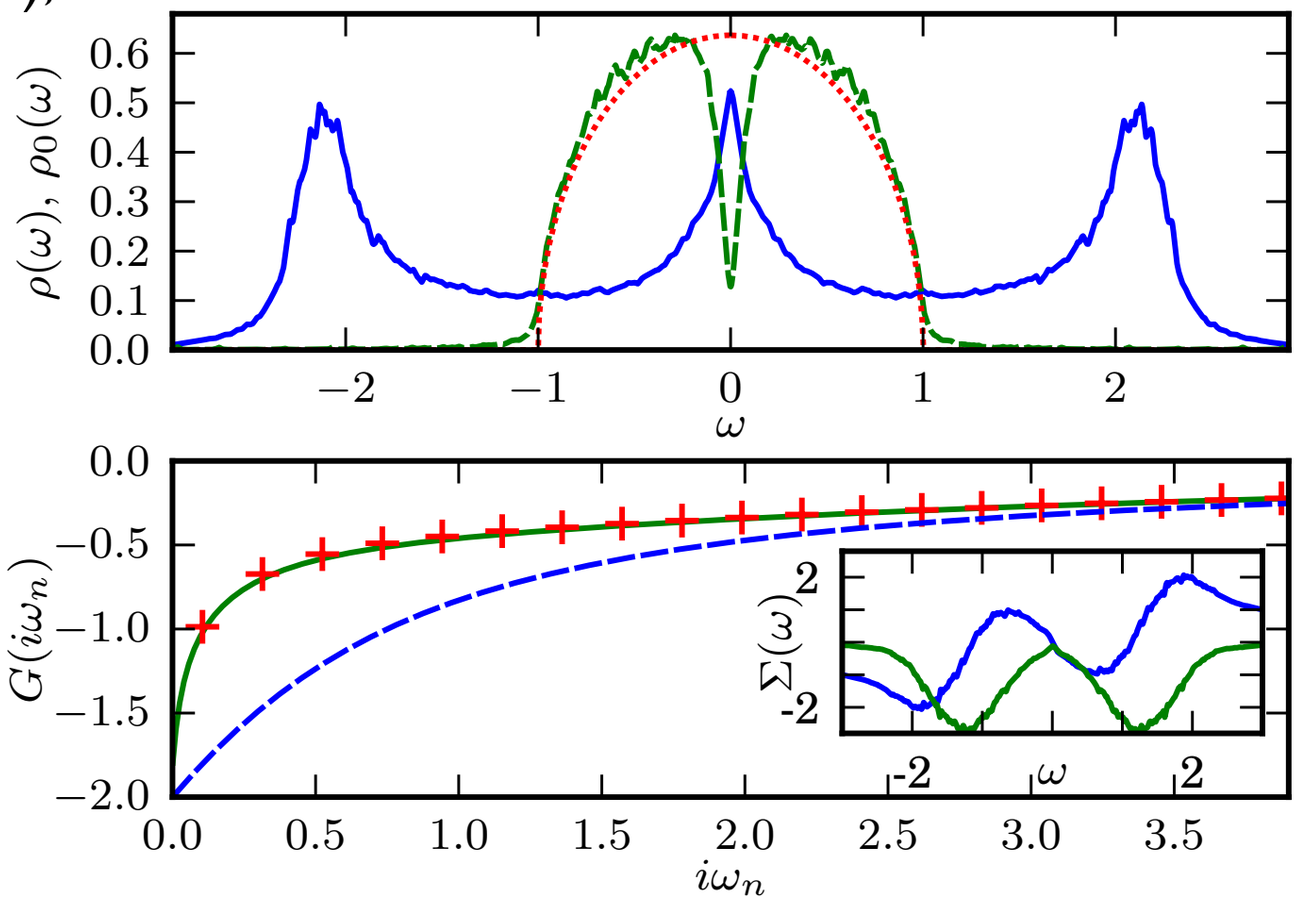
T=0, U=1

NRG from Grete et al. PRB 2011

compared to CT-QMC, crosses, within 4%

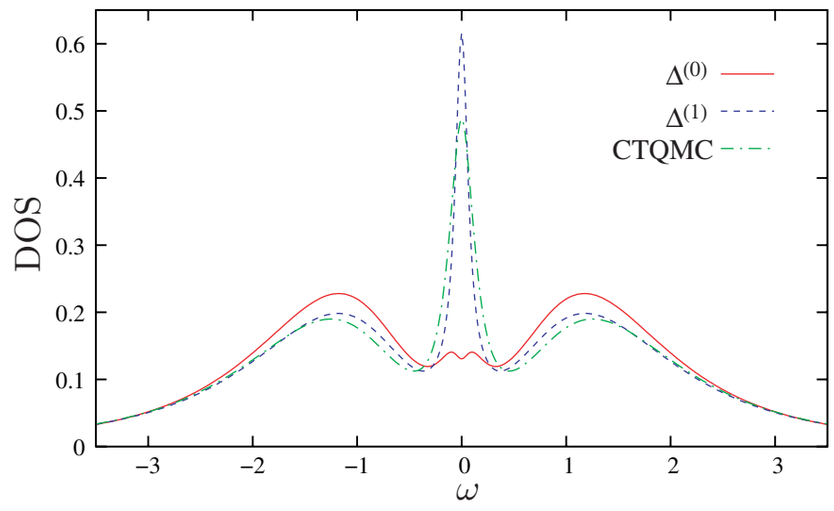
Impurity ("One-shot"),
Semicircular DOS
n=6

$$\beta = 30\,, U = 3$$



Noisy due to little poor statistics
finite T slower

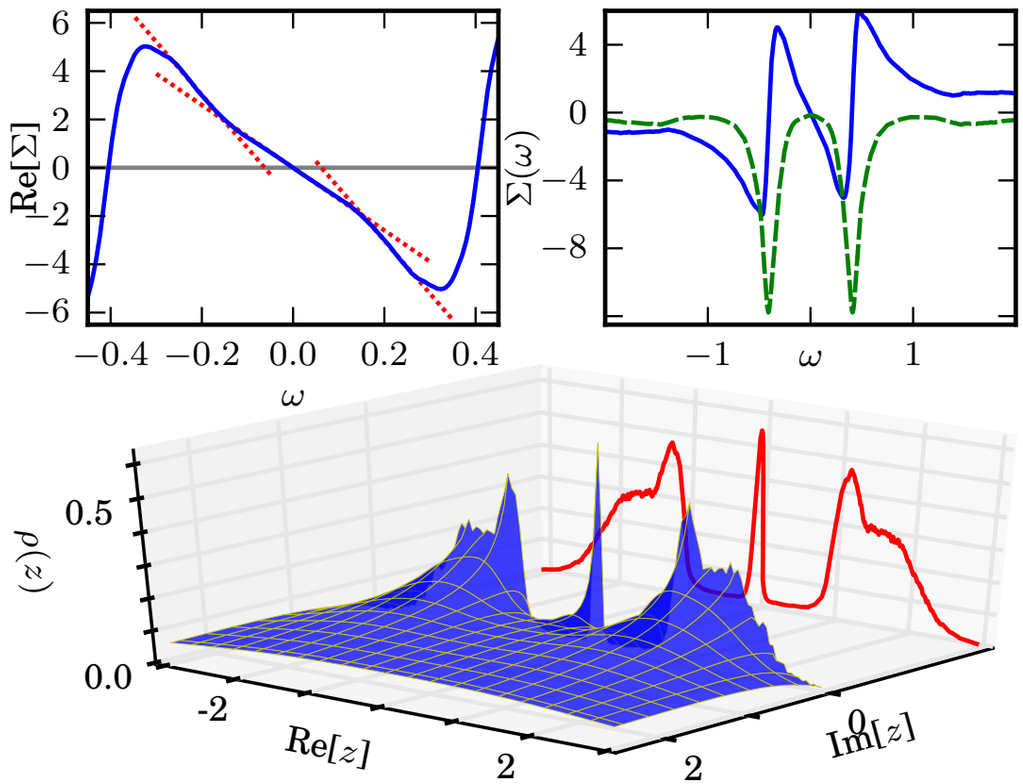
CT-QMC using Triqs-code



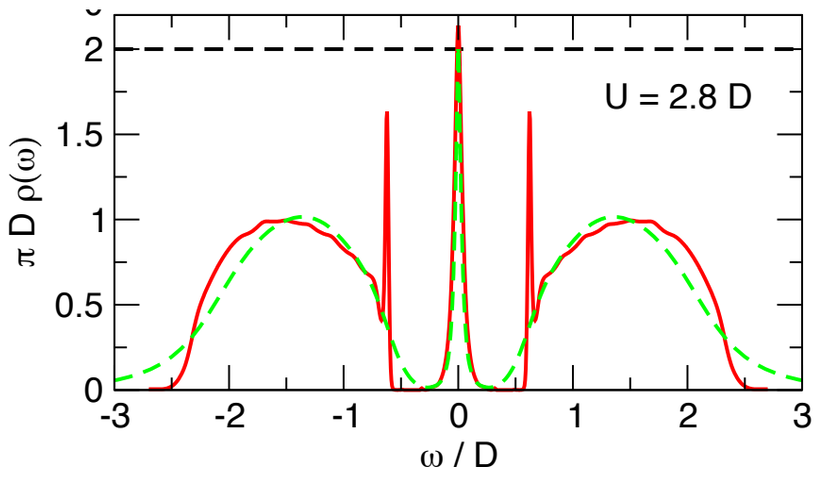
MAXENT,
broad Hubbard bands

Hafermann et al. , EPL 2009

Compared to DMRG-DMFT



Captures structure, such as dispersion kinks and Hubbard band peaks



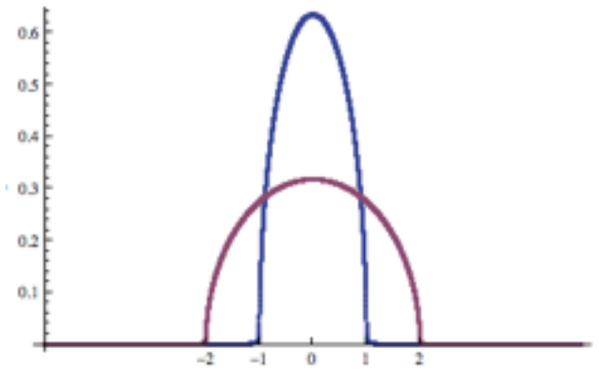
Karski et al. 2008

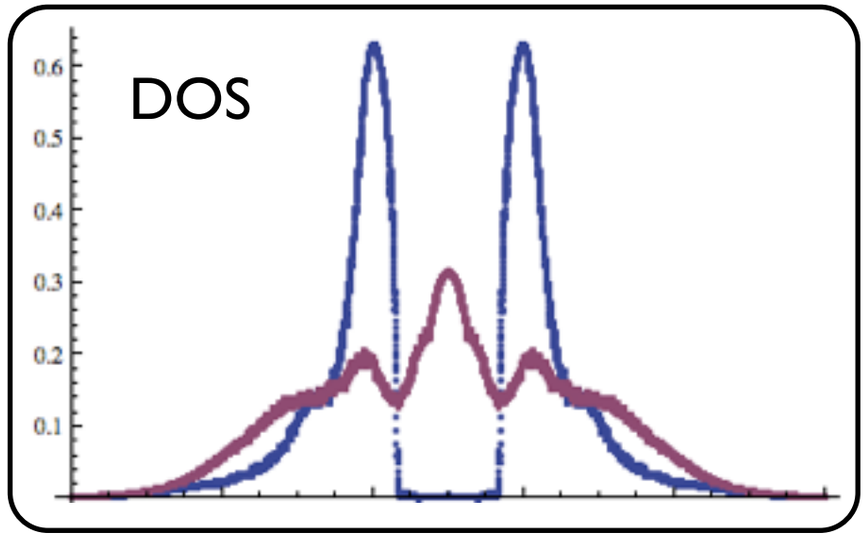
2-orbital Hubbard, in progress

Rotationally invariant Hund's J

Orbital selective Mott transition

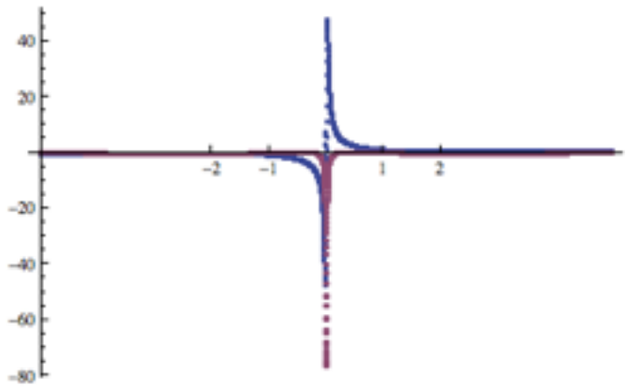
Bare DOS

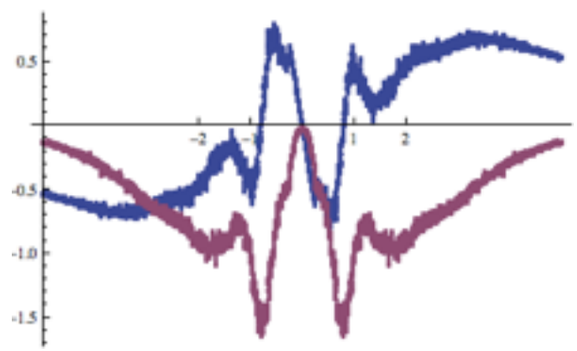




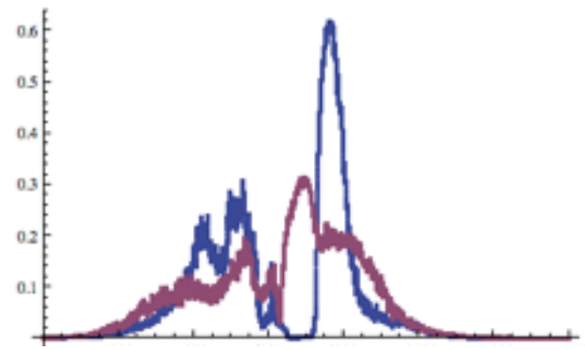
U=2.4 J=U/4

Self energies:





away from half filling:



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Compared to "standard" Exact diagonalization DMFT

ED

- Approximate G_0
- Fit on Matsubaras
- "Exact" self energy
- Very accurate on Matsubaras

Distributional ED

- "Exact" G_0
- No fitting, stochastic generation of n-level Anderson models
- Approximate self-energy
- Full analytic and continuous self-energy
- T=0, no problem

Summary

- Use non-interacting impurity-bath DOS as probability distribution for generating n-level Anderson models.

$$-\frac{1}{\pi} Im\, G_0(\omega + i\delta) \longrightarrow G_0^\nu = \sum_{j=1}^{n} \frac{a_j^\nu}{z - b_j^\nu} \qquad \nu = 1, 2, ..., \text{large}$$

- Calculate the sample self energy by exact diagonalization

$$\Sigma^\nu(z) - \mu = (G_0^\nu(z))^{-1} - (G^\nu(z))^{-1}$$

- Self energy is the sample averaged self energy

$$\Sigma \approx \frac{1}{N} \sum_\nu \Sigma^\nu$$

- Completely Parallelizable
- Results for Real and imaginary frequencies
- 0 or finite temperature
- "Scale free", shows fine structure even at high energy

M. Granath and Hugo U.R. Strand
arXiv:1201.6160v1