Optical and DC conductivity in the 2D *t-t'-t''* Hubbard model near the antiferromagnetic quantum critical point

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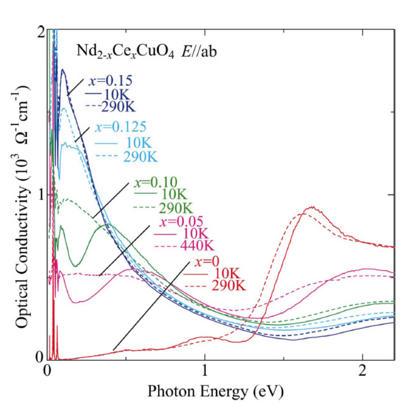
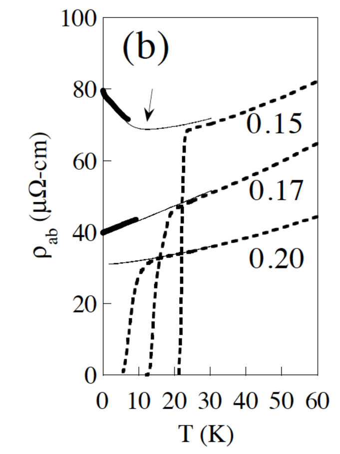
Introduction

- Transport in *e*-doped cuprates:
  - Mid-infrared peak in *Re* σ(ω)
  - Three regimes in *ρ*(*T*)
    - *T*<*T** : *ρ*↗ (or *ρ*↘)
    - doping n_c : $\rho \propto T$
    - overdoped: $\rho \propto T^2$



Y. Onose et al., Phys. Rev. B, 69, 24504 (2004)



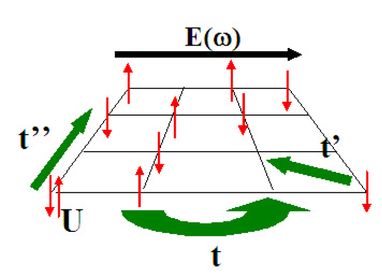
Fournier et al., Phys. Rev. Lett., 81, 4720 (1998)

- Are those features present in 2D Hubbard model?

Methodology

Model:

$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Two-Particle Self-Consistent (TPSC) approach:

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1-\frac{U_{sp}}{2}\chi_0(q)} \qquad \chi_{ch}(q) = \frac{\chi_0(q)}{1+\frac{U_{ch}}{2}\chi_0(q)}$$

$$\frac{T}{N}\sum_q \chi_{sp}(q) = n - 2\langle n_\uparrow n_\downarrow\rangle = n - \frac{U_{sp} n^2}{2U}$$

$$\frac{T}{N}\sum_q \chi_{ch}(q) = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2$$

$$\Sigma^{(2)}_\sigma(k) = U n_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right] G^{(1)}_\sigma(k+q)$$

Impose
- Conservation laws
- Pauli principle $\langle n_\sigma^2\rangle = \langle n_\sigma\rangle$
- sum rules $\langle n^2\rangle$ and $\langle S_z^2\rangle$

⇒
- Respect Mermin-Wagner theorem
- Kanamori-Brückner screening

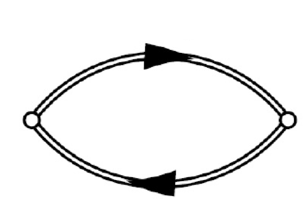
Optical conductivity:

$$Re\,\sigma_{xx}(\omega) = \frac{\chi''_{j_x j_x}(\omega)}{\omega}$$

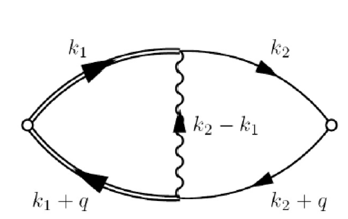
Current-current correlation function:

$$\chi_{j_x j_x}(iq_n, \mathbf{q}=0) =$$

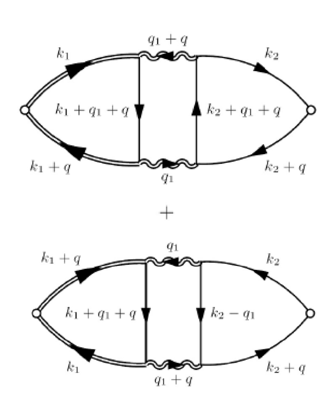
$$-\frac{2T}{N}\sum_k \left(\frac{\partial \epsilon_k}{\partial k_x}\right)^2 G^{(2)}(k)G^{(2)}(k+iq_n)$$



$$-\frac{U}{4}\left(\frac{T}{N}\right)^2 \sum_{k_1 k_2} G^{(2)}(k_1)G^{(2)}(k_1+iq_n)G^{(1)}(k_2)G^{(1)}(k_2+iq_n) \times \frac{\partial\epsilon_k}{\partial k_x}(k_1)\frac{\partial\epsilon_k}{\partial k_x}(k_2)\left[3U_{sp}\chi_{sp}(k_2-k_1) + U_{ch}\chi_{ch}(k_2-k_1)\right]$$



$$+\frac{U}{2}\left(\frac{T}{N}\right)^3 \sum_{k_1,k_2,q_1} \frac{\partial\epsilon_k}{\partial k_x}(k_1)\frac{\partial\epsilon_k}{\partial k_x}(k_2) G^{(2)}(k_1)G^{(2)}(k_1+iq_n) \times G^{(1)}(k_2)G^{(1)}(k_2+iq_n)\left[G^{(1)}(k_2+q_1+iq_n) + G^{(1)}(k_2-q_1)\right] \times G^{(1)}(k_1+q_1+iq_n)\left(3U_{sp}\frac{1}{1-\frac{U_{sp}}{2}\chi_0(q_1)}\frac{1}{1-\frac{U_{sp}}{2}\chi_0(q_1+iq_n)} + U_{ch}\frac{1}{1+\frac{U_{ch}}{2}\chi_0(q_1)}\frac{1}{1+\frac{U_{ch}}{2}\chi_0(q_1+iq_n)}\right)$$



Numerical results (U=6t, t'=-0.175t, t''=0.05t)

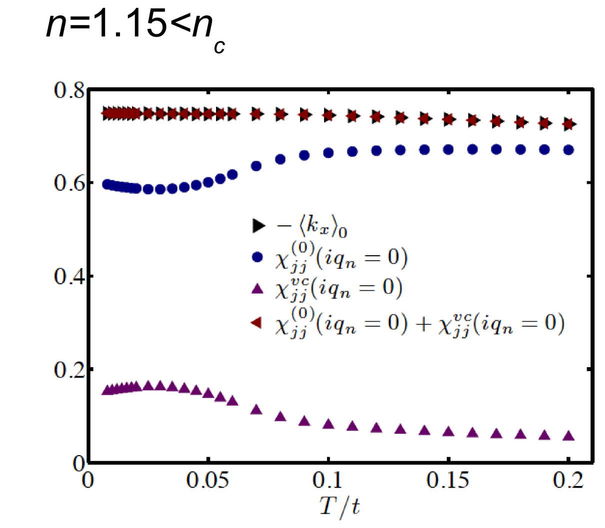
Particle conservation: *f*-sum-rule

$$\int \frac{d\omega}{\pi} Re\,\sigma_{xx}(\omega) = \chi_{j_x j_x}(iq_n=0) = -\langle k_x\rangle_0 \quad ,$$

$$\langle k_x\rangle_0 = -\frac{1}{N}\sum_{\mathbf{k}\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_x^2} n_{\mathbf{k}\sigma} = -\frac{1}{N}\sum_{\mathbf{k}\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_x^2} G^{(2)}_\sigma(\mathbf{k},\tau=0^-)$$

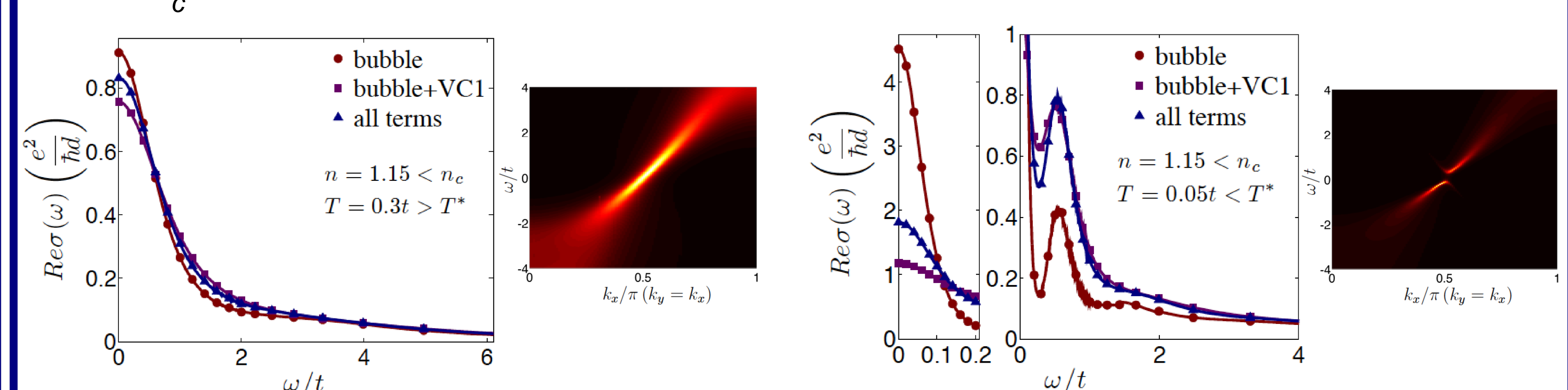
- Sum-rule satisfied with relative error $<10^{-7}$ for all *T* range with first vertex correction

n=1.15<n_c

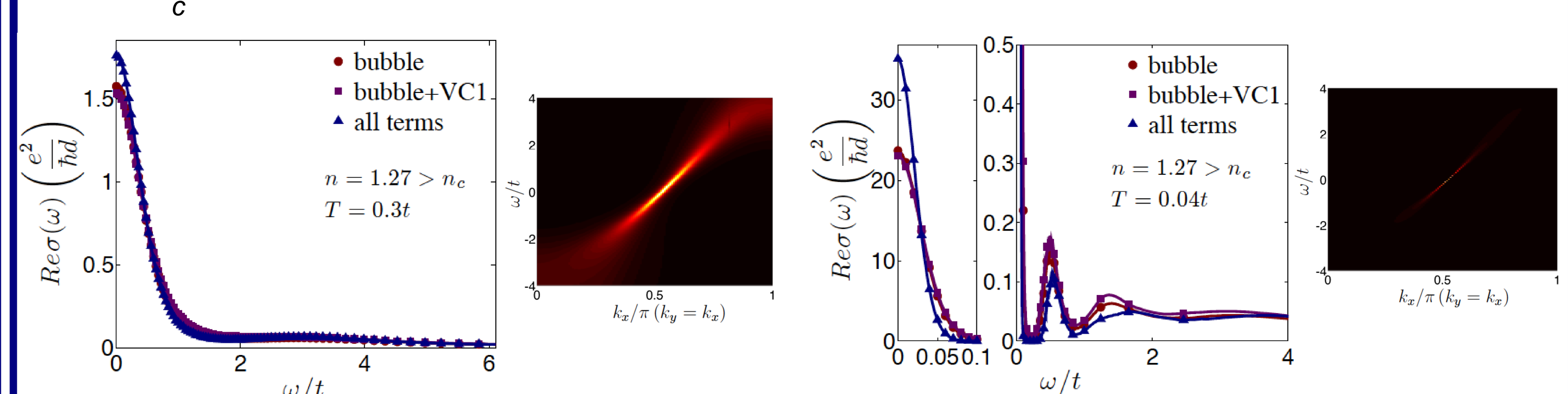


Optical conductivity:

$n < n_c$:

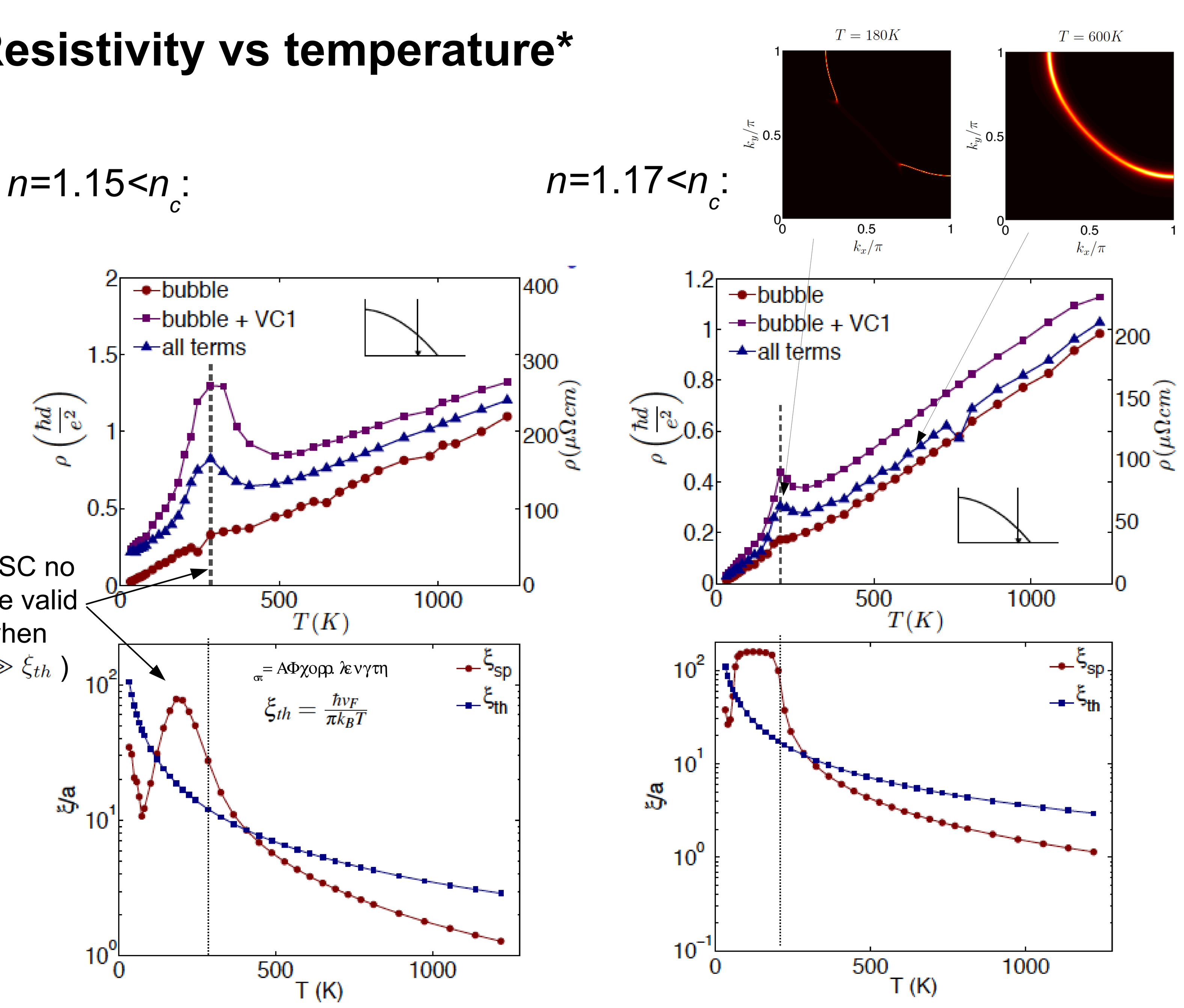


$n > n_c$:



Resistivity vs temperature*

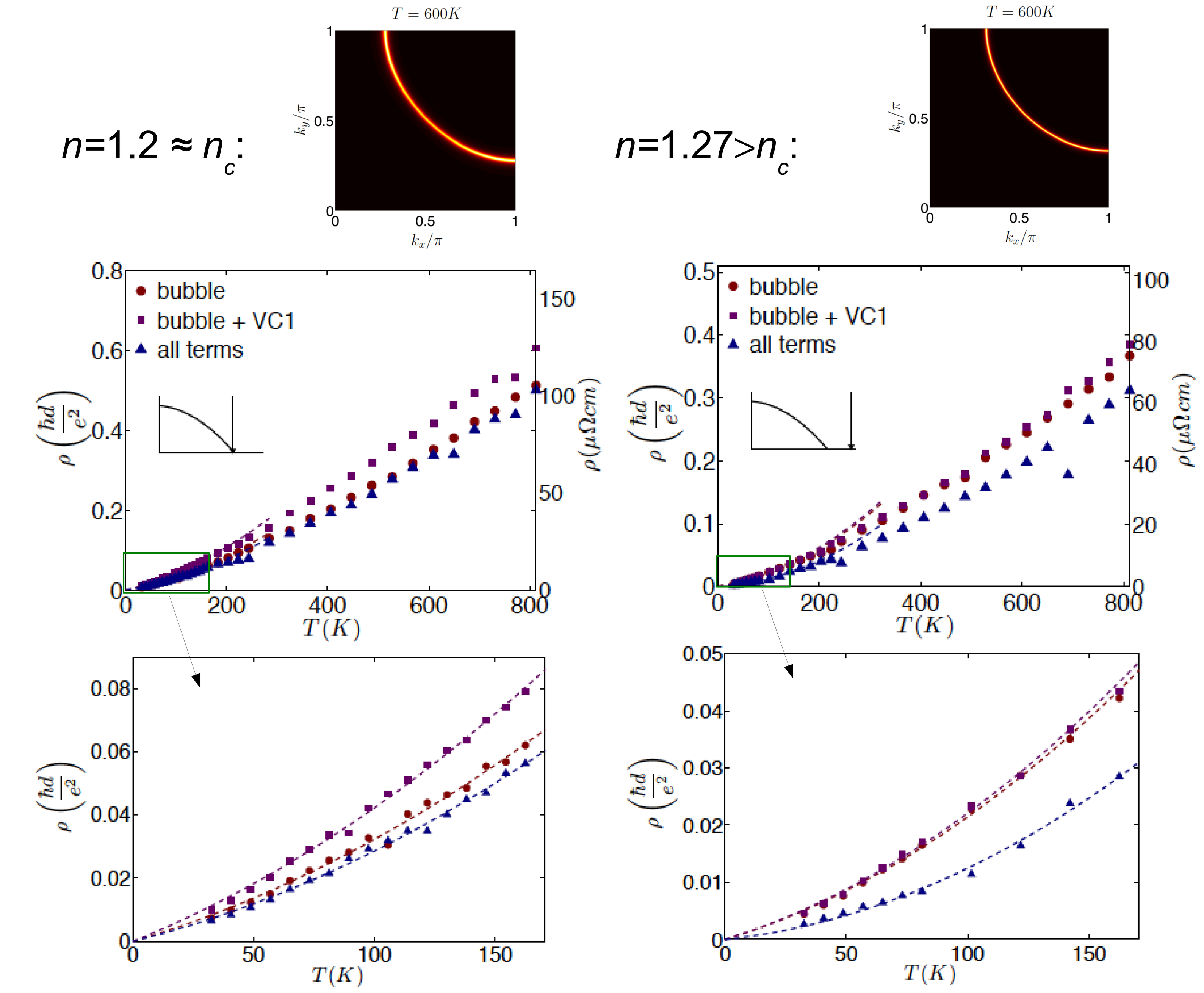
n=1.15<n_c: n=1.17<n_c:



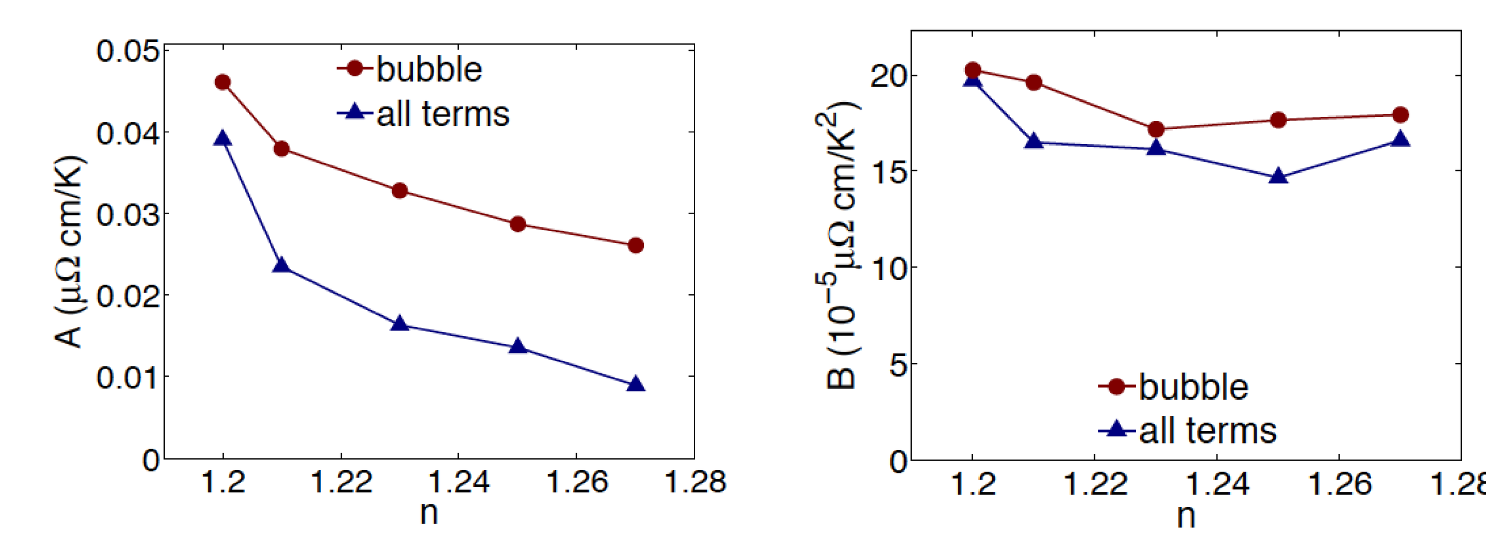
(TPSC no more valid when $\xi_{sp} \gg \xi_{th}$)

*(t=0.35eV, d=5Å)

n=1.2 ≈ n_c: n=1.27>n_c:



Fitting $\rho(T) = AT + BT^2$ for $n \geq n_c$:



Conclusion

- *f*-sum-rule satisfied with vertex corrections
- *ρ*(*T*), $n < n_c$
  - Insulating behavior with vertex corrections when $\xi_{sp} > \xi_{th}$, (*T*<*T**)
  - $\rho \propto T$ for *T*>*T**
- *ρ*(*T*), $n \geq n_c$
  - *ρ*(*T*) ≈ $AT+BT^2$ at low *T*, *A* decreases with doping
- Mid-infrared peak in *Re* σ(ω) due to antiferromagnetic fluctuations

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