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Dynamical mean-field theory study of electron-electron correlation effects in multilayered structures

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- We have seen in most of the previous talks a general approach to optimizing the figure of merit in thermoelectric materials.
- Jim Freericks showed that one could actually get unexpected thermal properties by sandwitching a correlated insulator between two metallic leads.
- In the current work we look at the same geometry and at a more realistic model, namely the Hubbard model, for the correlated insulator that makes the barrier.

- Model Hamiltonian

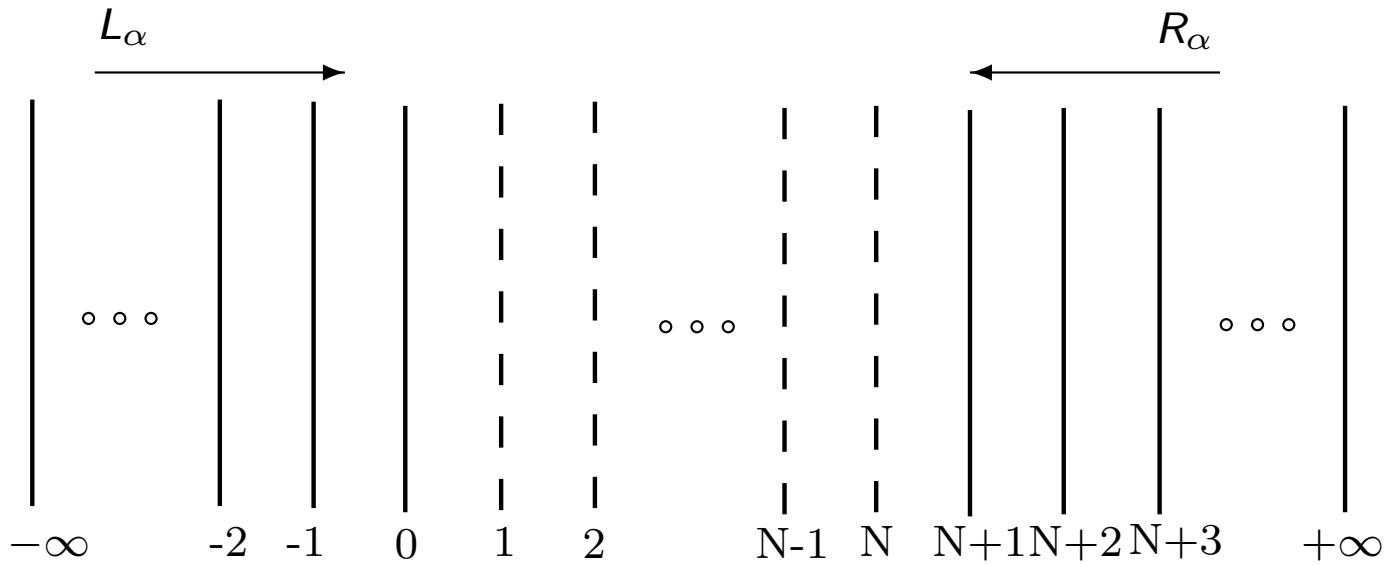
$$\begin{aligned}\mathcal{H} &= -\sum_{ij\alpha\sigma} t_{ij}^{\parallel} c_{i\alpha\sigma}^{\dagger} c_{j\alpha\sigma} - t\sum_{i\alpha\sigma}[c_{i\alpha\sigma}^{\dagger} c_{i\alpha+1\sigma} + h.c.] \\ &\quad -\mu\sum_{i\alpha\sigma} c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma} + \sum_{i\alpha} U_{\alpha}(n_{i\alpha\uparrow} - \frac{1}{2})(n_{i\alpha\downarrow} - \frac{1}{2}),\end{aligned}$$

  where α is the plane index, i is the site index within the plane. We assume that the inplane hopping $t_{ij}^{\parallel}$ is equal to the interplane hopping t which we take as the unit of energy.
- We assume particle-hole symmetry ($\mu = 0$) $\longrightarrow$ no charge reconstruction
- We work in the paramagnetic phase.

- Within the IDMFT the self-energy $\Sigma_\alpha(\omega)$ is assumed local but plane-dependent
- We want to calculate the local Green's function

$$G_\alpha(\omega) = \int d\epsilon \rho_{2d}(\epsilon) \frac{1}{L_\alpha(\epsilon,\omega) + R_\alpha(\epsilon,\omega) - Z_\alpha(\omega) + \epsilon},$$

L_α and R_α are two continued fractions which we know how to calculate and $Z_\alpha(\omega) \equiv \omega - \Sigma_\alpha(\omega)$.



- The two continued fractions are given by

$$L_\alpha(\epsilon,\omega) = Z_\alpha(\omega) - \epsilon - \cfrac{1}{Z_{\alpha-1}(\omega) - \epsilon - \ddots - \cfrac{1}{z_1 - \epsilon - \cfrac{1}{\frac{1}{2}(\omega-\epsilon) \pm \frac{1}{2}\sqrt{(\omega-\epsilon)^2-4}}}}}$$

$$R_\alpha(\epsilon,\omega) = Z_\alpha(\omega) - \epsilon - \cfrac{1}{Z_{\alpha+1}(\omega) - \epsilon - \ddots - \cfrac{1}{z_N - \epsilon - \cfrac{1}{\frac{1}{2}(\omega-\epsilon) \pm \frac{1}{2}\sqrt{(\omega-\epsilon)^2-4}}}}}$$

We have

$$\begin{cases} L_\alpha(\epsilon,\omega) &= g_{1d}^{-1}(\omega-\epsilon) \qquad \alpha \le 0 \\ R_\alpha(\epsilon,\omega) &= g_{1d}^{-1}(\omega-\epsilon) \quad \alpha \ge N+1 \end{cases}$$

where $g_{1d}^{-1}(\omega) \equiv \frac{1}{2}\omega \pm \frac{1}{2}\sqrt{\omega^2-4}$ is the inverse local Green's function for a 1-d tight-binding band.

- For large U we assume that the density of states due to the normal state proximity effect decreases as we move towards the center of the barrier. Therefore the following assumption holds

$$\begin{aligned} |\Sigma_{N/2}(\omega \approx 0)| &\gg |\Sigma_{N/2\pm 1}(\omega \approx 0)| \gg |\Sigma_{N/2\pm 2}(\omega \approx 0)| \\ &\gg \cdots \gg |\Sigma_{N/2\pm N/2}(\omega \approx 0)|. \end{aligned}$$

Hence we can write

$$L_\alpha(\epsilon, \omega) \approx Z_\alpha(\omega) - \epsilon + \bar{\gamma}_\alpha^L(\epsilon, \omega)$$

and

$$R_\alpha(\epsilon, \omega) \approx Z_\alpha(\omega) - \epsilon + \bar{\gamma}_\alpha^R(\epsilon, \omega).$$

where

$$\begin{cases} \bar{\gamma}_\alpha^L(\epsilon,\omega) & = -g_{1d}(\omega - \epsilon) \quad \alpha = 1 \\ \bar{\gamma}_\alpha^L(\epsilon,\omega) & = 1/\Sigma_{\alpha-1}(\omega) \qquad \alpha > 1 \end{cases}$$

and

$$\begin{cases} \bar{\gamma}_\alpha^R(\epsilon,\omega) & = -g_{1d}(\omega - \epsilon) \quad \alpha = N \\ \bar{\gamma}_\alpha^R(\epsilon,\omega) & = 1/\Sigma_{\alpha+1}(\omega) \qquad \alpha < N \end{cases}$$

Using the fact that $|\Sigma_\alpha(\omega \approx 0)| \gg |\bar{\gamma}_\alpha^{L,R}(\epsilon,\omega)|$, and after expanding the fraction and integrating over ϵ, we obtain

$$G_\alpha(\omega \approx 0) \approx -\frac{1}{\Sigma_\alpha(\omega \approx 0)} \left[1 + \frac{\omega + \gamma_\alpha^L + \gamma_\alpha^R}{\Sigma_\alpha(\omega \approx 0)} + \cdots\right],$$

with

$$\gamma_\alpha^{L,R} = \int d\epsilon\, \rho_{2d}(\epsilon)\, \bar{\gamma}_\alpha^{L,R}(\epsilon, \omega \approx 0)$$

Performing the integrals yields

$$\begin{cases} \gamma_\alpha^L & = 0.525i & \alpha = 1 \\ \gamma_\alpha^L & = 1/\Sigma_{\alpha-1}(\omega \approx 0) & \alpha > 1 \end{cases}$$

and

$$\begin{cases} \gamma_\alpha^R & = 0.525i & \alpha = N \\ \gamma_\alpha^R & = 1/\Sigma_{\alpha+1}(\omega \approx 0) & \alpha = N \end{cases}$$

The Green's function of the effective medium is defined as

$$G_{0\alpha}^{-1} = G_\alpha^{-1} + \Sigma_\alpha$$

and the hybridization function is then found to be

$$\Gamma_{0\alpha} = \mathrm{Im}\, G_{0\alpha}^{-1}(\omega \approx 0) = \mathrm{Im}(\gamma_\alpha^L + \gamma_\alpha^R)$$

In the bulk system and in the Mott insulting phase, the self energy is given by

$$\Sigma_{\mathrm{bulk}}(\omega \approx 0) = \frac{r(U)}{\omega + i\delta}$$

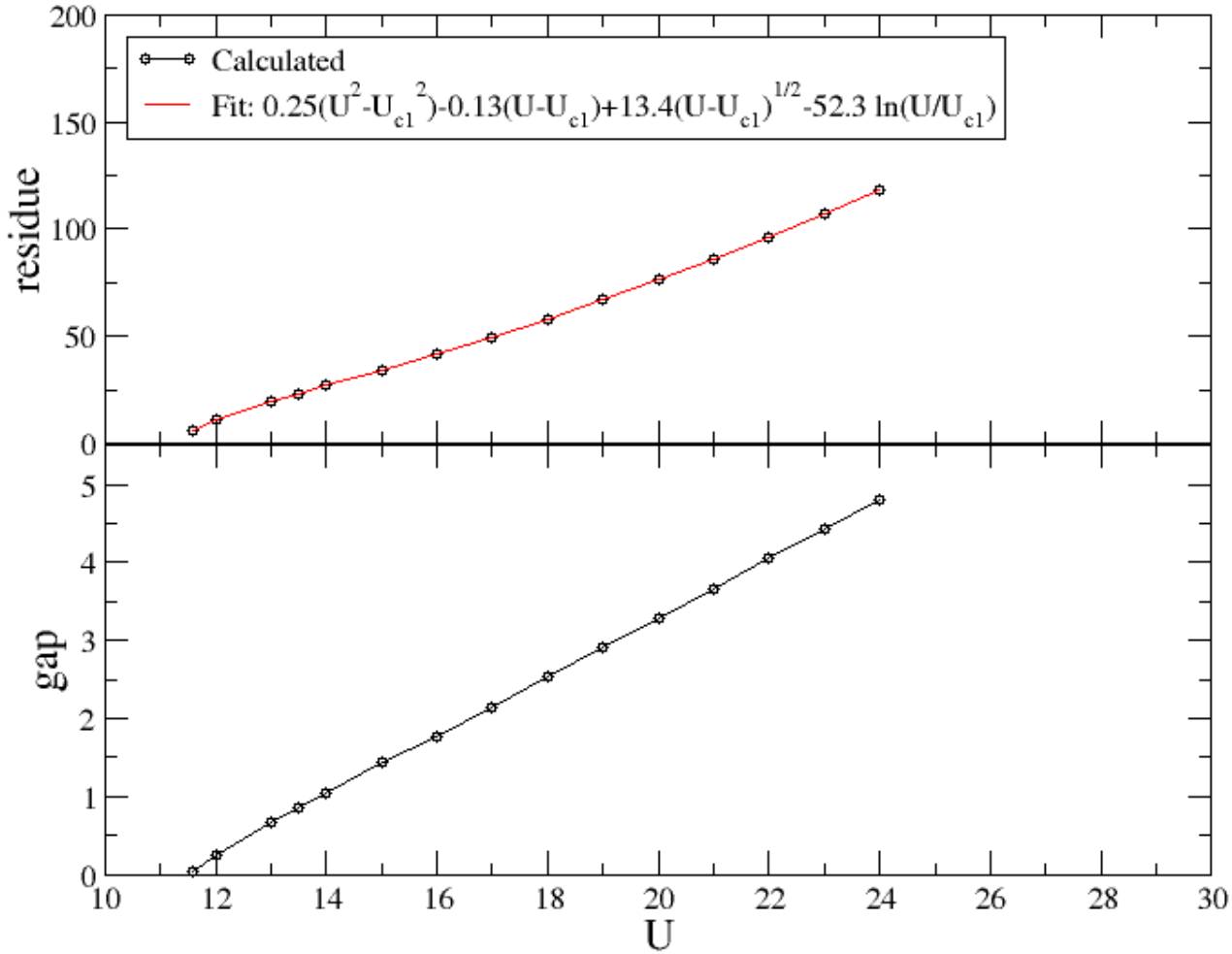
In the spirit of Hubbard III approximation we write

$$G_\alpha = \frac{w_1}{G_{0\alpha}^{-1}} + \frac{1 - w_1}{G_{0\alpha}^{-1} - U}$$

we find that

$$\Sigma_\alpha(\omega \approx 0) = \frac{r(U)}{\omega + \gamma_\alpha^L + \gamma_\alpha^R}$$

We found a functional form for the residue by fitting the values extracted from our numerical calculations.



$$r(U) \simeq (U^2 - U_{c1}^2)/4 - \ 0.13(U - U_{c1}) + \ 13.4\sqrt{U - U_{c1}} - \ 52.3 \ln(U/U_{c1})$$

We finally find that the hybridization function is such that

$$\Gamma_{0\alpha}(\omega \approx 0) \gtrsim \begin{cases} 0.525/[r(U)]^{\alpha-1} & 1 \leq \alpha \leq \frac{N-1}{2} \\ 1.05/[r(U)]^{\frac{N-1}{2}} & \alpha = \frac{N+1}{2} \\ 0.525/[r(U)]^{N-\alpha} & \frac{N+3}{2} \leq \alpha \leq N \end{cases}$$

$\longrightarrow$ It never vanishes and as we will se below this means that the only fixed point as the temperature is lowered is the Fermi liquid one.
This result is obtained for a tunnelling DOS that decays exponentially with a correlation length given by

$$\xi = 1/\ln r(U)$$

The Fermi temperature is given for each plane by

$$T_{F\alpha} \propto \exp[-8U/\pi\Gamma_{0\alpha}]$$

This important result means that at $T = 0$ the system becomes a Fermi liquid that leads in the special case of half-filling to the restoration of translational invariance and the Fermi surface. The system acquires as a result a perfect ballistic conductivity.

In the DMF the self-energy is local and therefore the local Green's function is given by

$$G(\omega) = \int d\epsilon \frac{\rho_0(\epsilon)}{\omega + \mu - \epsilon - \Sigma(\omega)}$$

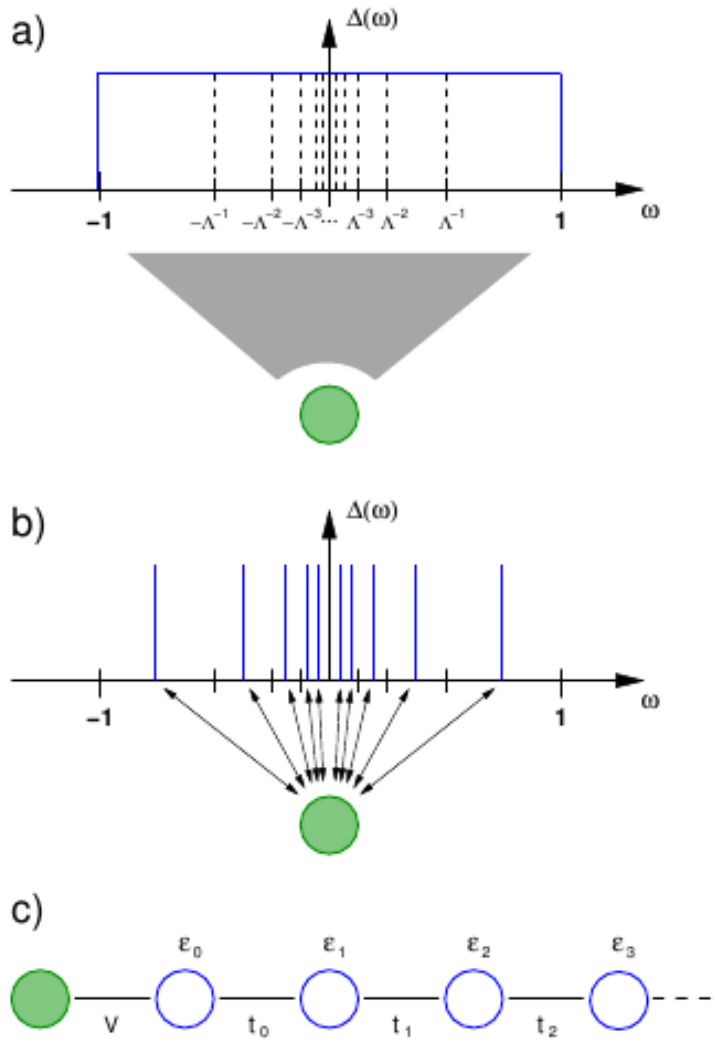
Hubbard model is mapped onto an Anderson impurity model with the hybridization function

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

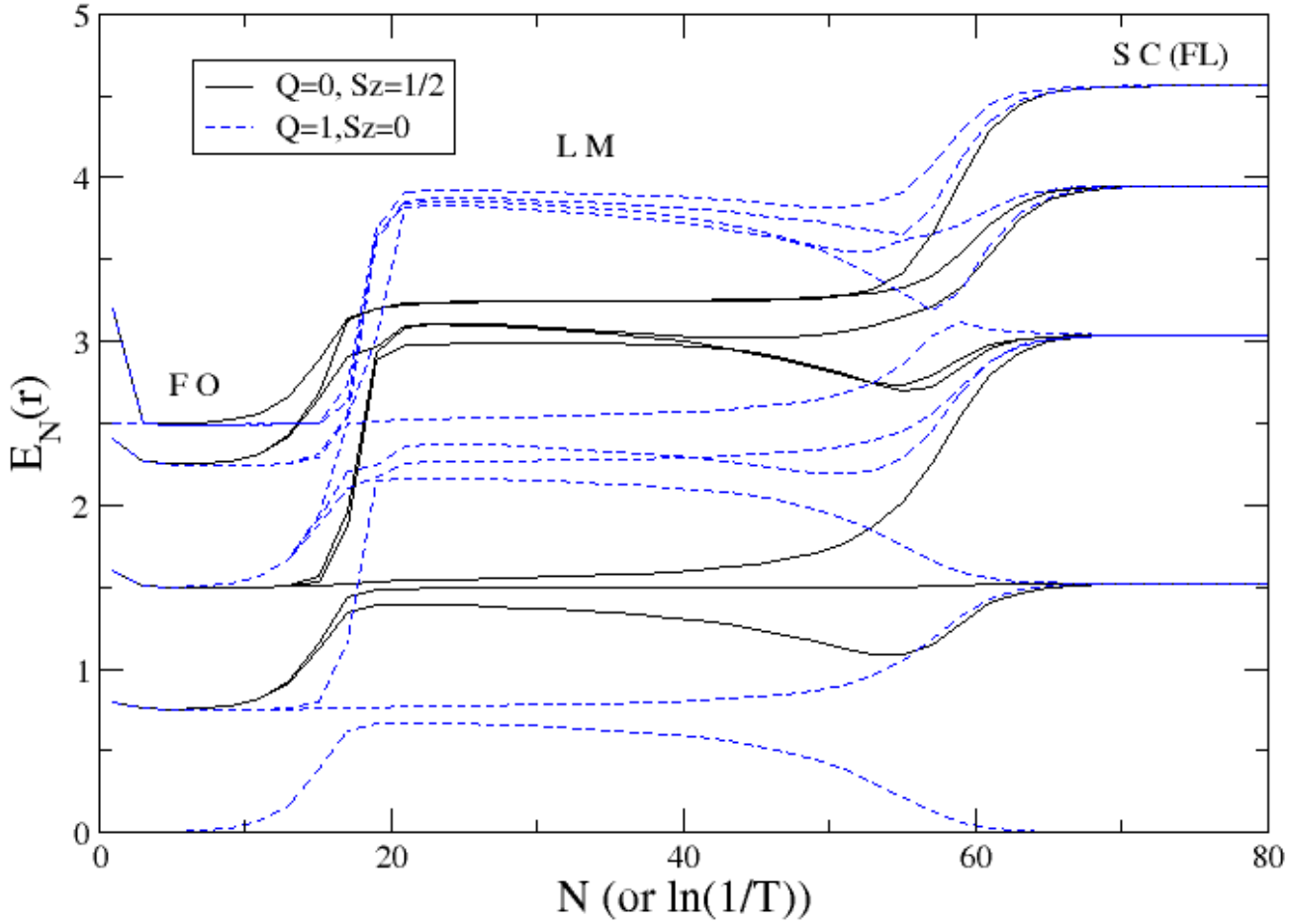
is determined self-consistently.

The Anderson impurity is solved using the Numerical Renormalization Group (NRG) method.

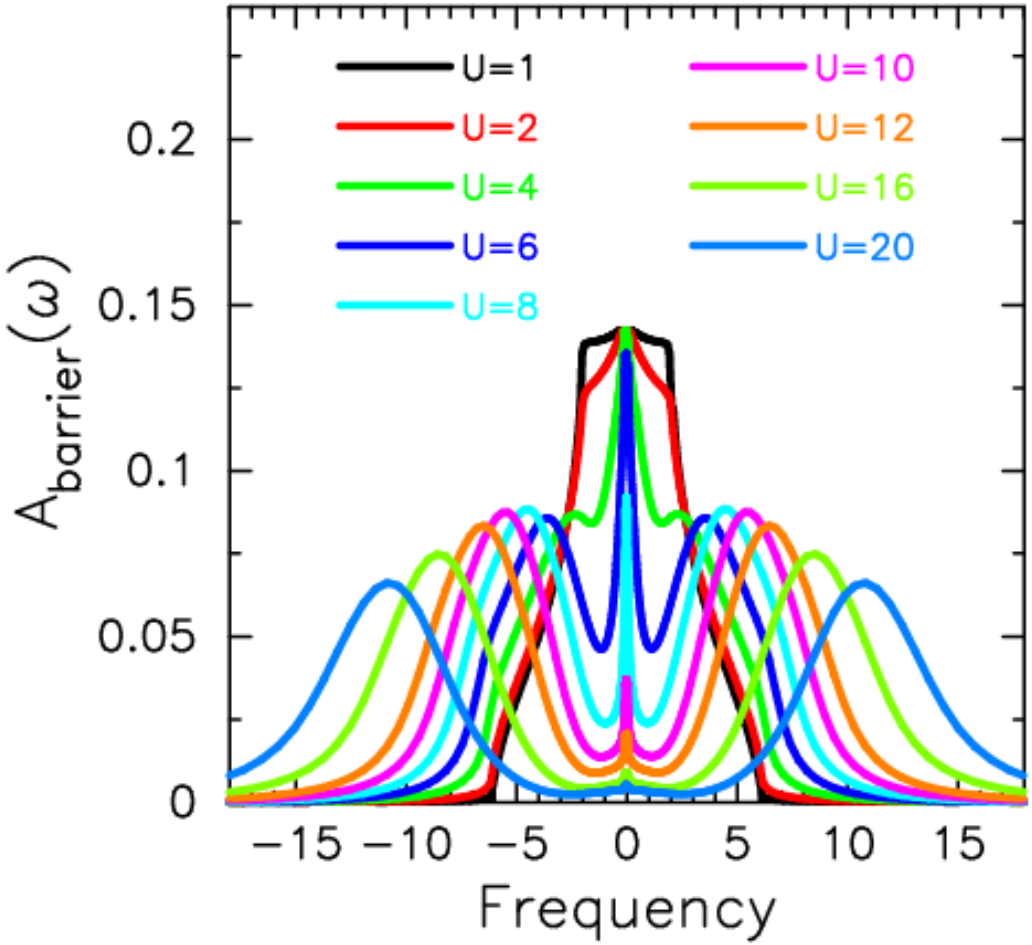
NRG maps the impurity problem onto a semi-infinite chain with the impurity at one end and the hopping parameters decreasing exponentially as we move further from the impurity



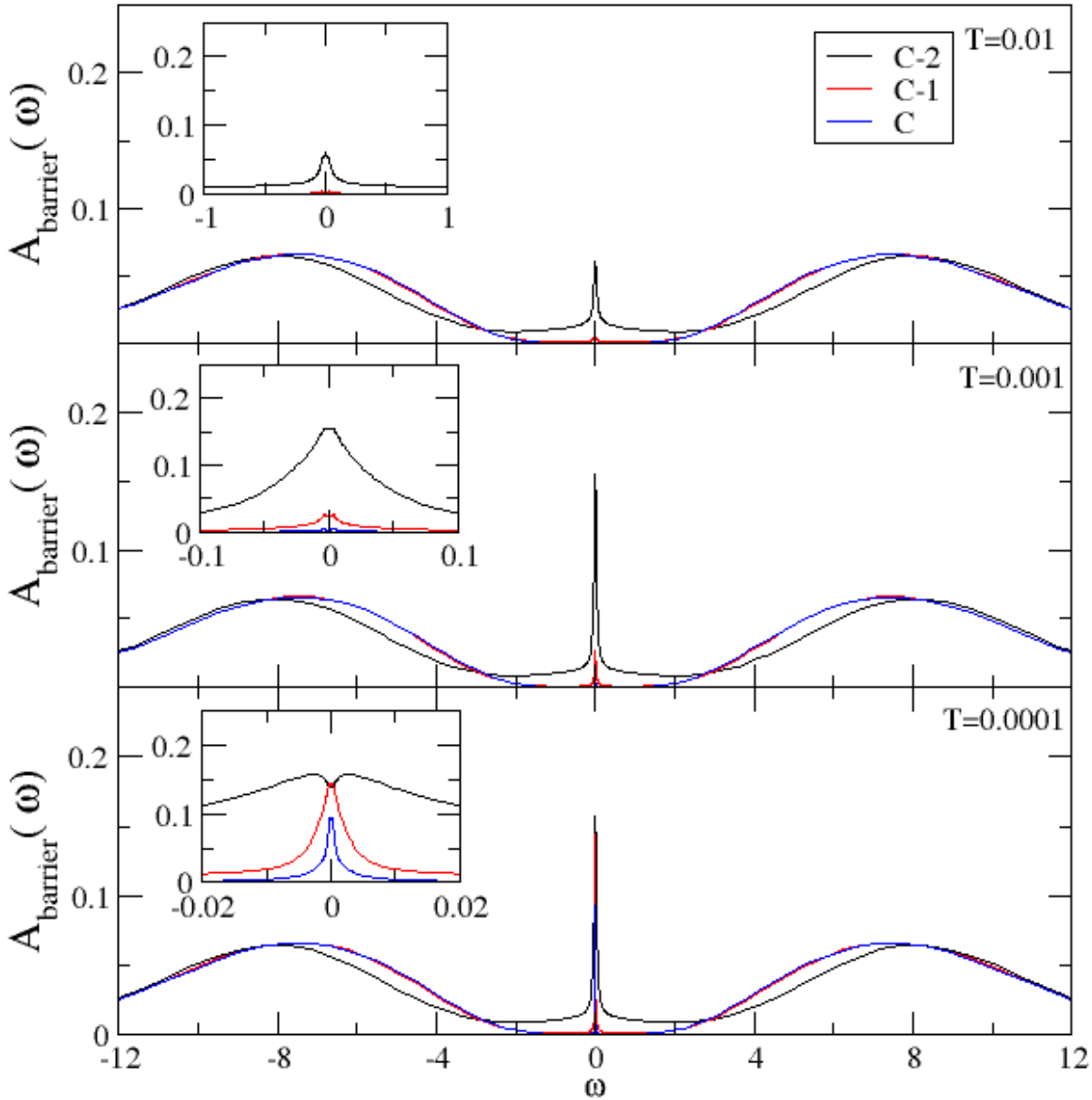
R. Bulla, T. A. Costi and Th. Pruschke, Rev. Mod. Phys. **80**, 395 (2008)



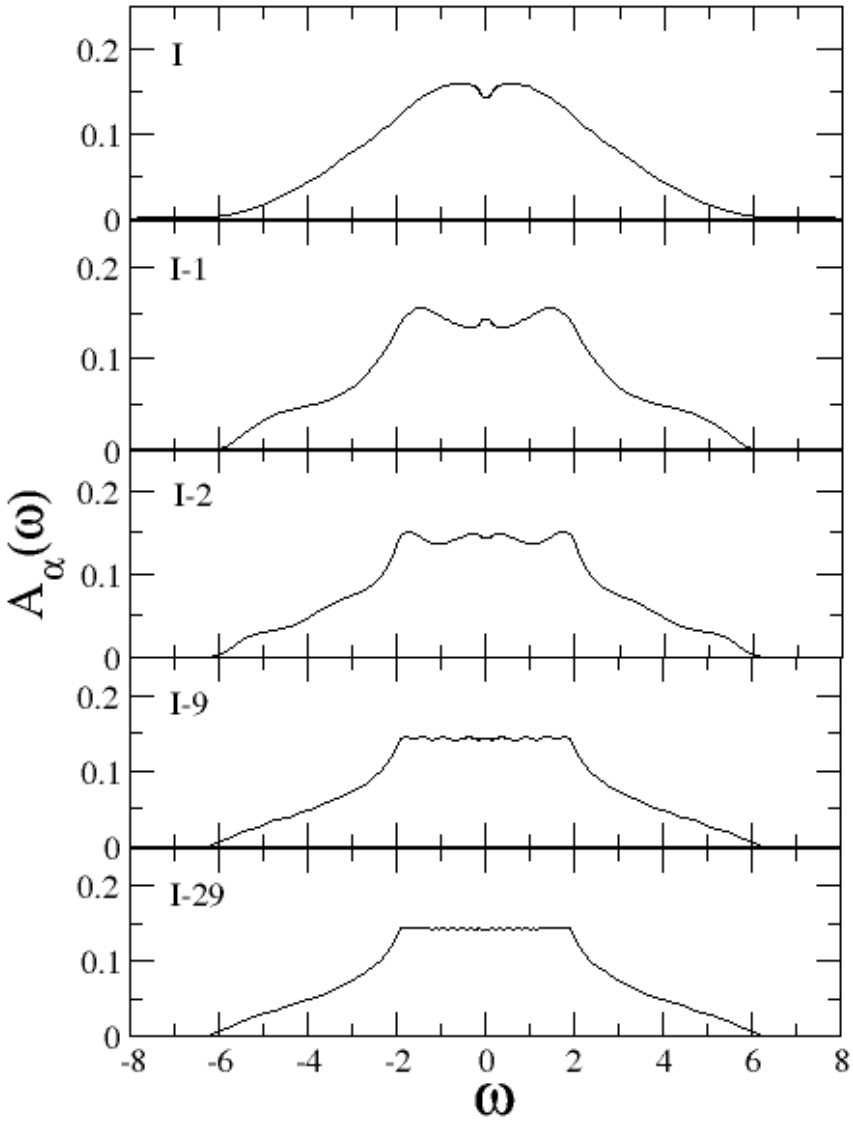
Evolution of the many-body energy levels with the chain length or equivalenty with the inverse temperature.



Local spectral function at the barrier plane for a single-barrier-plane multilayer, for $T = 0.01$, and a range of U's (increasing from top to bottom near zero frequency).



Local spectral function of the five-barrier-plane multilayer for $U = 16$, and three different temperatures.



Lead spectral functions: I stands for the interface layer. The parameters are $U = 12.9$ and $T = 0.01$.

- We have argued that a finite-size Mott insulator sandwitched between two metallic leads always becomes a Fermi liquid at low enough temperature.
- The numerical results corroborate our analytical argument for a reasonably thick Mott insulator with a large gap.
- The Fermi liquid state is however fragile with respect to
  - finite ω
  - finite T
  - disorder which we know is always present in real materials
  - magnetism

  In the presence of which the tunnelling regime through a Mott insulator is restored.
- However, we expect this phenomenon to be observed for not too large interaction U and not too thick barriers.
- An outlook: We are now looking at a very accurate way to find low frequency part of the self-energy needed to study thermal transport properties.