Combined CDW and Peierls Distortion in Cuprates

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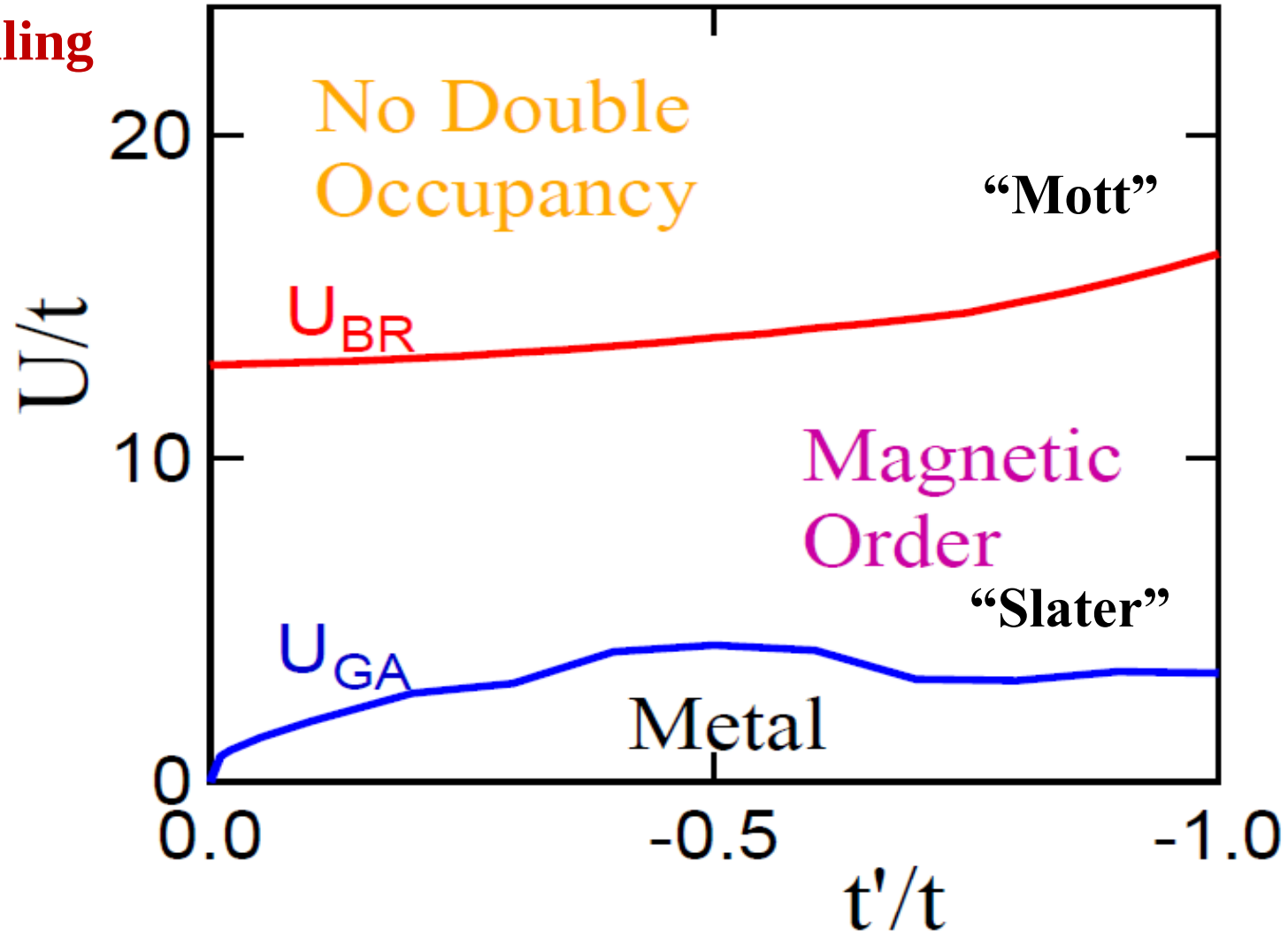
Outline

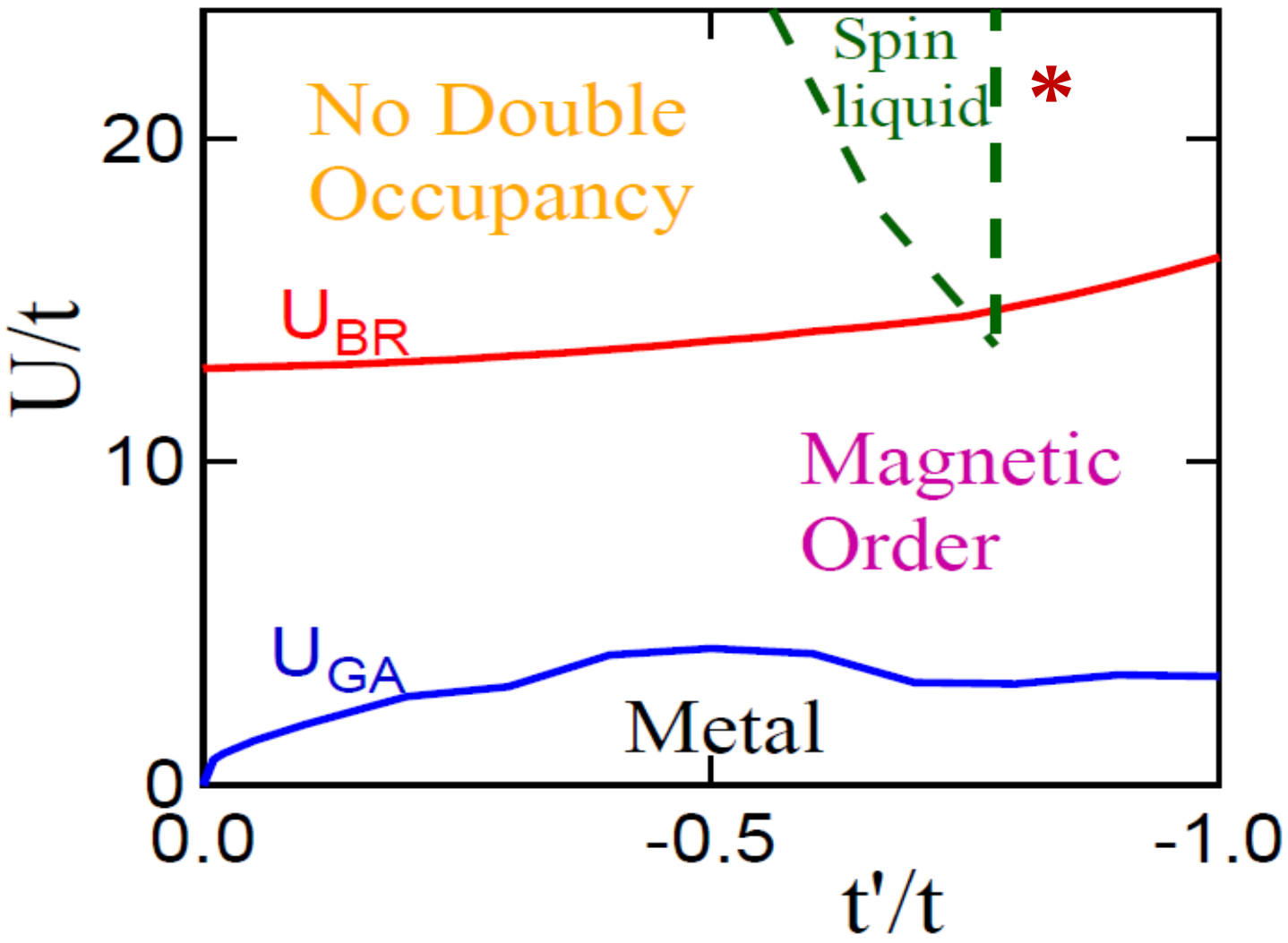
- Intermediate Coupling Theory (QP-GW)
- Magnetic Phase Diagram
- Charge Phase Diagram

Correlations in Cuprates

Half filling

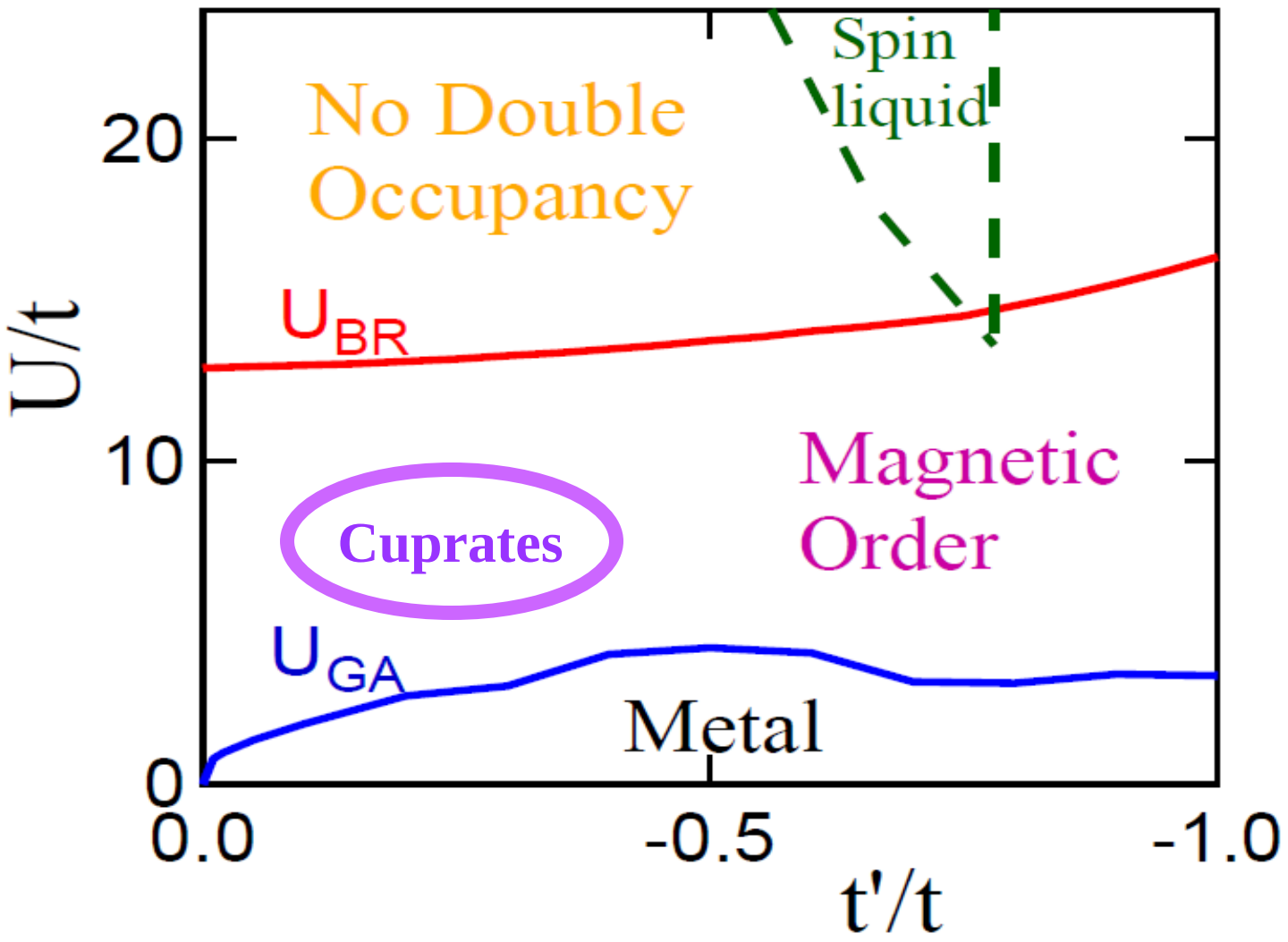


Correlations in Cuprates



*: Tocchio, Becca, Parola, and Sorella, PRB **78**, 041101(R) (2008).

Correlations in Cuprates

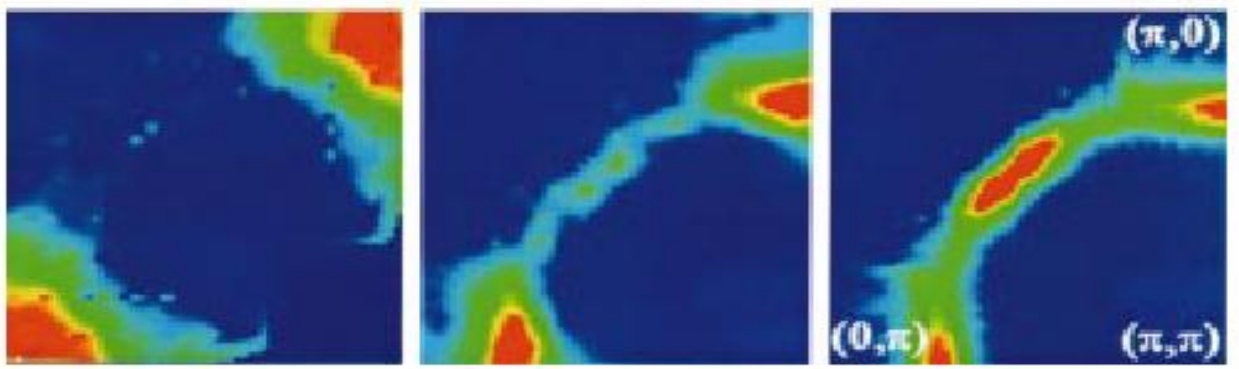


QP-GW Model

- Susceptibility $\chi(\omega,k)$
  - LDA bands
  - RPA Correction (U)
- Dressing: Self-energy Σ
  - $\Sigma(\omega,k)=U^2\int G(\omega',k')\chi(\omega-\omega',k-k')dk'd\omega'$
  - R.H.S.: G, χ renormalized by Z
  - Z found self-consistently
  - Few free parameters (U)

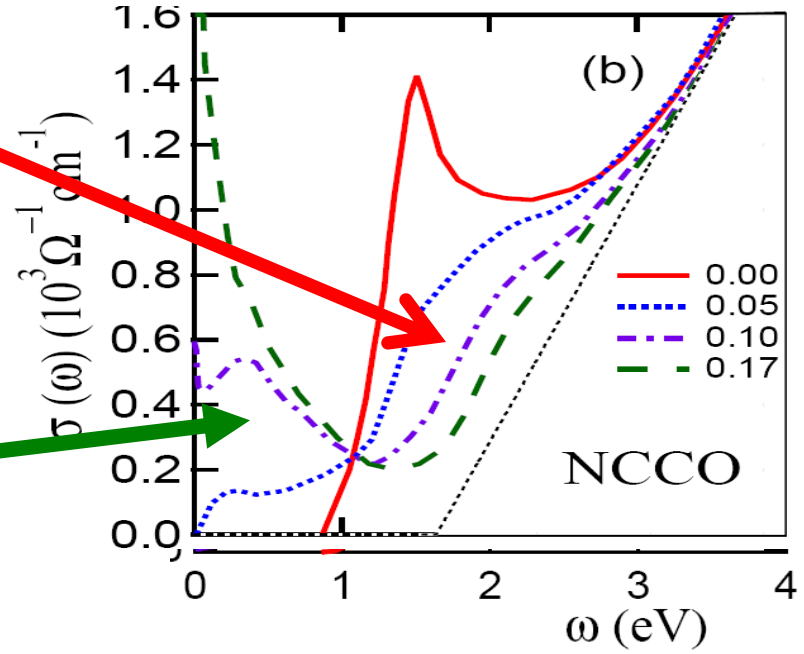
Explains Gap Collapse Problem

ARPES sees gap collapse …



0.04 0.10 0.15

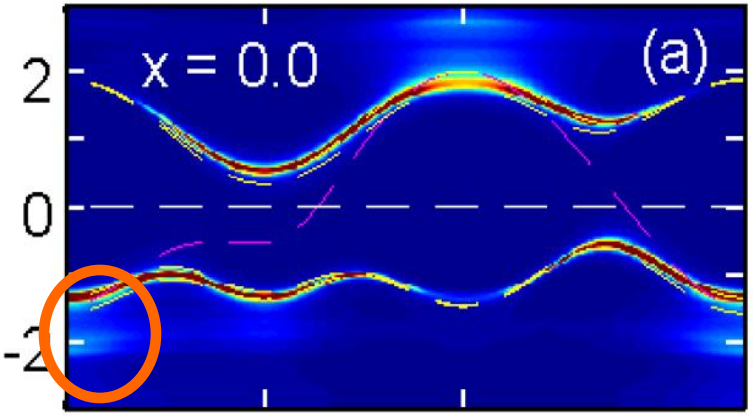
but optical gap remains large



Solution: the 'mid-infrared peak' tracks the gap collapse in the coherent states

Intermediate Coupling:
Add fluctuations

ARPES: waterfalls

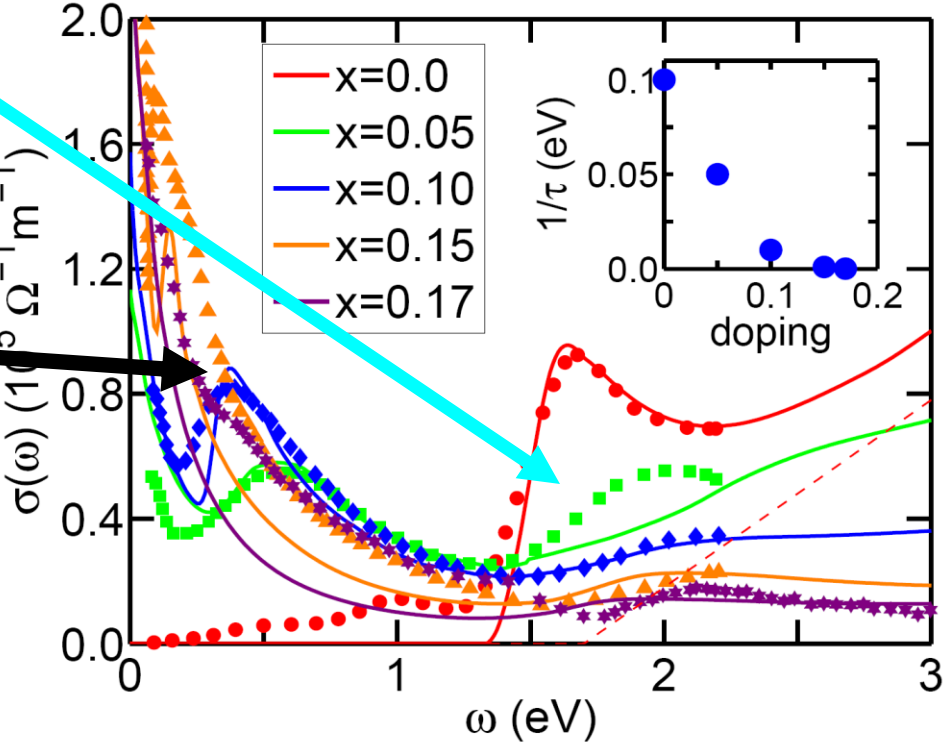


Optical:

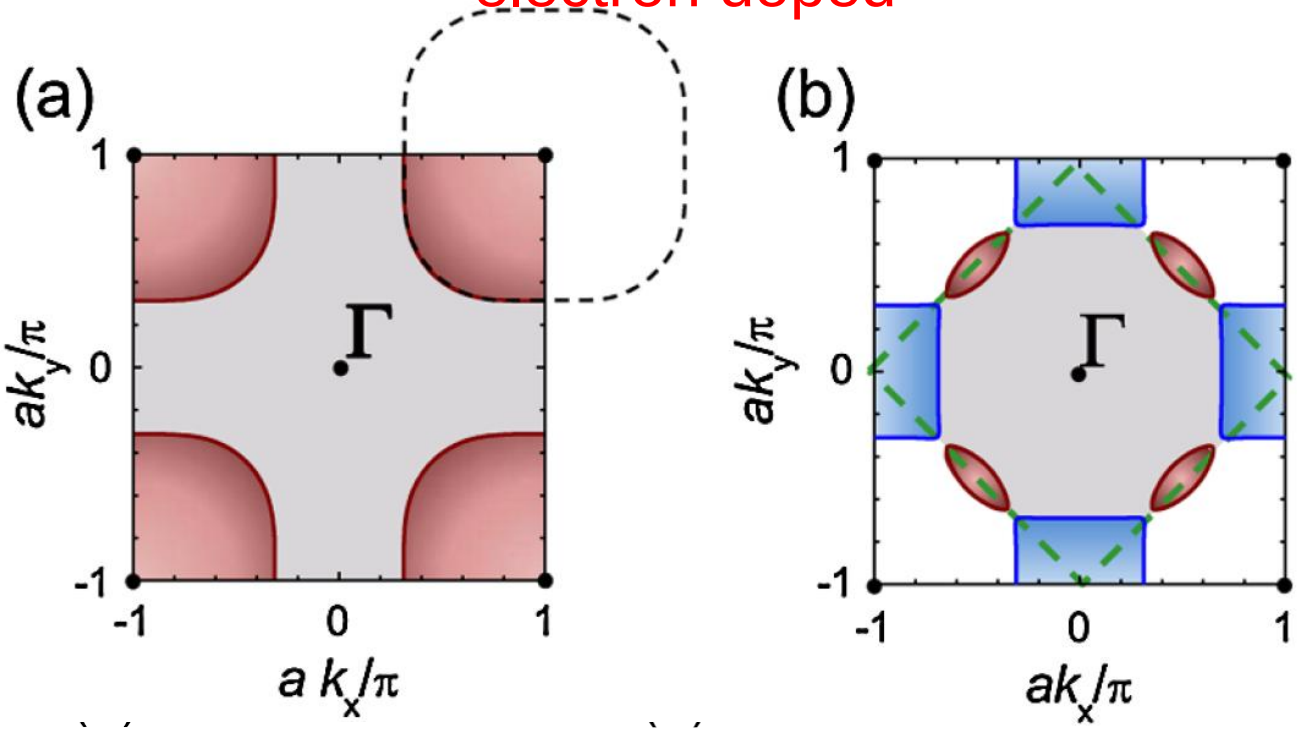
Tanmoy Das, R.S. Markiewicz, A. Bansil
PRB 81, 174504 (2010)

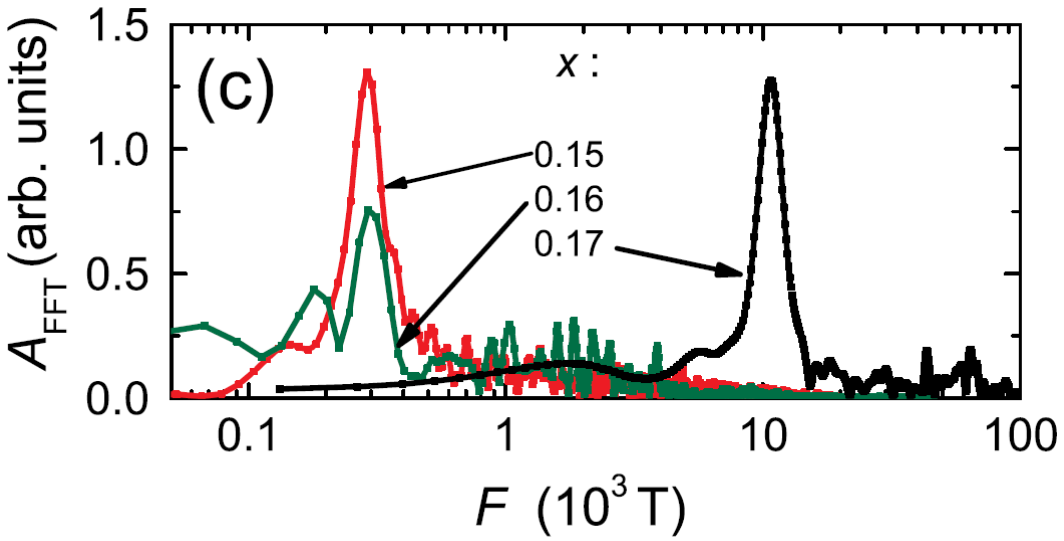
Incoherent: remnant Mott gap

Coherent:
Mid-infrared peak
= magnetic gap



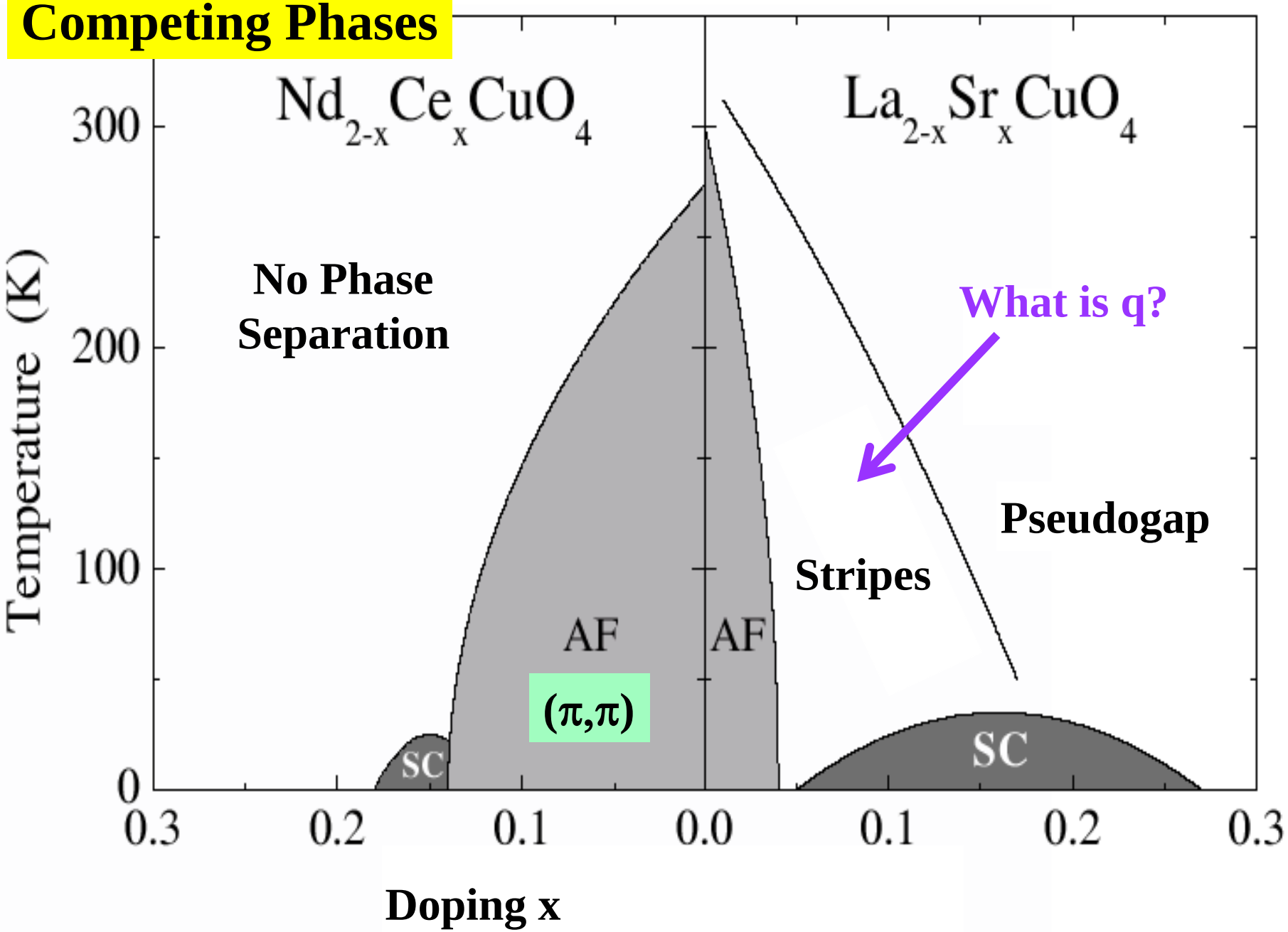
Model gets right quantum oscillations for electron doped





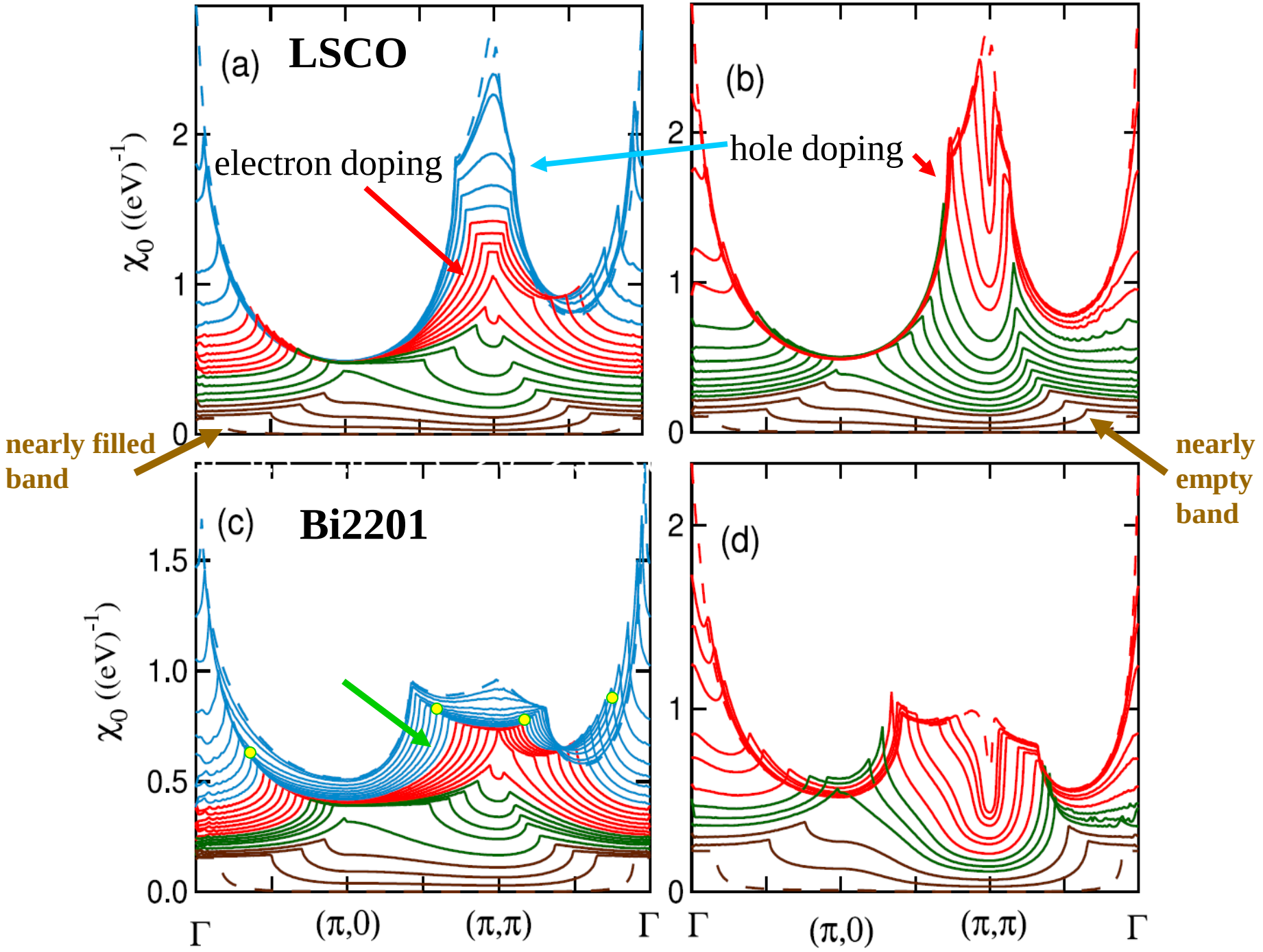
Experiment:
T. Helm, et al., PRL 103, 157002 (2009);
Theory:
Kusko, Markiewicz, Lindroos, Bansil, PRB 66, 140513 (2002)

Competing Phases

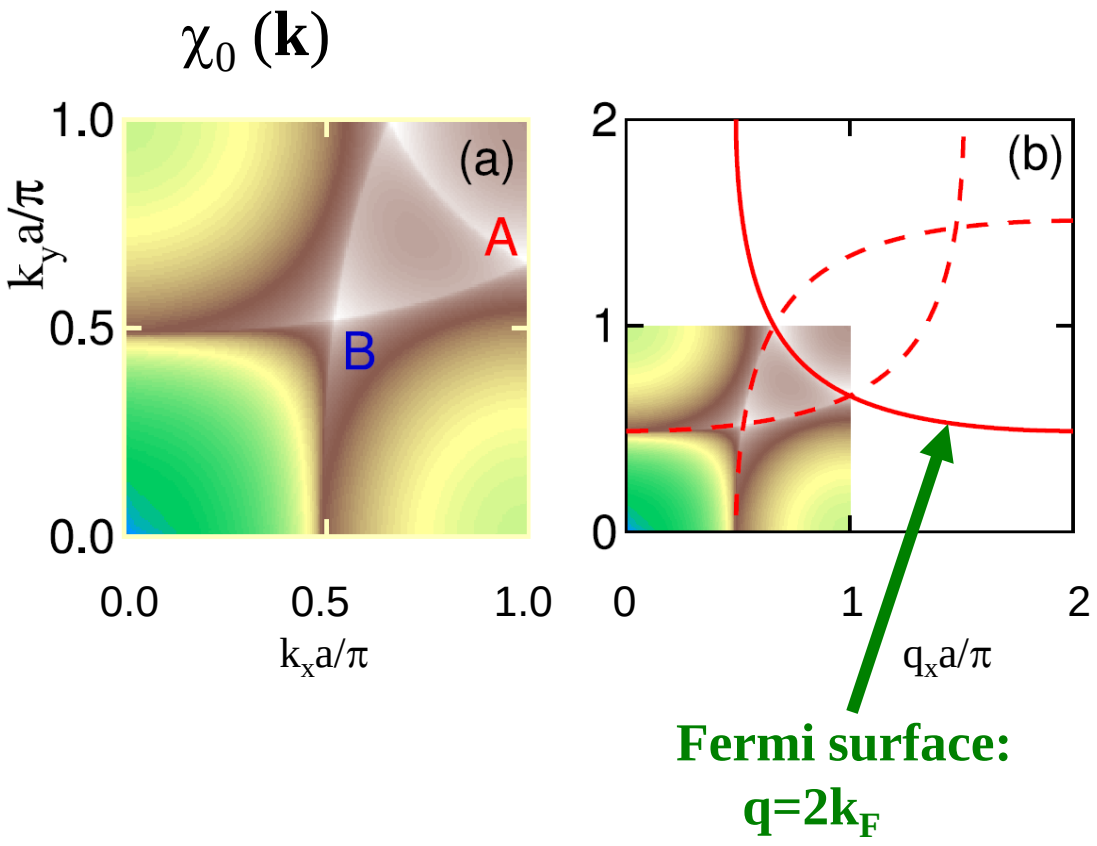


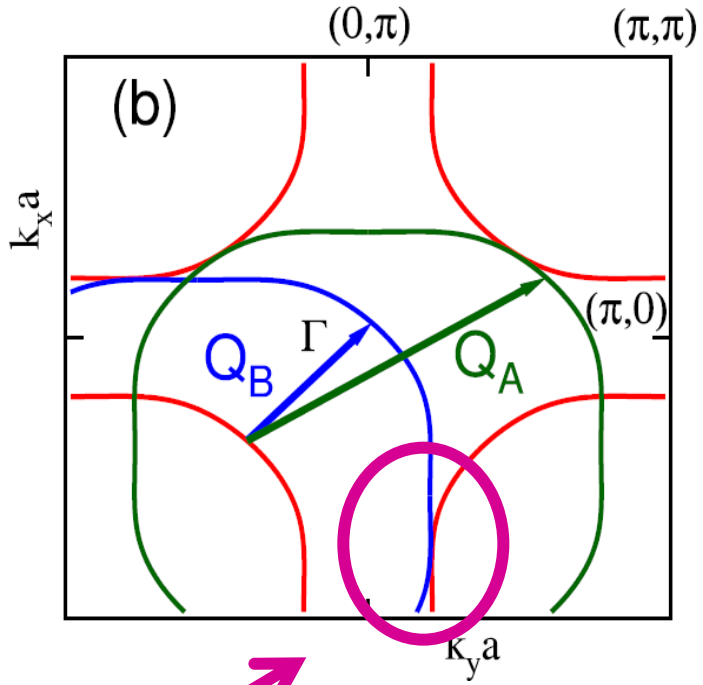
Applied Slater Physics

- $\chi = \chi_0/(1-U\chi_0)$
- Calculate bare susceptibility
- Gutzwiller-corrected U [~slave boson]
- Phase diagrams: $U\chi_0(q)=1$


(a) LSCO
(b)
(c) Bi2201
(d)
electron doping
hole doping
nearly filled band
nearly empty band
χ_0 ((eV)$^{-1}$)
Γ
(π,0)
(π,π)
Γ

Leading Instability controlled by Double Nesting

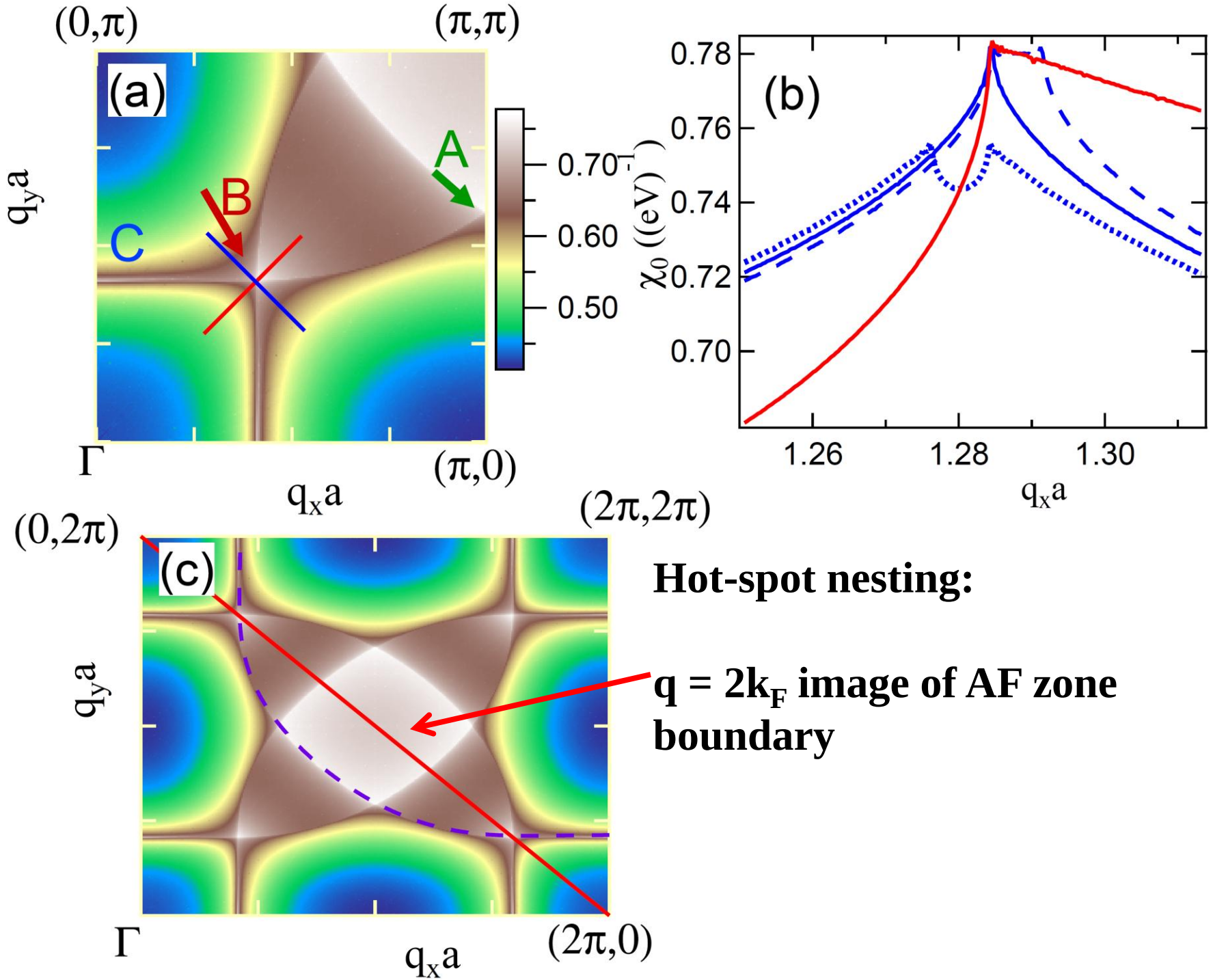




Fermi surface:
$q=2k_F$

~~**Anti-Nodal Nesting**~~

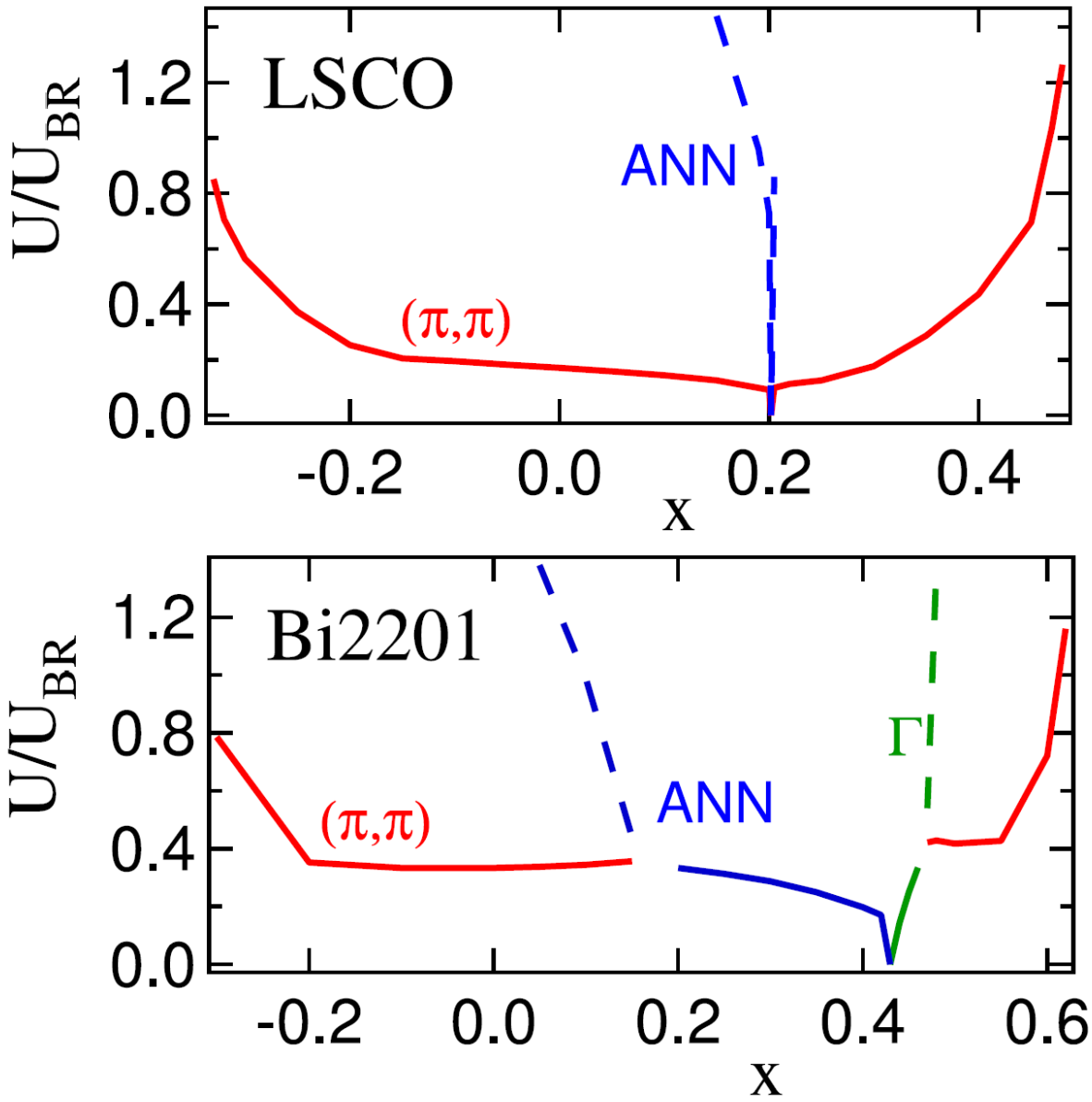
Hot-spot

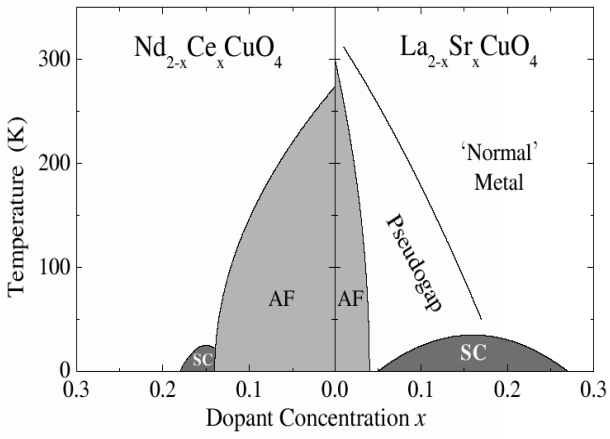


Hot-spot nesting:

q = $2k_F$ image of AF zone boundary

Magnetic Phase Diagrams of Cuprates





CDW + Peierls distortion

- Chang *et al*., Nature Physics **8**, 871 (2012): x-ray study of YBCO
- $I \sim |\Sigma_i n_i|^2$
- For electronic CDW, $\Sigma_i n_i = x$ or $(1-x)$
- For Peierls distortion, $\Sigma_i n_i$ = all electrons in unit cell [acoustic wave]

Electron-phonon coupling

Modulated hopping: t → t±δt, δt/t = - γδr/r

$$H_{el-ph} = -\sum_{ij} \frac{t_{ij}\gamma_{ij}}{r_{ij}} \sum_{\sigma\mu=x,y} (u_j^\mu - u_i^\mu)(c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

$$H_{ph} = \frac{1}{2N} \sum_{\alpha\beta\mathbf{q}} u_{\mathbf{q}}^\alpha K_{\alpha\beta\mathbf{q}} u_{-\mathbf{q}}^\beta + \frac{1}{2N} \sum_{\alpha\mathbf{q}} p_{\mathbf{q}}^\alpha \frac{1}{M} p_{-\mathbf{q}}^\alpha$$

$$\lambda_{ep} = \frac{\gamma^2 t}{K a^2}$$

Strong correlations

- GA ~ slave bosons: $Z=z_0^2$

$$z_0 = \sqrt{\frac{2x^2 - x^4 - \delta^2}{1 - \delta^2}}$$

$$x = \sqrt{\delta + D} + \sqrt{D}$$

D = double occupancy
δ = doping

$$\frac{x^4(1-x^2)}{x^4 - \delta^2} = (1 - \delta^2)\frac{U}{U_{BR}}$$

Di Ciolo, Lorenzana, Grilli, and Seibold, PR**B79**, 085101 (2009)

CDW: Stoner denominator → 0:

$$1 + U_{\text{eff}}(q)\chi_0(q, \omega = 0) = 0$$

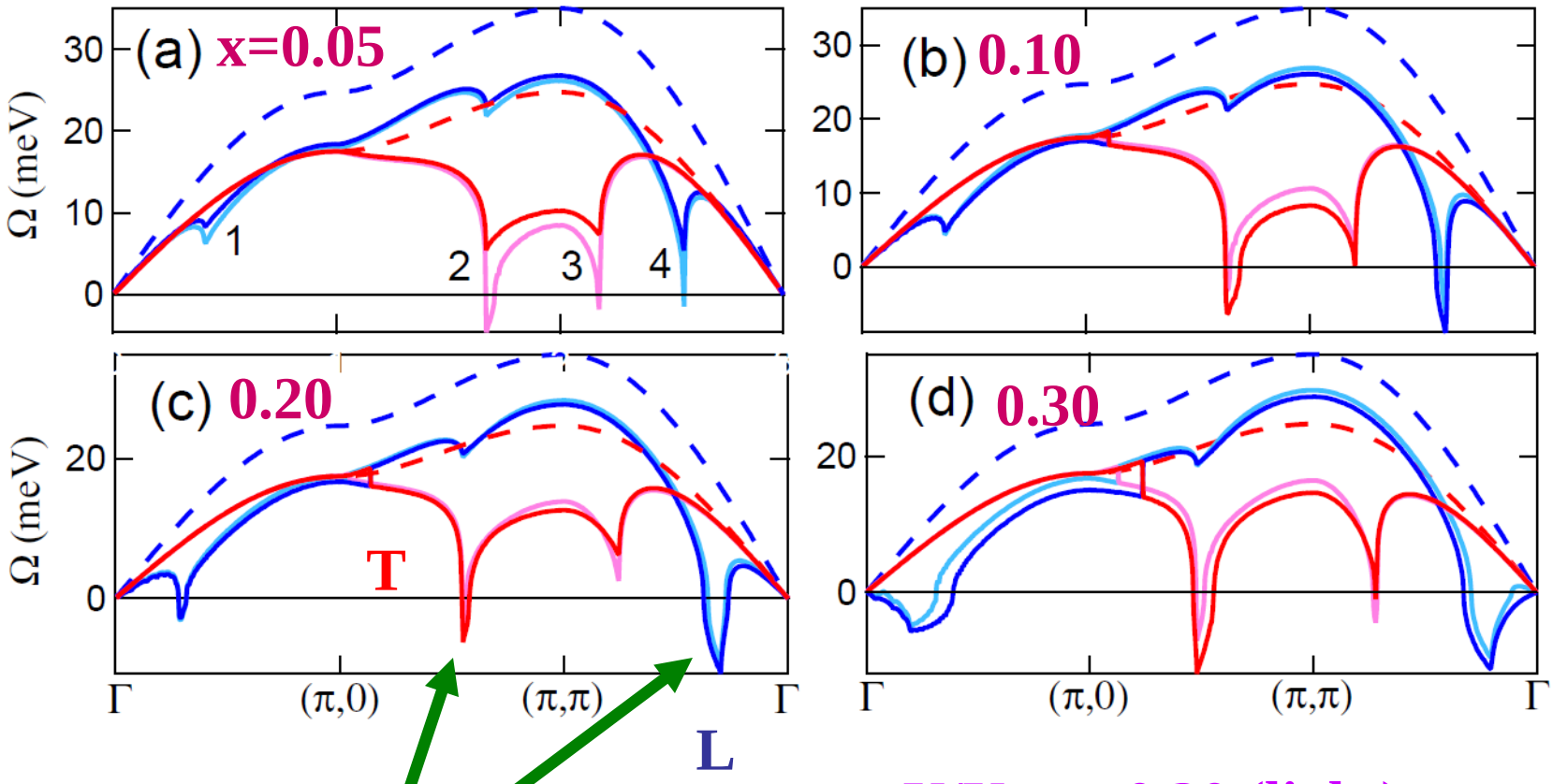
Peierls: Phonon softening:

$$\Omega^2_{q\mu} = \Omega^2_{0q\mu} + \frac{\delta K_{\mu\mu}}{M}$$
$$= \Omega^2_{0q}[1 - U_{eff,q}\chi_{0q}]$$

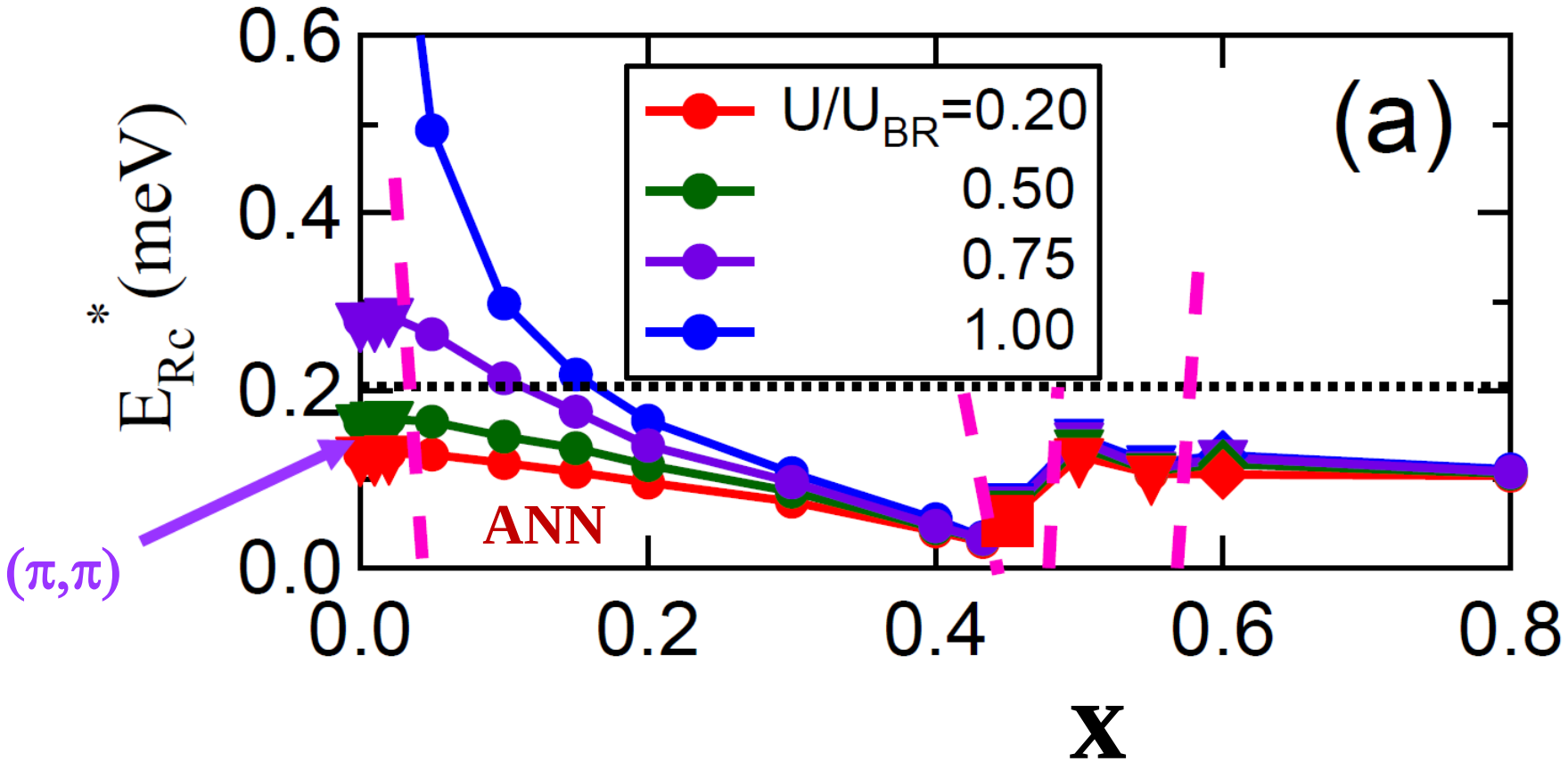
$$U_{eff,q}\chi_{0q} = [\chi^0_{ff\mu\mu} - \tilde{\chi}^0_{f\mu}\hat{W}(1 + \tilde{\chi}_0\hat{W})^{-1}\tilde{\chi}^0_{f\mu}]/z_0^2\Omega^2_{0q}$$

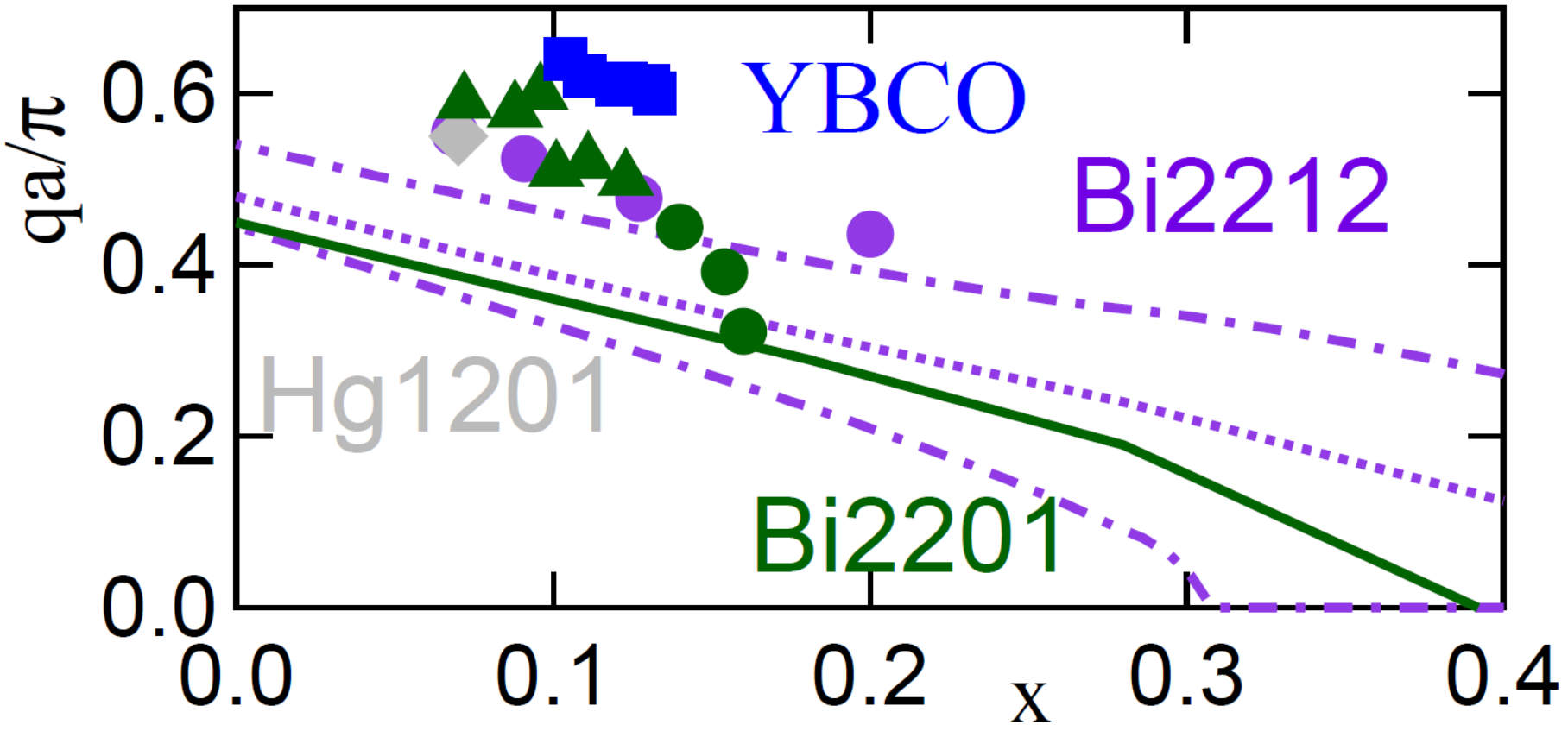
The meaning of Eq. A.38 is clear. If all the terms were scalars and all χ's equal to χ_0, the term in brackets would be $\chi_0[1-\chi_0 W/(1+\chi_0 W)] = \chi_0/(1+\chi_0 W)$ – the electron-phonon interaction would be screened by the e-e dielectric constant.

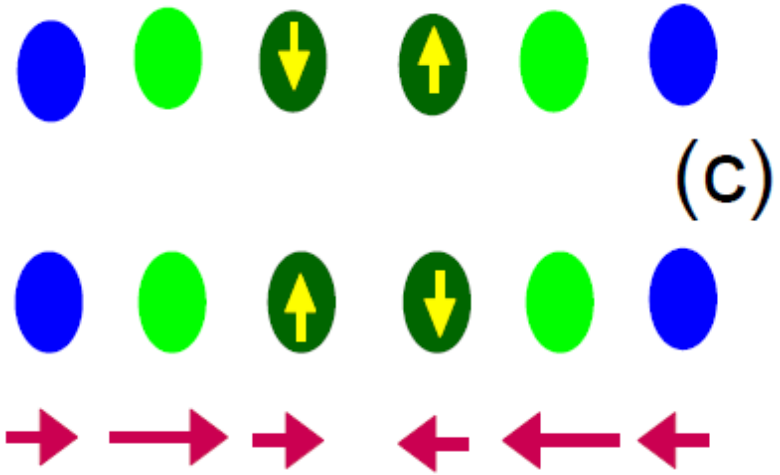
Phonon Dispersion Bi2201



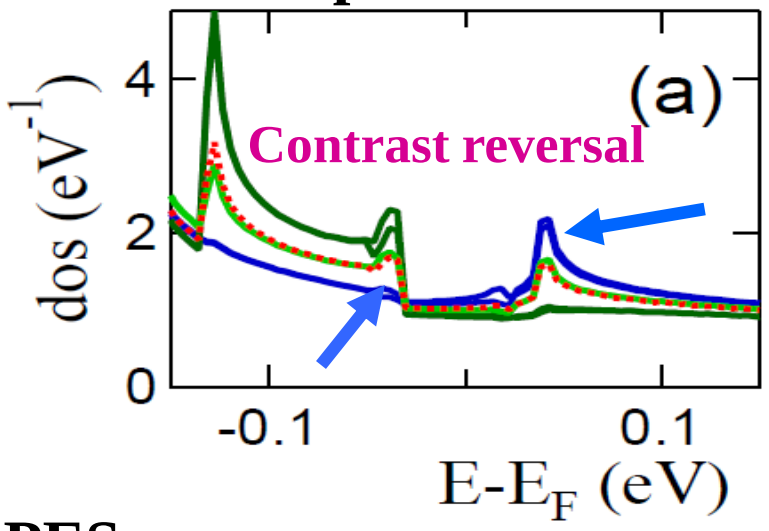
Charge Phase Diagram of Cuprates



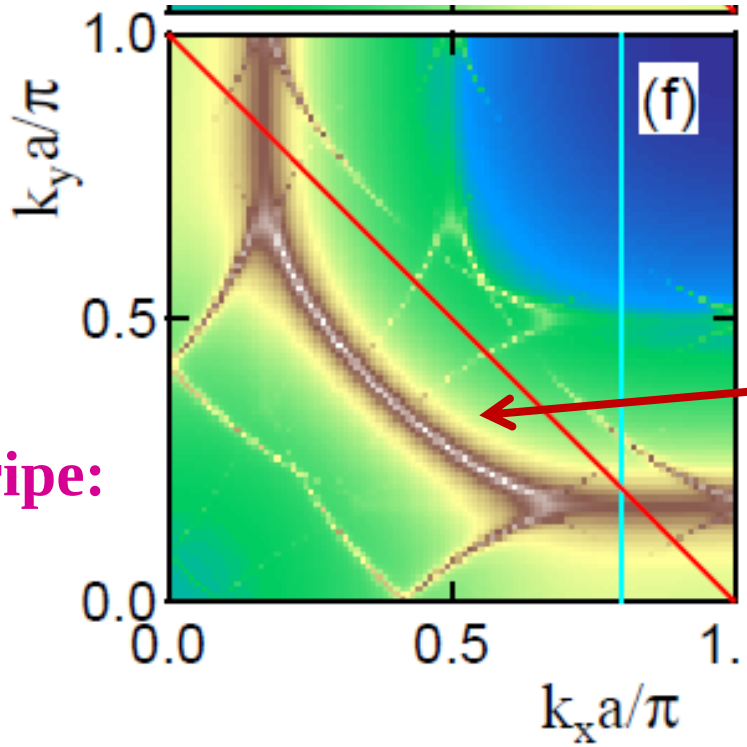

YBCO
Bi2212
Hg1201
Bi2201
qa/π
0.0
0.2
0.4
0.6
0.0
0.1
0.2
0.3
0.4
x



1D Stripe **STM**



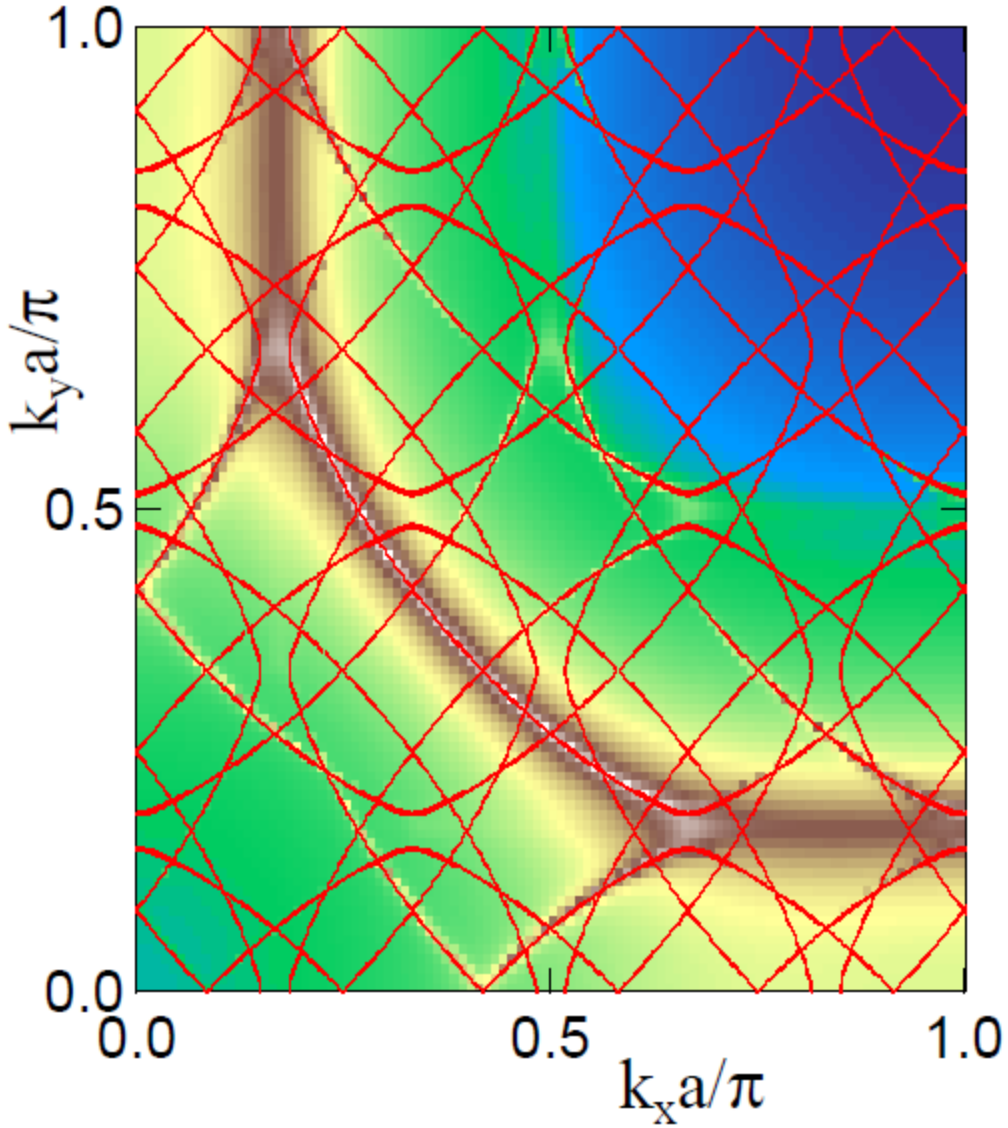
CDW: **ARPES**

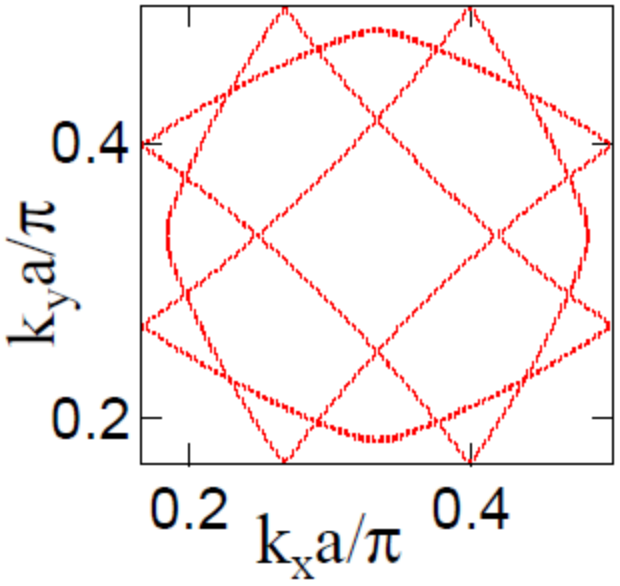


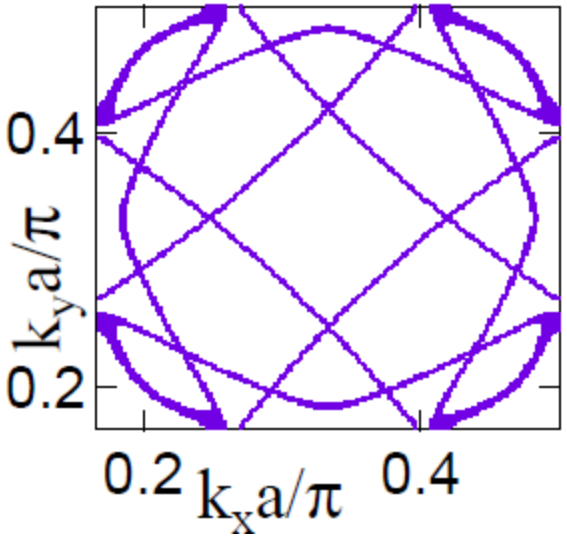
log scale

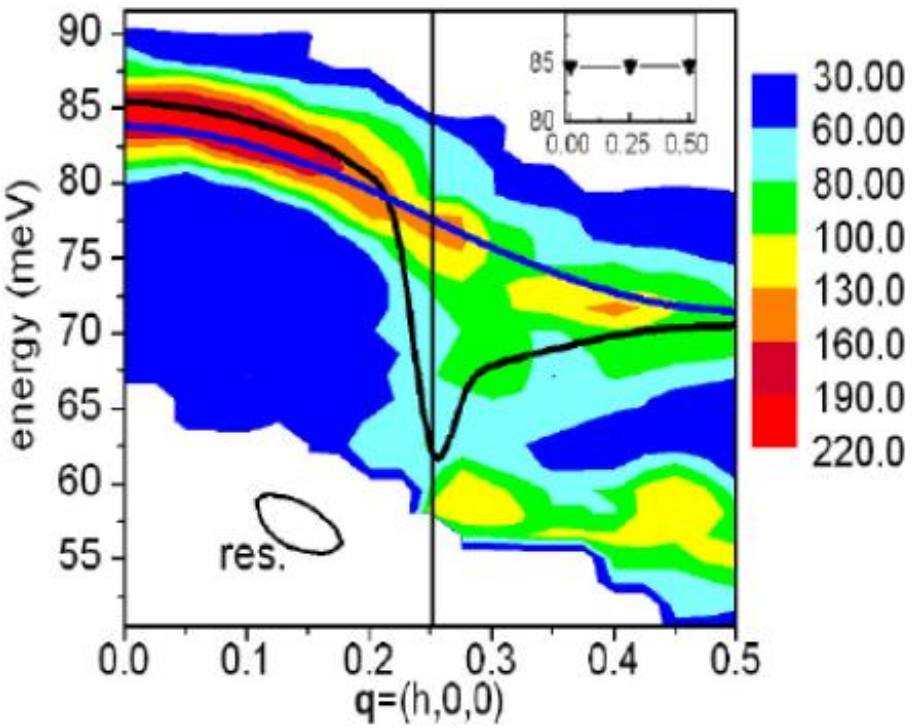
Fermi surface ~ QO

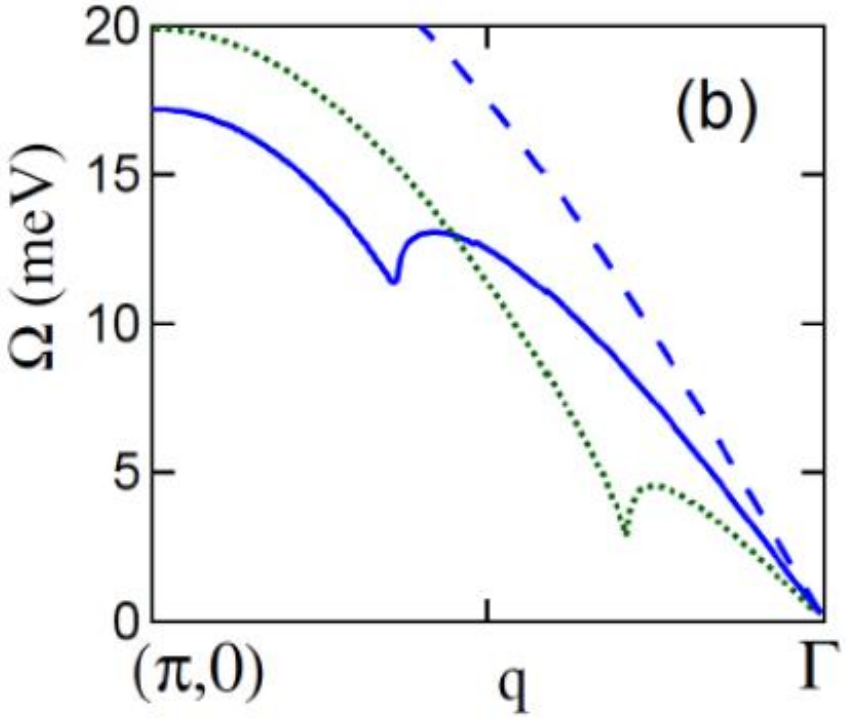
2D stripe:


1.0
0.5
0.0
0.0
0.5
1.0
$k_y a/\pi$
$k_x a/\pi$

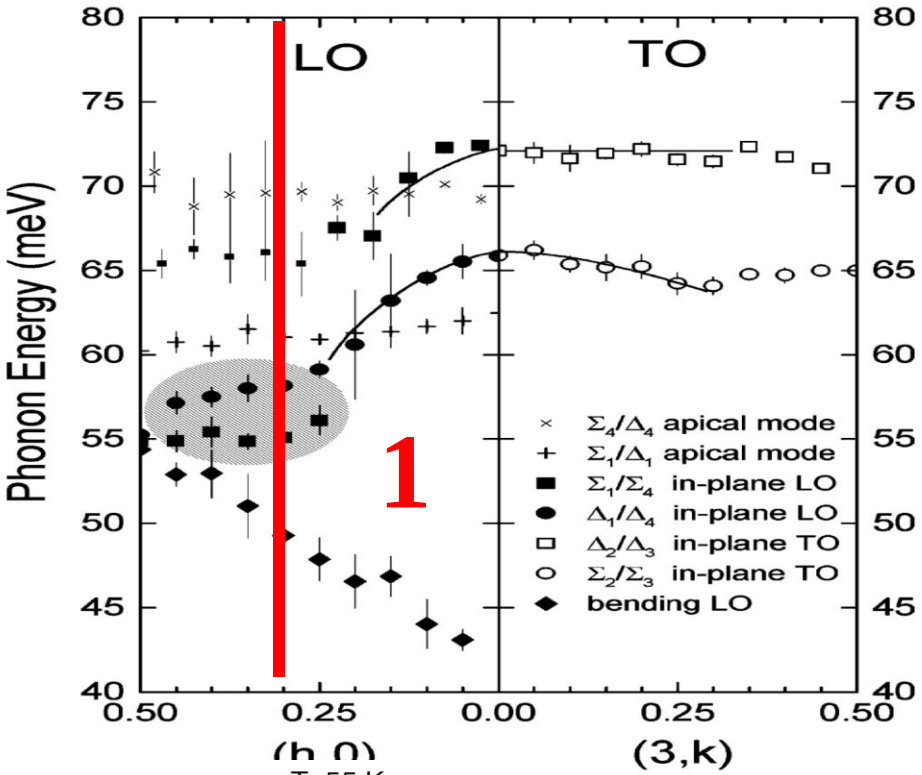

0.4
0.2
0.2
0.4
$k_y a/\pi$
$k_x a/\pi$

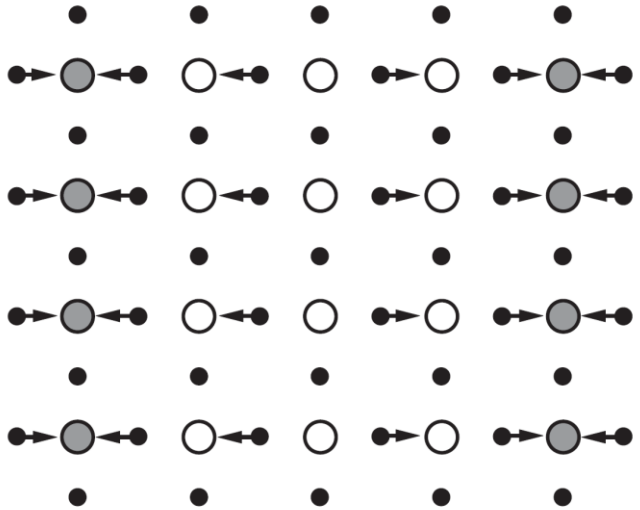

0.4
0.2
0.2
0.4
$k_y a/\pi$
$k_x a/\pi$

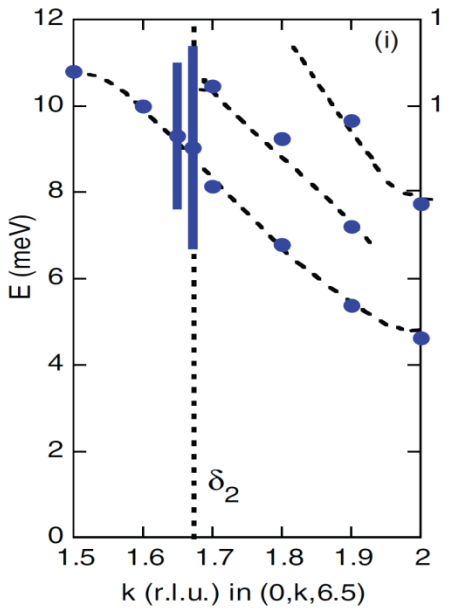


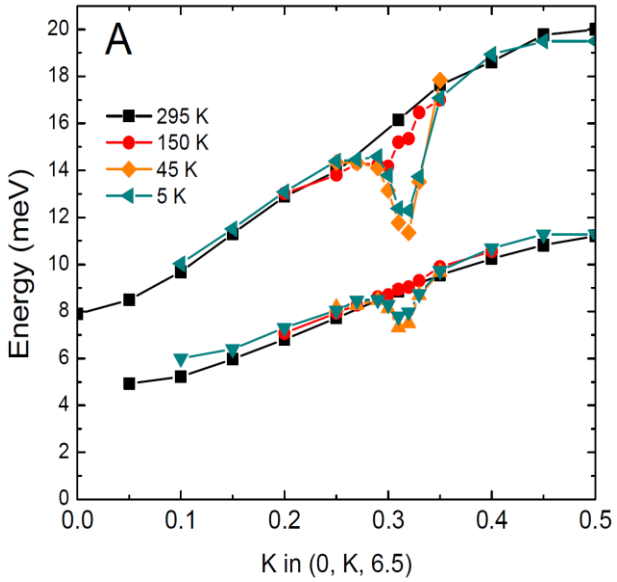


Bond-stretching phonon branch in La1.875Ba0.125CuO4
Nature 440, 1170 (2006)


LO
TO
Phonon Energy (meV)
1
Σ_4/Δ_4 apical mode
Σ_1/Δ_1 apical mode
Σ_1/Σ_4 in-plane LO
Δ_1/Δ_4 in-plane LO
Δ_2/Δ_3 in-plane TO
Σ_2/Σ_3 in-plane TO
bending LO
(h,0)
(3,k)




T=55 K
(i)
E (meV)
δ_2
k (r.l.u.) in (0,k,6.5)


A
295 K
150 K
45 K
5 K
Energy (meV)
K in (0, K, 6.5)

Conclusions

- Intermediate Correlations in Cuprates
- QP-GW captures most features
- Competing orders:
  - Nesting
  - SDWs
  - CDWs
    - Peierls distortion
  - …