Strong correlation effects on the electrical permittivity of two-dimensional systems

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Outline

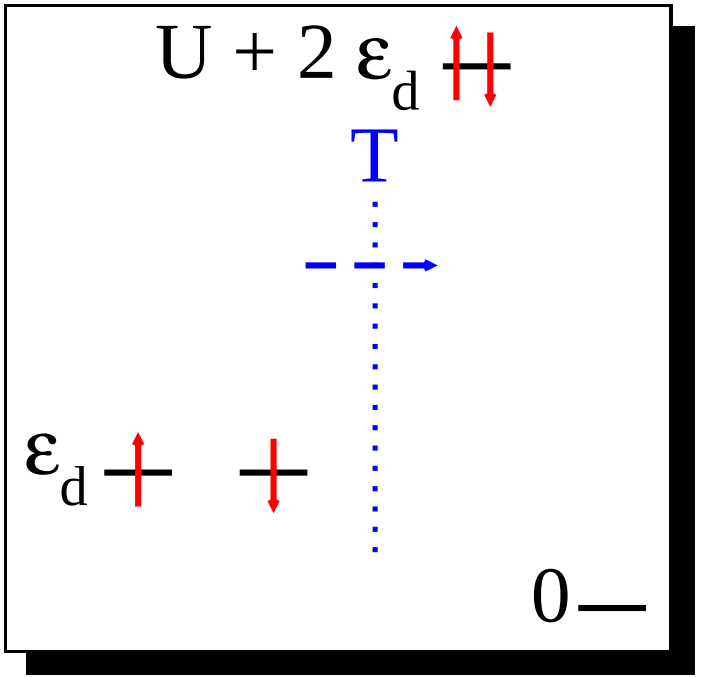
- Motivation
- The Kotliar and Ruckenstein slave boson representation of the Hubbard model
- Mott transition
- Magnetic and charge instabilities
- Charge dynamics: from weak coupling to Hubbard split bands
- Summary and outlook

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Prominent models for strongly correlated electrons

☞ The Hubbard model:

$$H = \sum_{i,j,\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i,\sigma} \varepsilon_d a^{\dagger}_{i\sigma} a_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



- Metallic magnetism
- Hubbard, Kanamori, Gutzwiller
- Screened Coulomb interaction
- Superconducting cuprates (2D)
- Cold atoms

☞ The single impurity Anderson model:

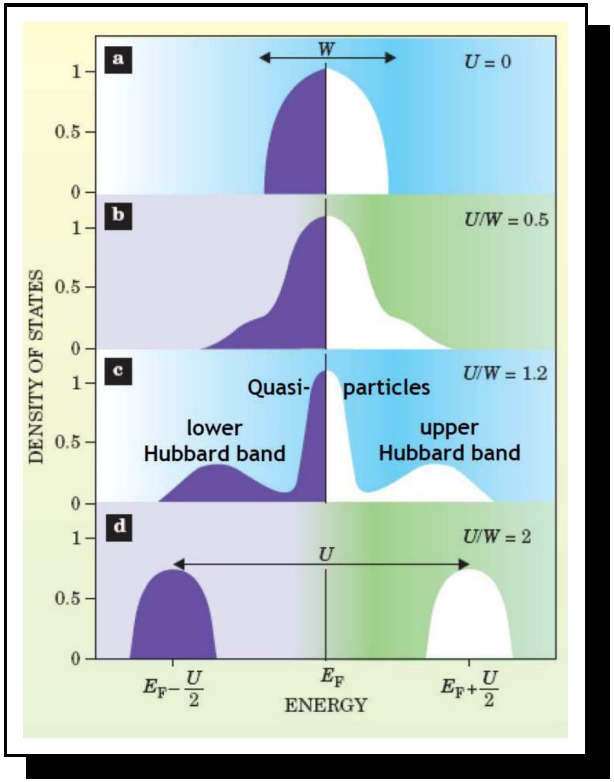
$$H = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \varepsilon_f \sum_{\sigma} a^{\dagger}_{\sigma} a_{\sigma} + V \sum_{\vec{k}\sigma} \left(c^{\dagger}_{\vec{k}\sigma} a_{\sigma} + a^{\dagger}_{\sigma} c_{\vec{k}\sigma} \right) + U a^{\dagger}_{\uparrow} a_{\uparrow} a^{\dagger}_{\downarrow} a_{\downarrow}$$

- Formation of a singlet involving the correlated impurity and the band
- Deep impact on the physical properties (Kondo effect)
- Connection with the Hubbard Model in the DMFT context

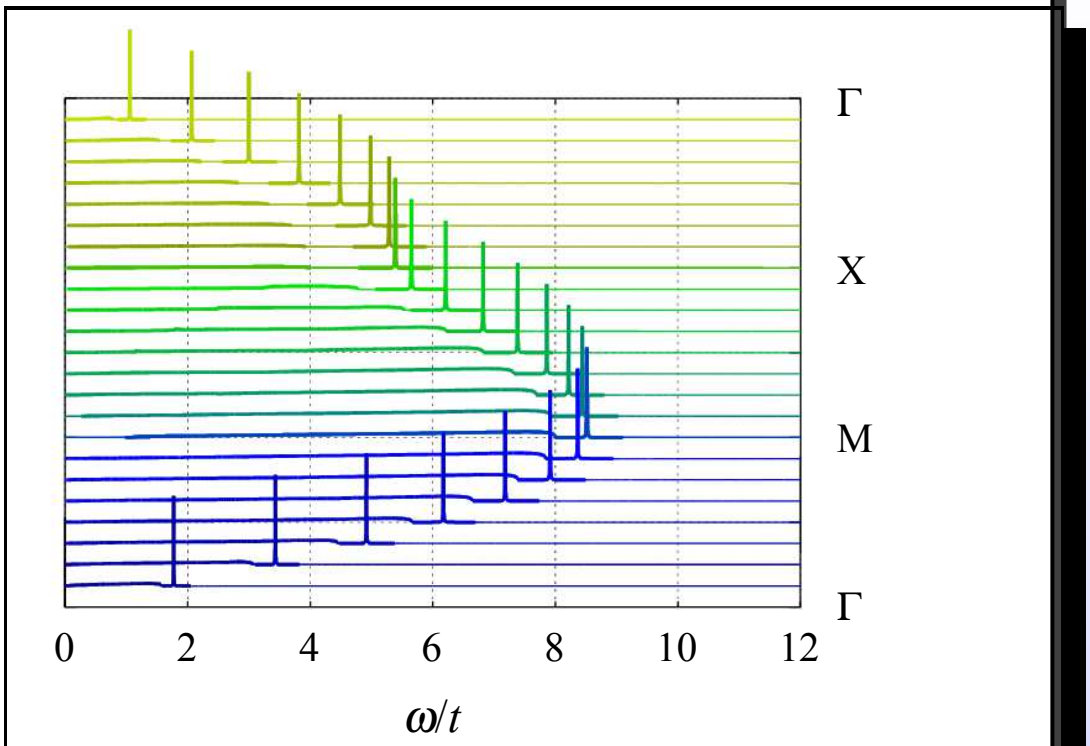
Motivation

Excitations

Mott transition: density of states



Charge excitations in RPA: $\Im(\chi_c(\mathbf{q}, \omega))$



Quasi-particle peak; Hubbard split bands

Continuum and collective modes

How can one mary both in the thermodynamical limit?

Extension to the Kotliar and Ruckenstein representation

Principle: Introduce the auxiliary particles f_σ, e, p_σ, and d to represent the physical states:

$$\begin{aligned} |0\rangle &= e^\dagger |\text{vac}\rangle \\ |\sigma\rangle &= p_\sigma^\dagger f_\sigma^\dagger |\text{vac}\rangle \\ |2\rangle &= d^\dagger f_\uparrow^\dagger f_\downarrow^\dagger |\text{vac}\rangle \end{aligned}$$

There are now three constraints:

$$\begin{aligned} 1 &= e^\dagger e + \sum_\sigma p_\sigma^\dagger p_\sigma + d^\dagger d \\ f_\sigma^\dagger f_\sigma &= p_\sigma^\dagger p_\sigma + d^\dagger d \,, \ \sigma = \uparrow, \downarrow \end{aligned}$$

which are implemented in path integral.

The phase of 3 slave boson fields may be gauged away.
Operators: $a_\sigma^\dagger = \tilde{z}_\sigma^\dagger f_\sigma^\dagger$ with $\tilde{z}_\sigma^\dagger = p_\sigma^\dagger e + d^\dagger p_{-\sigma}$. Problematic. Yet, with:

$\tilde{z}_\sigma^\dagger = p_\sigma^\dagger L_\sigma R_\sigma e + d^\dagger L_\sigma R_\sigma p_{-\sigma}$; $L_\sigma \equiv \left(1 - d^\dagger d - p_\sigma^\dagger p_\sigma\right)^{-\frac{1}{2}}$; $R_\sigma \equiv \left(1 - e^\dagger e - p_{-\sigma}^\dagger p_{-\sigma}\right)^{-\frac{1}{2}}$
the Gutzwiller approximation is recovered as a saddle-point.

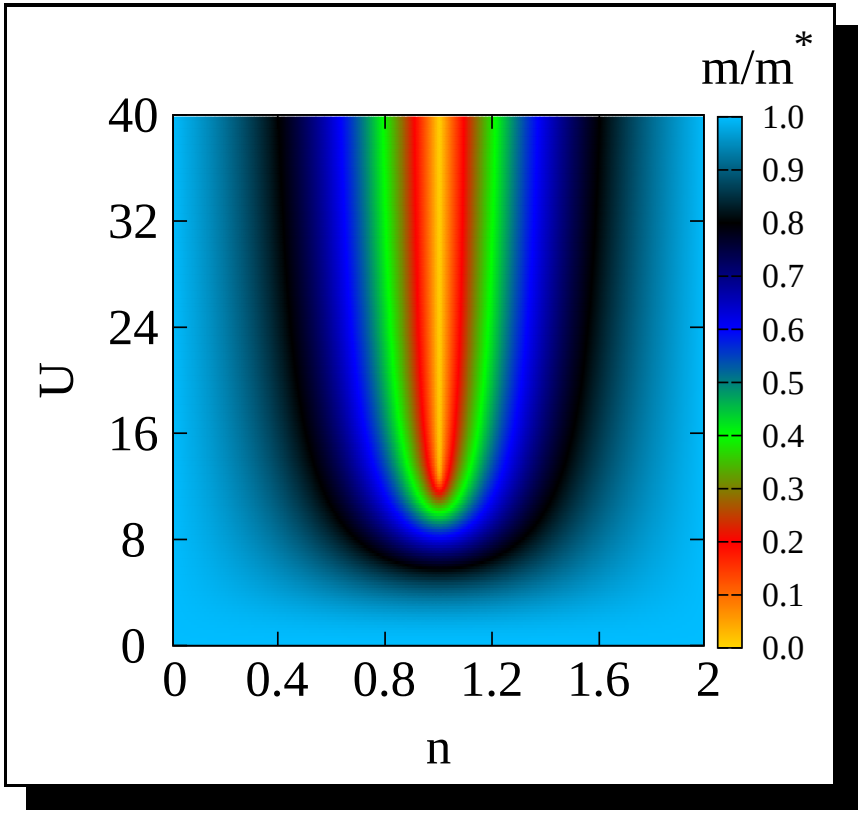
Operators : $\hat{n} = \sum_\sigma p_\sigma^\dagger p_\sigma + 2 d^\dagger d$ $\quad \hat{\mathbf{S}} = \frac{1}{2} \sum_{\sigma,\sigma'} a_\sigma^\dagger \tau_{\sigma,\sigma'} a_{\sigma'}$ $\quad \hat{D} = d^\dagger d$

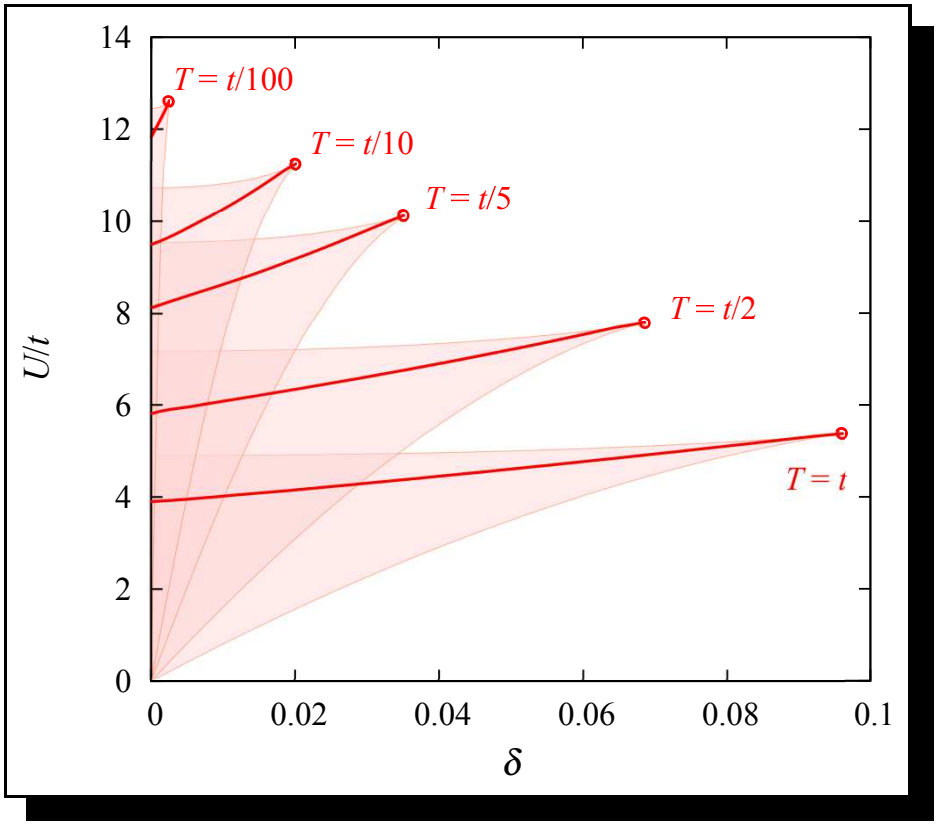
Asymmetry

G. Kotliar, A. Ruckenstein, PRL **57** 1362 (1986)
RF and T. Kopp, Ann. Phys. (Berlin) **524** 175 (2012)

Mott transition

All saddlepoint equations equations may be merged into: $y^3 + (u-1)y^2 = u\delta^2$ with: $y = (e+d)^2; u = U/U_0; U_0 = -8\sum_{\vec{k},\sigma} t_{\vec{k}} n_F(E_{\vec{k}})/(1-\delta^2)$





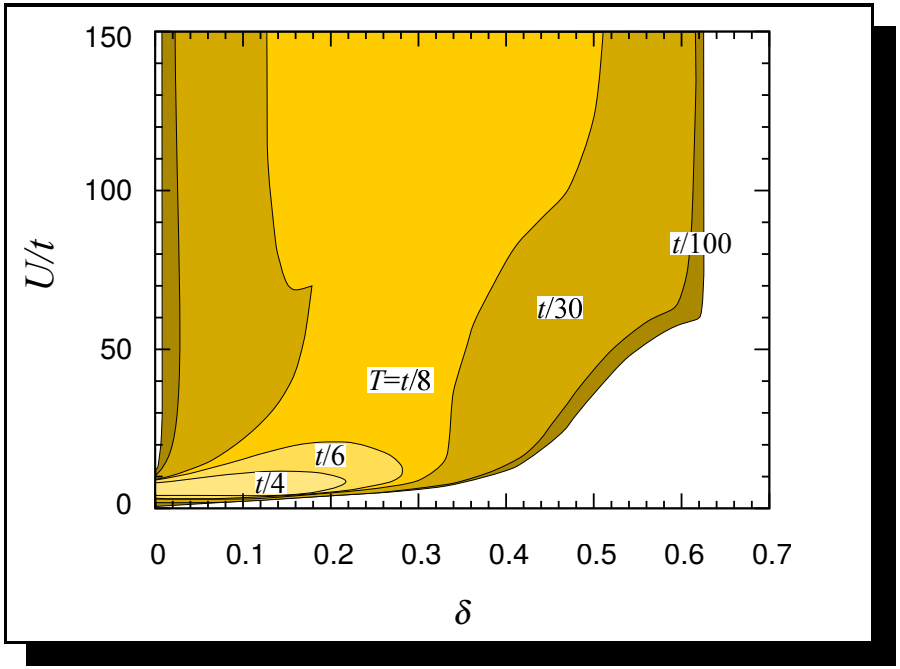
Second order transition at zero temperature

First order transition at finite temperature

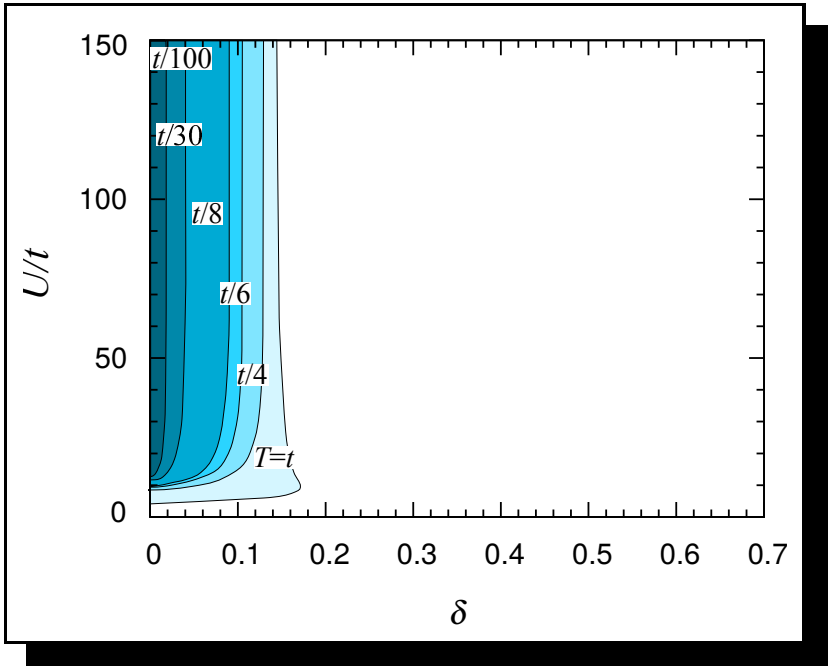
V. H. Dao and RF, PRB **95**, 165127 (2017)

Instabilities on the square lattice

Magnetic instabilities



Charge instabilities



Suppression of magnetic instabilities with increasing temperature

Enhancement of charge instabilities with increasing temperature

V. H. Dao and RF, PRB **95**, 165127 (2017)

Charge dynamics

The gaussian fluctuation separate into a charge channel and a spin channel. Here:

$$S_c = \sum_q \sum_{\mu,\nu} \delta\psi_\mu(-q) S_{\mu,\nu}(q) \delta\psi_\nu(q)$$

with $\delta\psi_1(q) = \delta e(q)$, $\delta\psi_2(q) = \delta d'(q)$, $\delta\psi_3(q) = \delta d''(q)$, $\delta\psi_4(q) = \delta p_0(q)$, $\delta\psi_5(q) = \delta\beta_0(q)$, $\delta\psi_6(q) = \delta\alpha(q)$. The "main" contribution to $S_{\mu,\nu}(q)$ reads:

$$S^{(1)}(q) = \begin{pmatrix} \alpha & 0 & 0 & 0 & 0 & e \\ 0 & \alpha - 2\beta_0 + U & \nu_n & 0 & 0 & d \\ 0 & -\nu_n & \alpha - 2\beta_0 + U & 0 & -2d & 0 \\ 0 & 0 & 0 & \alpha - \beta_0 & -p_0 & p_0 \\ 0 & -2d & 0 & -p_0 & -\frac{1}{2}\chi_0(q) & 0 \\ e & d & 0 & p_0 & 0 & 0 \end{pmatrix},$$

which may be used to obtain the charge susceptibility as:

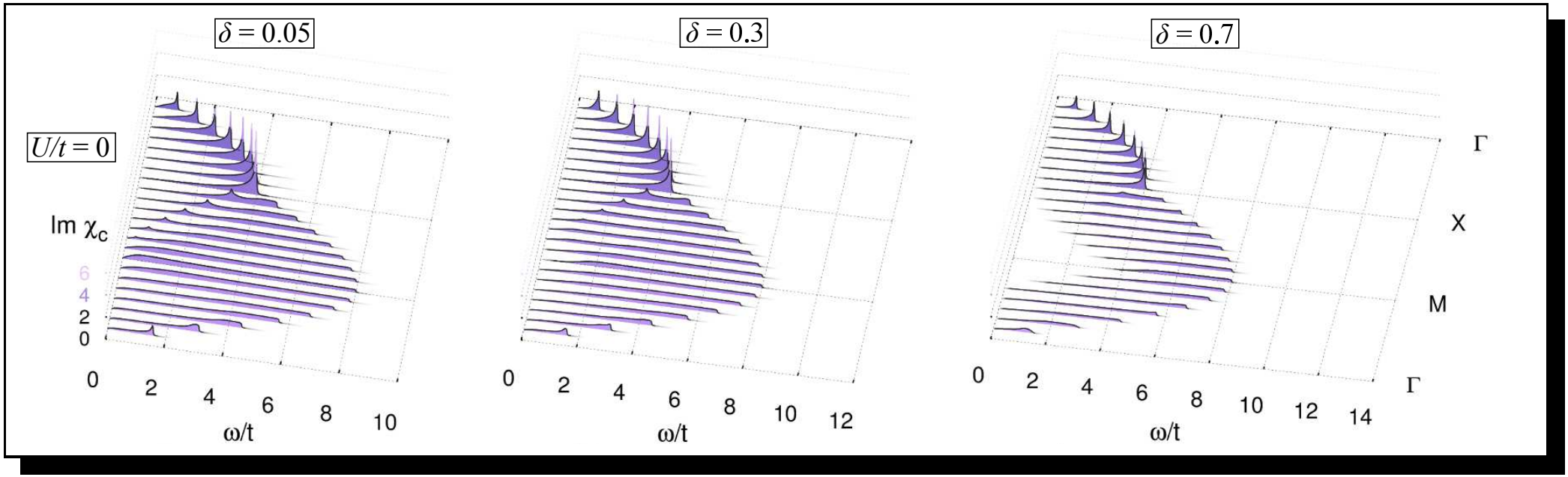
$$\chi_c(q) = 2e^2 S_{11}^{-1}(q) - 4ed S_{12}^{-1}(q) + 2d^2 S_{22}^{-1}(q).$$

A pole arises in the charge dynamics at $\omega \simeq \alpha - 2\beta_0 + U \simeq U$. Upper Hubbard band?

Charge dynamics on the square lattice

Performing the full one-loop calculation of the charge autocorrelation function yields $\chi_c(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega)$ in the non-interacting limit, though this is a fully interacting problem in slave boson representations.

$U/t = 0$



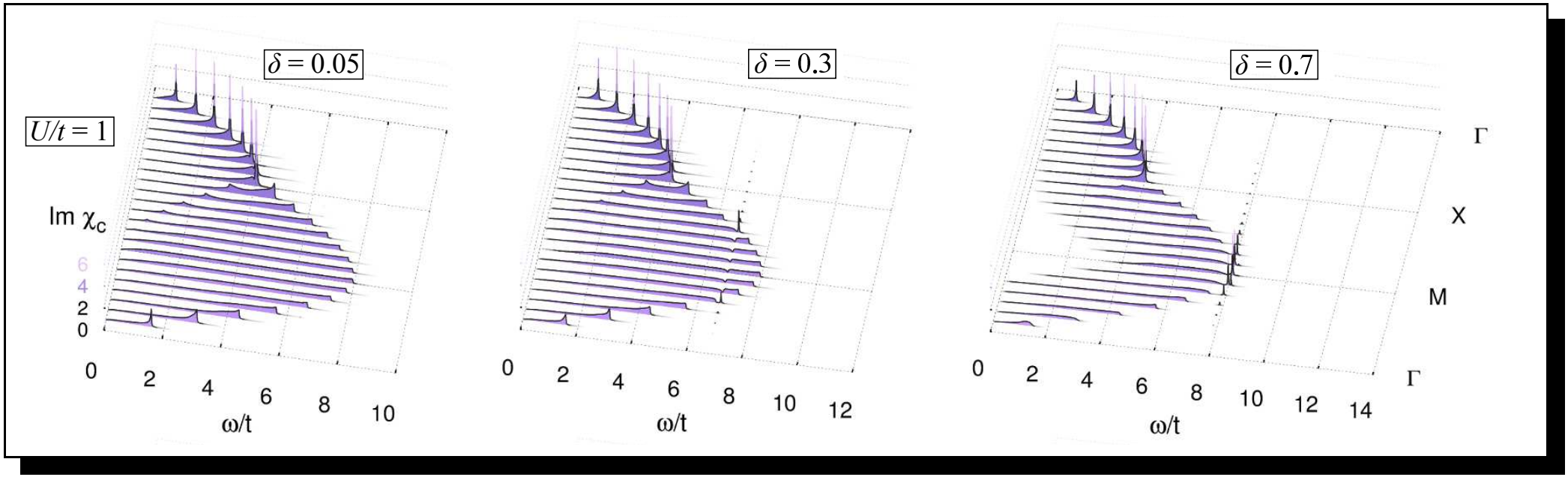
Particle-hole continuum. Logarithmic singularities along $\Gamma - X$.

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Charge dynamics on the square lattice

Performing the full one-loop calculation of the charge autocorrelation function yields $\chi_c(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega)/(1+\frac{U}{2}\chi_0(\mathbf{q},\omega))$ to lowest order in U. The RPA is recovered in this regime.

$U/t = 1$

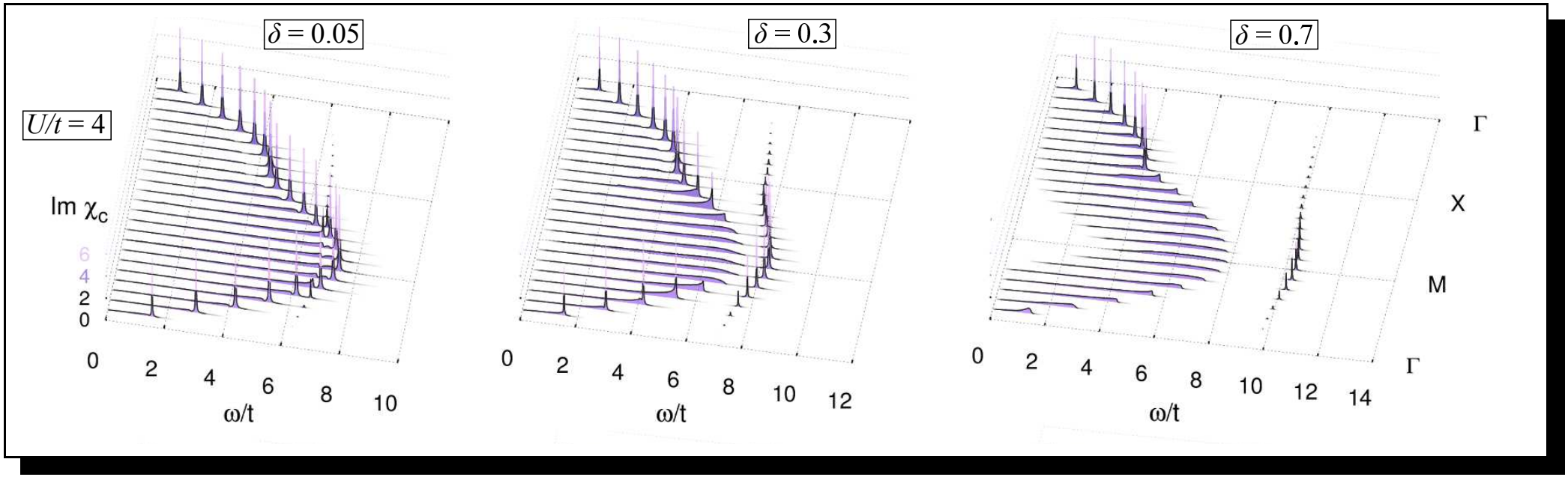


The edge peak is complemented by:

- An additional feature in the continuum: Damped collective mode
- A dispersionless mode

Charge dynamics on the square lattice

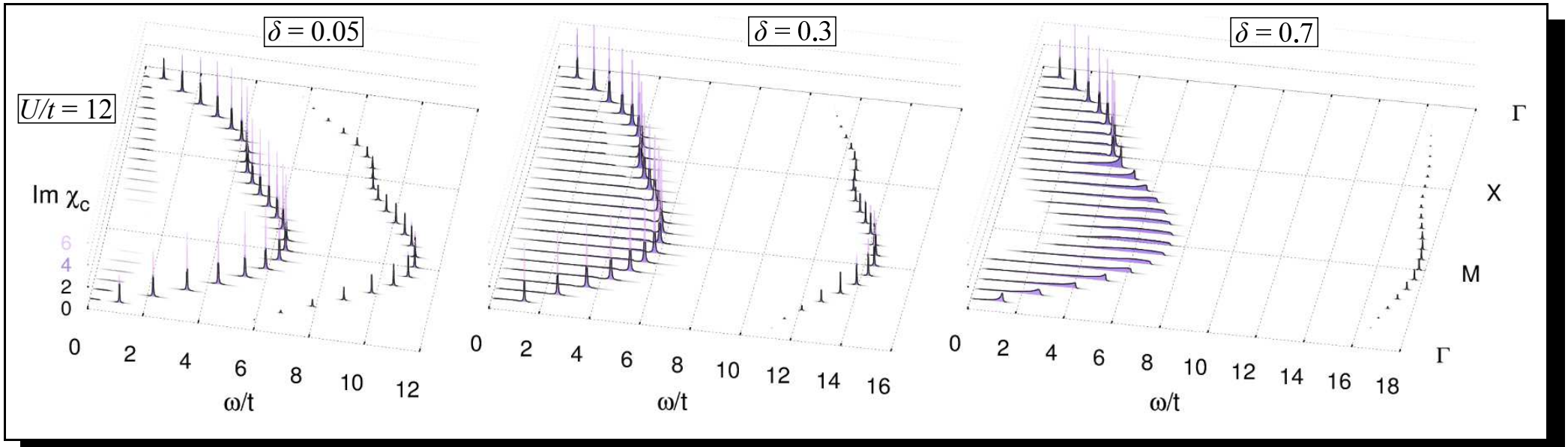
$U/t = 4$



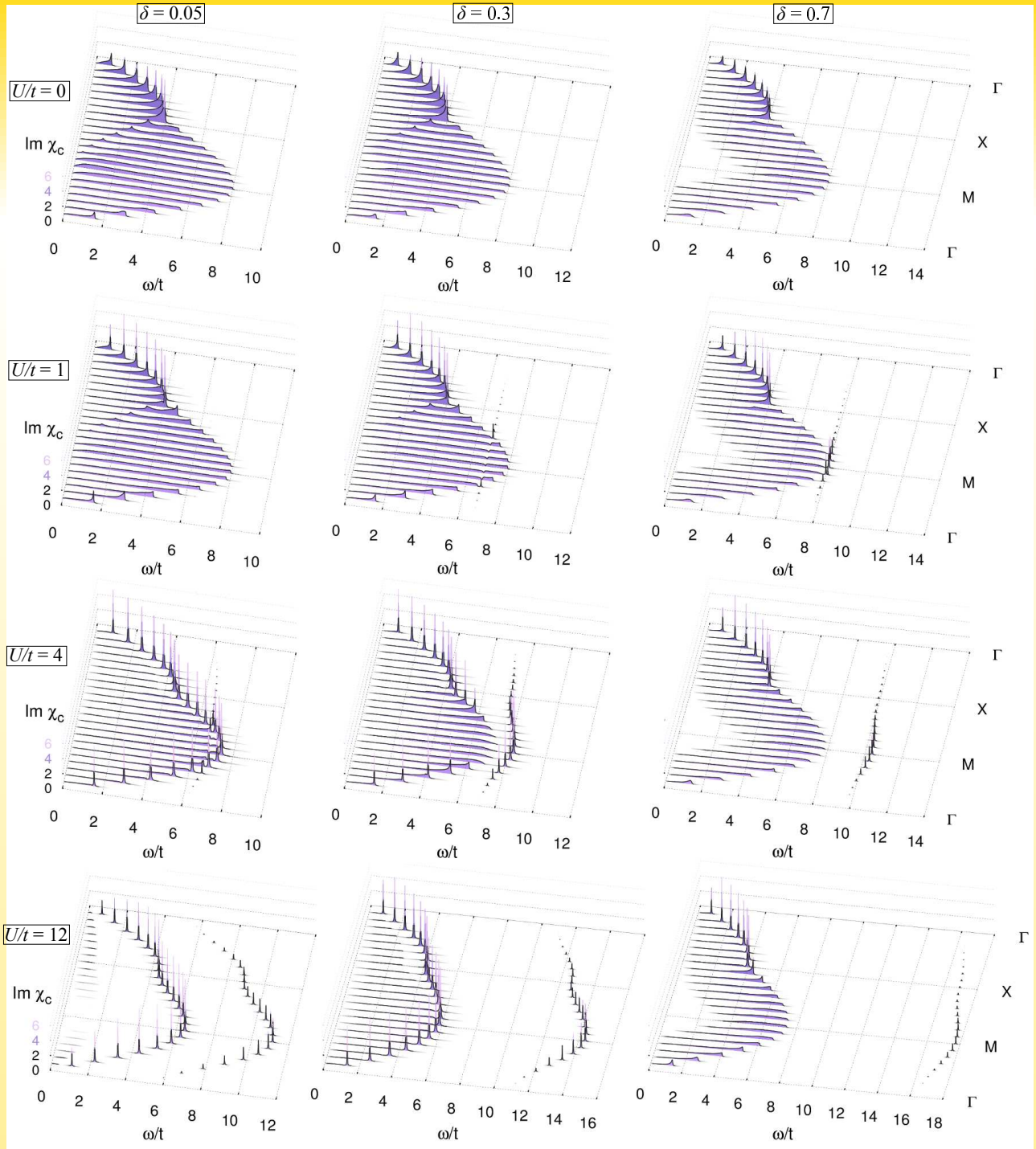
- The particle-hole continuum shrinks due to mass renormalization
- The collective mode separates from the continuum
- The upper mode gains weight and acquires dispersion. δ dependence

Charge dynamics on the square lattice

$U/t = 12$



- The particle-hole continuum further shrinks due to mass renormalization
- The collective mode is fully separated from the continuum
- The upper mode acquires further weight and dispersion. Upper Hubbard band
- $\Delta \sim U$



$U/t = 0$: Particle-hole continuum ending with an edge peak

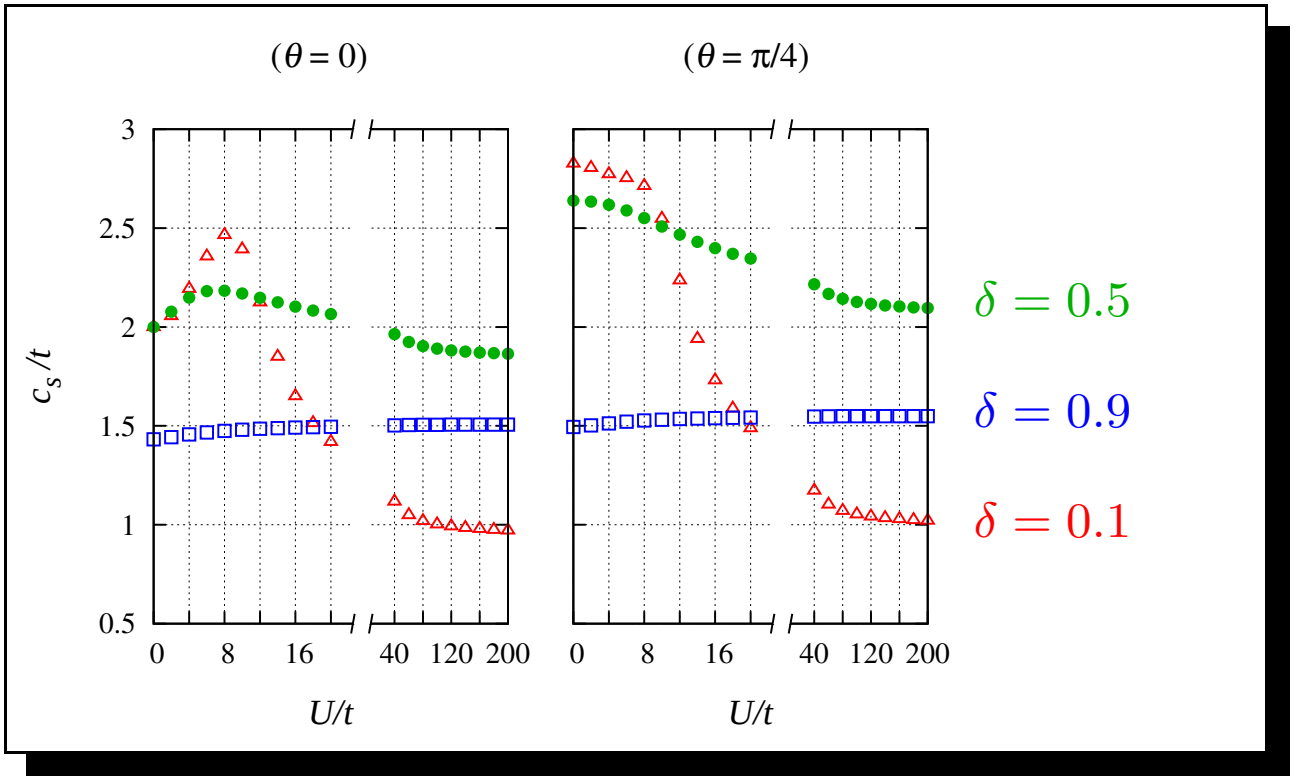
$U/t = 1$: A collective mode and an upper Hubbard band start to develop

$U/t = 4$: The collective mode separates from the continuum. The upper Hubbard band is clearly developed

$U/t = 12$: The upper Hubbard band is fully developed. $\Delta \simeq U$

V. H. Dao and RF, PRB **95**, 165127 (2017)

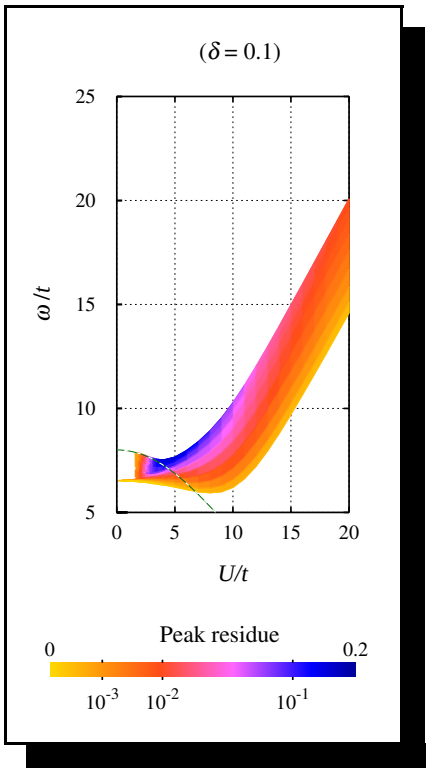
Charge dynamics on the square lattice: Zero-sound velocity

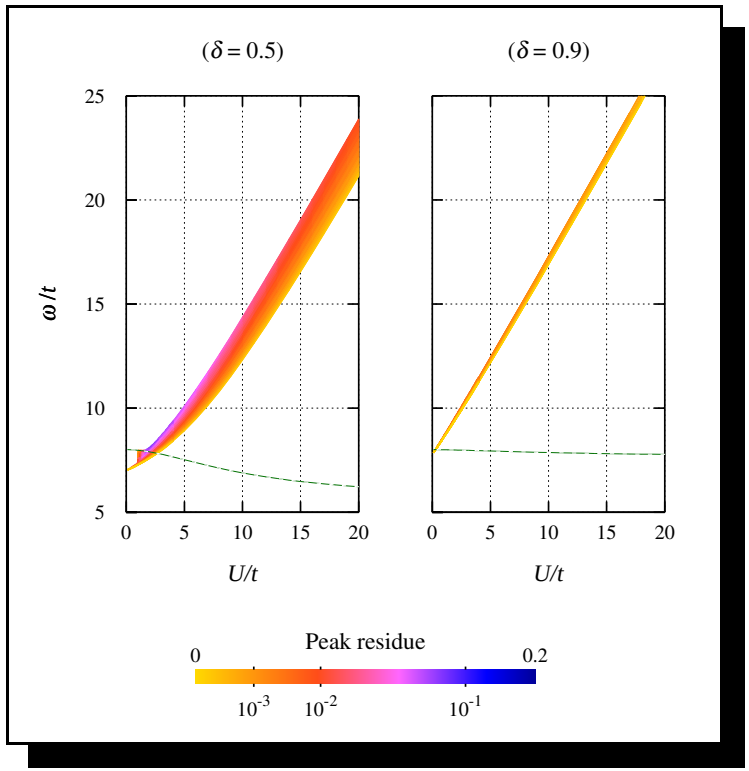


$$c_s(\theta_{\mathbf{k}}) = \frac{\omega_{\mathrm{ZS}}(\mathbf{k})}{|\mathbf{k}|}$$

- Suppression of the zero-sound velocity due to mass enhancement
- The strong weak-coupling anisotropy is suppressed by U
- Strong weak-coupling anisotropy, suppressed by the mass enhancement
- Weak increase of the zero-sound velocity with increasing U

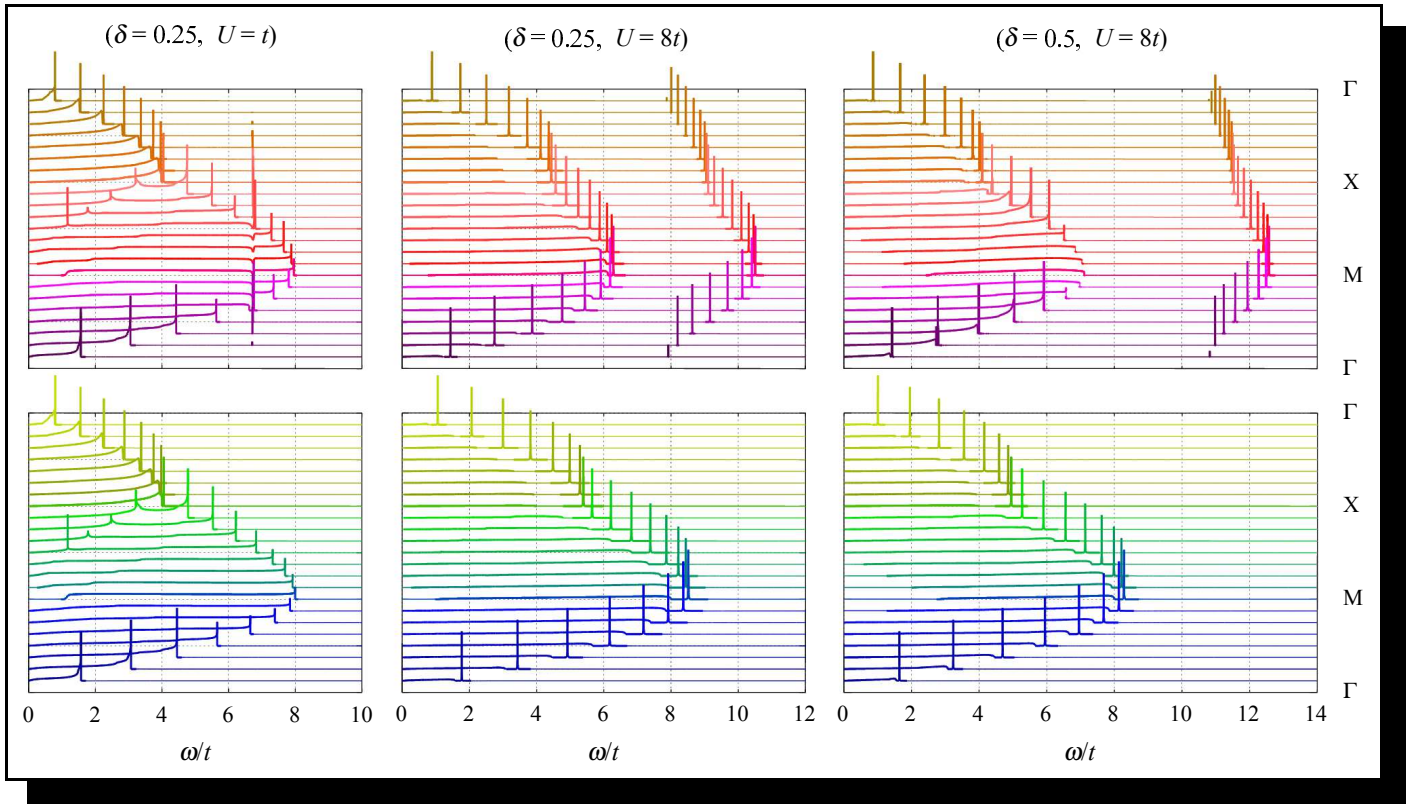
Charge dynamics on the square lattice: High-energy mode





- High-energy mode at $\omega \simeq U$, $\omega_{\rm UHB}(\mathbf{k}) \approx U\sqrt{1-\frac{U_0}{2U}\left(1-3|\delta|+(1-|\delta|)\frac{\varepsilon_{\mathbf{k}}}{\varepsilon_0}\right)}$
- Width $\approx (1-|\delta|)U_0/2$. It decreases with doping
- The weight is maximal for $U \simeq W$
- It fully separates from the continuum for a density-dependent U value

Charge dynamics on the square lattice: Comparison with RPA



$$\chi_{\rm RPA}(\mathbf{q},\omega) = \frac{\chi_0^{(0)}(\mathbf{q},\omega)}{1+\frac{U}{2}\chi_0^{(0)}(\mathbf{q},\omega)}$$

- The RPA misses the high energy mode
- The RPA misses the renormalization of the continuum
- The RPA overestimates the formation of the low-energy collective mode

Summary and outlook

- The Kotliar and Ruckenstein slave boson representation of the Hubbard model helps to unravel the physics of Hubbard split bands.
- The obtained charge excitation spectra generically consist of i) a continuum the width of which decreases with increasing interaction and density, ii) a collective mode with anisotropic zero-sound (ZS) velocity, and iii) a high frequency mode at $\omega \approx U$ which is the signature of the UHB.
- Qualitative differences with the RPA.
- Mass enhancement suppresses the ZS velocity.
- The width of the high-energy mode decreases with doping.
- The low-energy collective mode may be damped by t'.

Perspectives

- Longer-ranged interactions?
- Excitations of symmetry broken phases?

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THANKS TO

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- Thilo Kopp, Augsburg.

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