Signature of Collective Excitations close to the Metal-to-Insulator Transition

Michał Karski[1], Carsten Raas[2], Götz S. Uhrig[2]
[1]*Institut für Theoretische Physik • Universität zu Köln*
[2]*Institut für Theoretische Physik • Universität des Saarlandes*

Introduction

Mott-Hubbard metal-insulator transition

- correlation-driven transition from paramagnetic metallic to paramagnetic insulating phase
- essential features captured by the single-band Hubbard model

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\right) + U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right)$$

Dynamic mean-field theory (DMFT)

- non-perturbative approximation which becomes exact in the limit $d \to \infty$
- neglects spatial correlations, retains the dynamic correlations
- lattice problem is mapped onto an effective single-impurity model

$$\hat{H} = \sum_{n,\sigma} \gamma_n \left(\hat{c}^\dagger_{n\sigma}\hat{c}_{n+1\,\sigma} + \mathrm{h.c.}\right) + V \sum_\sigma \left(\hat{c}^\dagger_{d\sigma}\hat{c}_{0\sigma} + \mathrm{h.c.}\right) + U\left(\hat{n}_{d\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{d\downarrow} - \frac{1}{2}\right)$$

embedded in a self-consistently determined medium

$$G^{\mathrm{And}}_\sigma(\omega) = G^{\mathrm{Hub}}_\sigma(\omega)\,, \quad \Sigma^{\mathrm{And}}_\sigma(\omega) = \Sigma^{\mathrm{Hub}}_\sigma(\omega)$$

- effective single-impurity model must be solved for a single-particle Green function
- several numerical and analytical methods were applied as impurity solvers

Focus of investigation

- spectral densities close to the metal-insulator transition
- interplay of electronic degrees of freedom with collective modes in a highly correlated metal

Investigated model

- single-band Hubbard model at half band-filling and zero temperature on a Bethe lattice with infinite coordination

Motivation

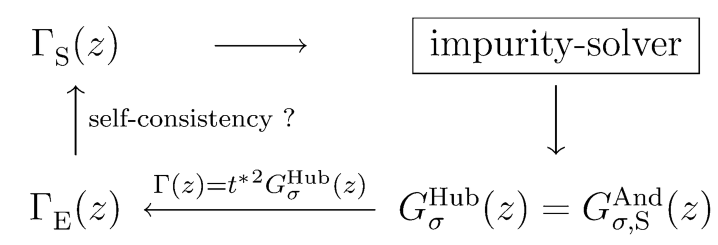
- Dynamic DMRG: well controlled energy resolution at all energy scales

Methods

Self-consistency cycle

- iterative determination of the hybridization function

$$\Gamma(z) = \cfrac{V^2}{z - \cfrac{\gamma_0^2}{z - \cfrac{\gamma_1^2}{z - \dots}}}$$



Impurity solver

- uses spin representation of the single-impurity Anderson Hamiltonian [1]

$$\hat{H} = V\left[\left(\hat{S}^+_{\mathrm{d}}\hat{S}^-_0 + \hat{T}^+_{\mathrm{d}}\hat{T}^-_0\right) + \mathrm{h.c.}\right] + \sum_n \gamma_n \left[\left(\hat{S}^+_n\hat{S}^-_{n+1} + \hat{T}^+_n\hat{T}^-_{n+1}\right) + \mathrm{h.c.}\right] + U\hat{S}^z_{\mathrm{d}}\hat{T}^z_{\mathrm{d}}$$

- based on correction vector DMRG

$$|c(z_i)\rangle = \frac{1}{z_i - (\hat{H} - E_0)}\hat{S}^+_{\mathrm{d}}|\Psi_0\rangle \qquad (z_i \equiv \omega_i + \mathrm{i}\eta_i)$$

$G^>_\sigma(z) = \langle\Psi_0|\hat{S}^-_{\mathrm{d}}|c(z)\rangle$ particle-hole symmetry → $G_\sigma(z) = G^>_\sigma(z) - G^>_\sigma(-z)$

$$\rho^{(\eta_i)}_\sigma(\omega_i) = -\frac{1}{\pi}\mathrm{Im}\,G_\sigma(\omega_i + \mathrm{i}\eta_i)$$

- the obtained spectral density is broadened and has to be deconvolved

Least-bias deconvolution

- continuous and positive semi-definite ansatz for the spectral density [2]

$$\rho_\sigma(\omega) = \exp\left[\mu + \sum_{i=1}^n \lambda_i \frac{\eta_i}{\pi\left[(\omega_i - \omega)^2 + \eta_i^2\right]}\right]$$

- maximize $-S = \int_{-\infty}^{\infty} \mathrm{d}\omega\, \rho_\sigma(\omega) \ln \rho_\sigma(\omega)$

under the side conditions $\rho^{(\eta_i)}_\sigma(\omega_i) = \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \frac{\eta_i \rho_\sigma(\zeta)}{\pi\left[(\omega_i - \zeta)^2 + \eta_i^2\right]}$

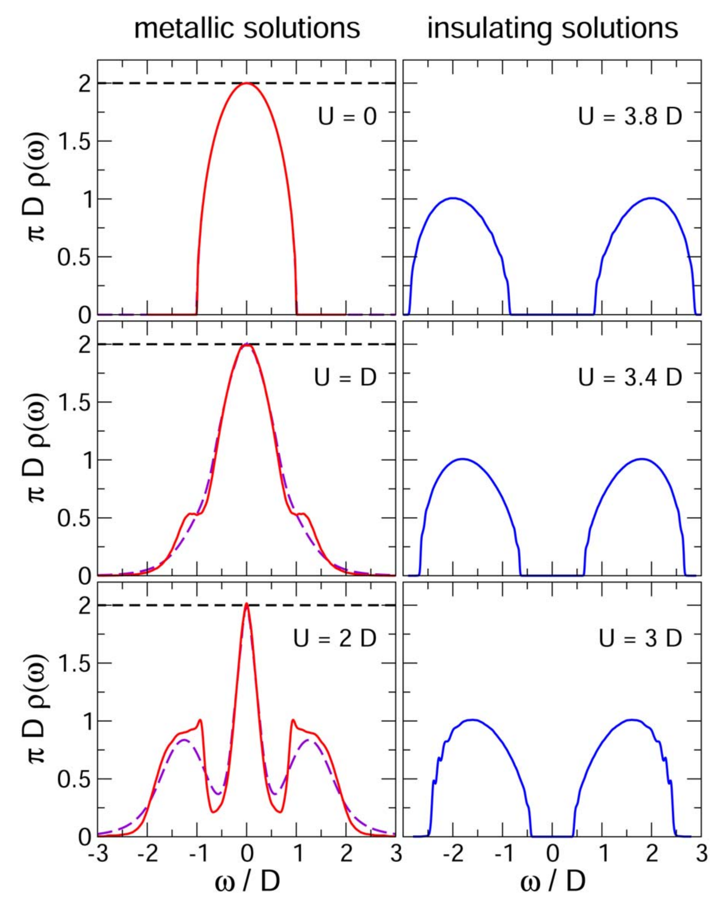
Single particle spectra far from transition

Weak interaction, metallic region

- Hubbard bands appear already for $U \approx D$
- no significant effects on collective modes (overdamped by Landau damping)

Strong interaction, insulating region

- charge and collective modes are well separated in energy
  → no significant interplay is to be expected

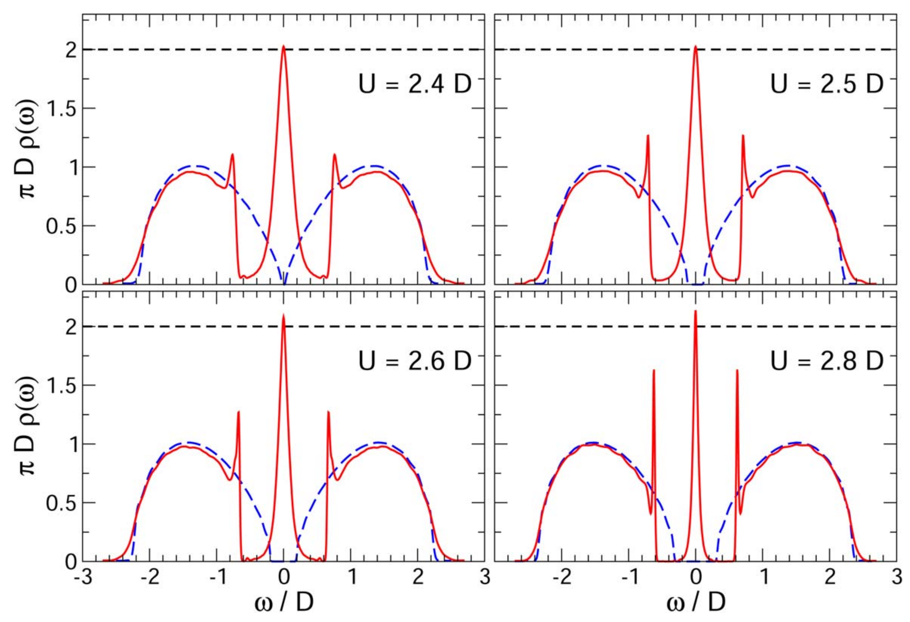


Spectral densities for the single-band Hubbard model at half band-filling and zero temperature deep in the metallic (red lines) and deep in the insulating regime (blue lines) calculated using a spin chain with 320 sites (160 fermionic sites). The dashed violet lines shows NRG-results [3].

Single particle spectra close to transition

Region close to transition

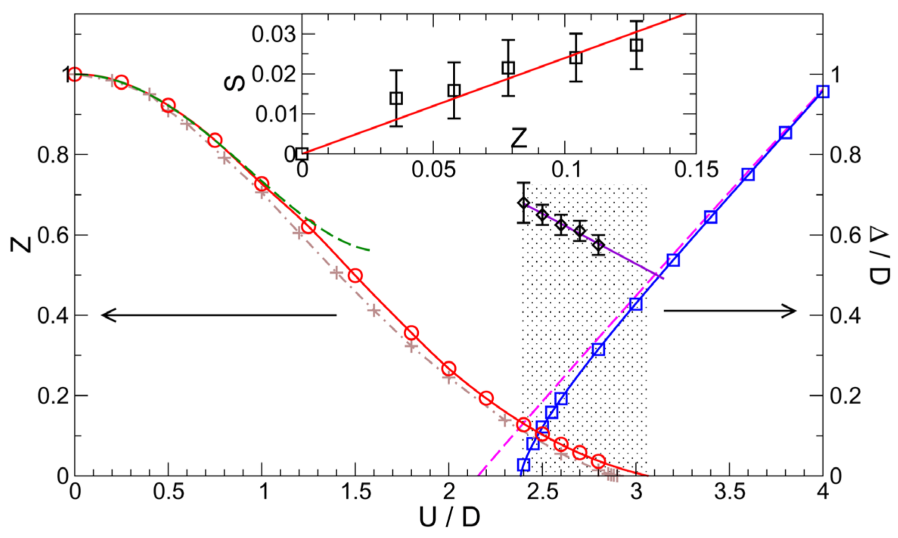
- no upturn [6] in the insulating solution close to $U_{c1} = (2.38 \pm 0.02)\ D$
- sharp peaks at inner edges of the Hubbard bands in the metallic solution close to transition at $U_{c2} = (3.07 \pm 0.1)\ D$
- preformed pseudo-gap in the metallic solution passes continuously into the insulating gap



Spectral densities for the single-band Hubbard model at half band-filling and zero temperature of the metallic (red solid) and the insulating solution (dashed blue) between U_{c1} and U_{c2}.

Interpretation

- signature of collective excitations with heavy quasiparticles involved
- due to the energy an antibound state or resonance of heavy quasiparticles with a collective spin excitation is expected
  → tentatively antipolaron
- scenario corroborated by the weight *S* of the side-peaks:
  S vanishes rather linearly with Z rather than quadratically or cubically



Dotted area: two-solution region. Left curves: metallic quasi-particle weight *Z*; red line with circles: interpolated DMRG, brown line with pluses: NRG [3]; dashed green line: perturbation up to U^4 [4]. Right curves: insulating gap Δ or pseudo-gap in the metal (violet line with diamonds); blue line with squares: DMRG; dashed magmata line: perturbation up to $1/U^2$ [5]. Inset: weight *S* of the peaks at inner Hubbard band edges.

Conclusions

- high-resolution calculation of the dynamic mean-field equations for the half-filled Hubbard model reveals a clear signature of collective excitations close to the metal-to-insulator transition
- effect of collective excitations is seen as sharp peaks at the inner edges of the Hubbard bands
- peaks evidence a strong interaction between charge and collective degrees of freedom
- tentative interpretation: antibound state (antipolaron)

References

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The results presented in this poster are published in the paper: "Electron Spectra close to a Metal-to-Insulator Transition", cond-mat/0507132