Plasmons and bond-charge excitations in layered *t-J* model

Hiroyuki Yamase[1,2], Andres Greco[3], and Matias Bejas[3]

[1] *National Institute for Materials Science (NIMS), Tsukuba, Japan*

[2] *Graduate School of Science, Hokkaido University, Sapporo, Japan*

[3] *Instituto de Fisuca Rosario (UNR-CONICET), Rosario, Argentina*

We employ the layered *t-J* model with the long-range Coulomb interaction and study the charge excitation spectrum at leading order in a large-*N* formalism. We find that the spectrum is characterized by a dual structure in energy space [1]. In the low-energy region typically less than the superexchange coupling *J*, various kinds of bond-charge excitations are dominant [1]. In particular, *d*-wave bond-charge excitations exhibit softening along the direction (0,0)-(π,0) [2], which explains the charge ordering tendency observed in $Nd_{2-x}Ce_xCuO_4$ [3]. The doping dependence of the *d*-wave bond-charge excitations [4] can also capture the experimental observations [5,6]. In the high-energy region typically larger than *J*, on the other hand, the usual on-site charge excitations become dominant and yield plasmons [1]. The plasmons exhibit a strong dependence on out-of-plane momentum q_z as is well known in a layered system [7,8,9]. In particular, acoustic-like plasmons are realized for finite q_z and show a V-shaped dispersion around in-plane momentum (0,0) with a gap proportional to interlayer hopping t_z [9]. The acoustic-like plasmons well explain [10,11,12] the charge excitation spectra observed around (0,0) in various electron-doped systems $Nd_{2-x}Ce_xCuO_4$ [13,14,15,16], $La_{2-x}Ce_xCuO_4$ [16,17], $Sr_{1-x}La_xCuO_2$ [18], and hole-doped systems $La_{2-x}(Sr,Ba)_xCuO_4$ [12,19] and $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ [12]. Furthermore, plasmons have a big impact on the electron self-energy and reduce the quasiparticle residue substantially [20].

[1] M. Bejas, H. Yamase, and A. Greco, Phys. Rev. B **96**, 214513 (2017).
[2] H. Yamase, M. Bejas, and A. Greco, Europhys. Lett. **111**, 57005 (2015).
[3] E. H. da Silva Neto et al., Science **347**, 282 (2015).
[4] H. Yamase, M. Bejas, and A. Greco, Phys. Rev. B **99**, 014513 (2019).
[5] E. H. da Silva Neto et al., Science Advances **2**, e1600782 (2016).
[6] E. H. da Silva Neto et al., Phys. Rev. B **98**, 161114 (2018).
[7] D. Grecu, Phys. Rev. B **8**, 1958 (1973).
[8] A. L. Fetter, Ann. Phys. **88**, 1 (1974).
[9] A. Greco, H. Yamase, and M. Bejas, Phys. Rev. B **94**, 075139 (2016).
[10] A. Greco, H. Yamase, and M. Bejas, Commun. Phys. **2**, 3 (2019).
[11] A. Greco, H. Yamase, and M. Bejas, Phys. Rev. B **102**, 024509 (2020).
[12] A. Nag et al., Phys. Rev. Lett. **125**, 257002 (2020).
[13] K. Ishii et al., Phys. Rev. Lett. **94**, 207003 (2005).
[14] K. Ishii et al., Nat. Commun. **5**, 3714 (2014).
[15] W. S. Lee et al., Nat. Phys. **10**, 883 (2014).
[16] M. Hepting et al., Nature **563**, 374 (2018).
[17] J. Lin et al., npj Quantum Materilas **5**, 4 (2020).
[18] G. Dellea et al., Phys. Rev. B **96**, 115117 (2017).
[19] K. Ishii et al., Phys. Rev. B **96**, 115148 (2017).
[20] H. Yamase, M. Bejas, and A. Greco, Phys. Rev. B **104**, 045141 (2021).

Renewed interests in charge orders

YBCO, Bi2201, Bi2212, Hg1201

charge order (no magnetic order)

$0.08 \lesssim p \lesssim 0.16$

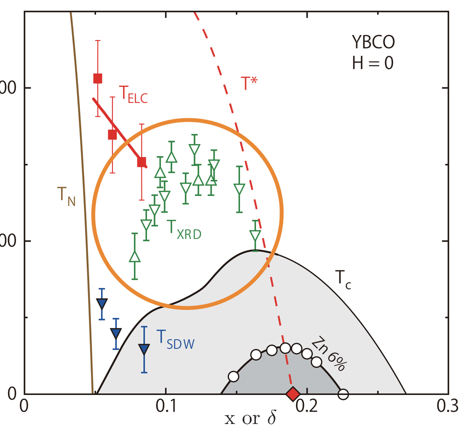
enhanced at $\delta \approx 0.11 - 0.12$

$T \lesssim 150\,\mathrm{K} < T^*$

$\mathbf{q} = (2\pi\eta, 0)$

$\eta \approx 0.30$

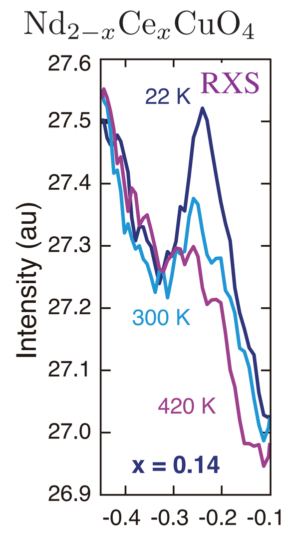
Ghiringhelli *et al.*, Science **337**, 821 (2012)
Chang *et al.*, Nat. Phys. **8**, 871 (2012)
Comin *et al.*, Science **343**, 390 (2014)
Hashimoto *et al.*, PRB **89**, 220511 (2014)
Tabis *et al.*, Nat. Commin. **5**, 5875 (2014)



Haug *et al.*, NJP **12**, 105006 (2010)
Badoux *et al.*, Nature **531**, 210 (2016)

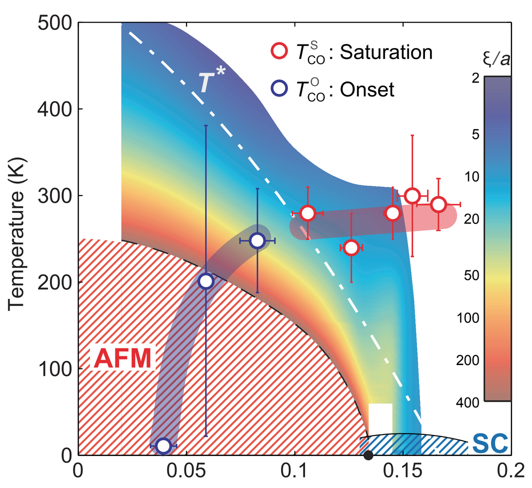
Charge-order tendency in electron-doped cuprates

$Nd_{2-x}Ce_xCuO_4$



$\mathbf{q} = (2\pi\eta, 0)$ $\eta \approx 0.24$

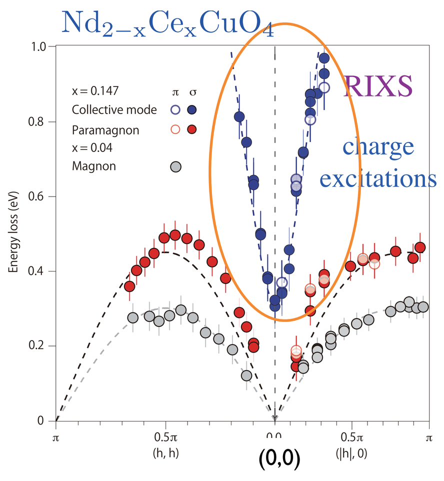
da Silva Neto *et al.*, Science **347**, 282 (2015)



da Silva Neto et al., Science Advances **2**, 16700782 (2016)

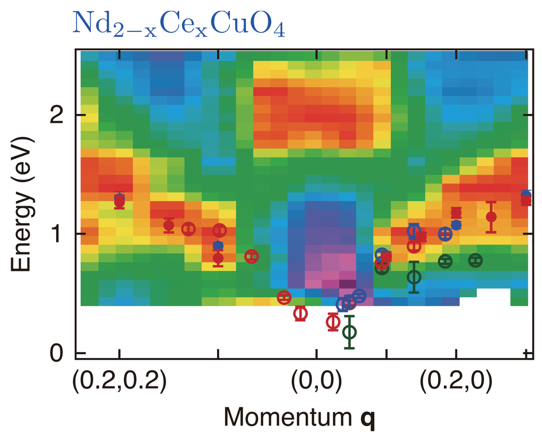
High-energy charge excitations

$Nd_{2-x}Ce_xCuO_4$



Lee et al., Nat. Phys. **10**, 883 (2014)

$Nd_{2-x}Ce_xCuO_4$



Ishii et al., Phys. Rev. Lett. **94**, 207003 (2005)
Ishii et al., Nat. Commun. **5**, 3714 (2014)

$La_{2-x}Ce_xCuO_4$ $Sr_{1-x}La_xCuO_2$

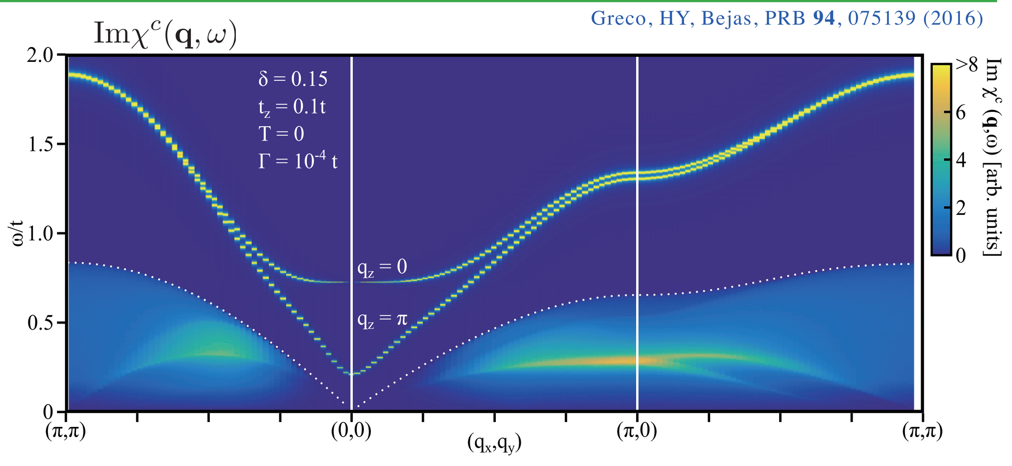
Hepting et al., Nature **563**, 374 (2018)
Lin et al., npj Quantum Materials **5**, 4 (2020)
Della et al., Phys. Rev. B **96**, 115117 (2017)

$La_{2-x}(Sr,Ba)_xCuO_4$
$Bi_2Sr_{2-x}La_xCuO_{6+\delta}$

Ishii et al., Phys. Rev. B **96**, 115148 (2017)
Nag et al., Phys. Rev. Lett. **125**, 257002 (2020)

On-site charge excitations: Plasmons

Greco, HY, Bejas, PRB **94**, 075139 (2016)



particle-hole continuum below $\omega \sim 0.8t$
no charge-order tendency

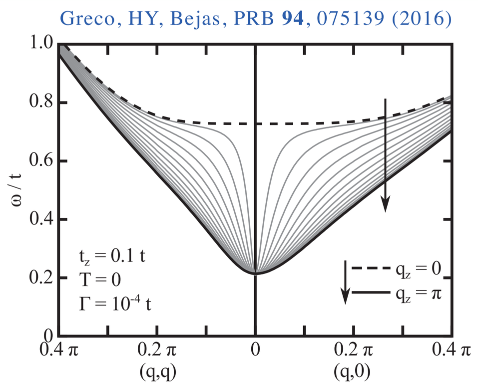
above the continuum : plasmons
$q_z = 0$: very flat dispersion around $\mathbf{q}_\parallel = (0,0)$
$q_z = \pi$: strong dispersion around $\mathbf{q}_\parallel = (0,0)$

optics, EELS: $q_z = 0$
large gap $\sim t$
Nuecker *et al.*, PRB **39**, 12 379 (1989)
Romberg *et al.*, Z. Phys. B **78**, 367 (1990)

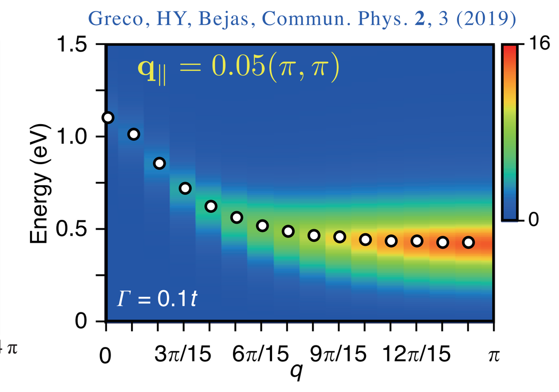
RIXS: finite q_z
small gap $\propto t_z$

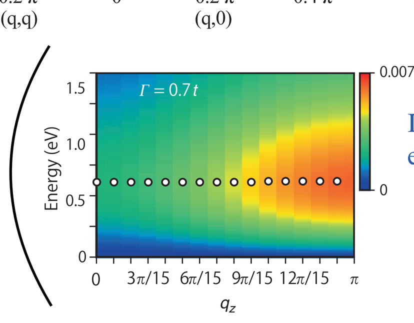
Characteristic *qz* dependence

Greco, HY, Bejas, PRB **94**, 075139 (2016)



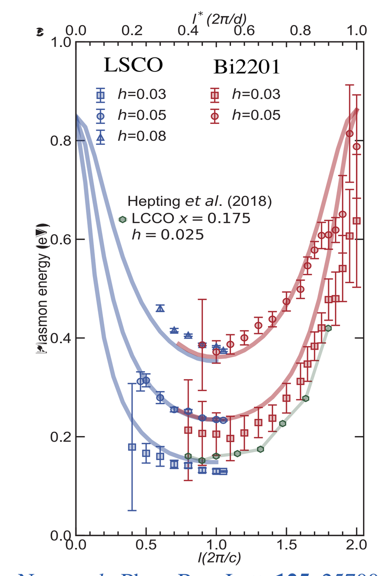
Greco, HY, Bejas, Commun. Phys. **2**, 3 (2019)



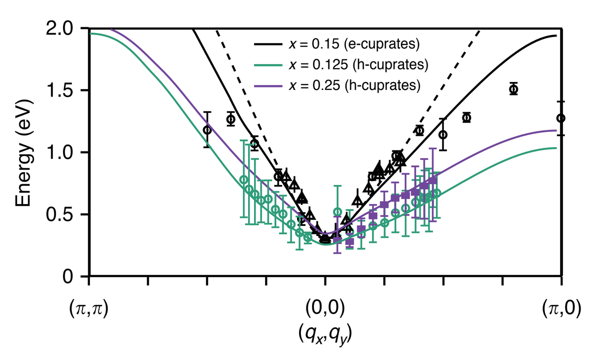


Incoherent particle-hole excitations
no qz dependence

Comparison with RIXS data



Nag et al., Phys. Rev. Lett. **125**, 257002 (2020)



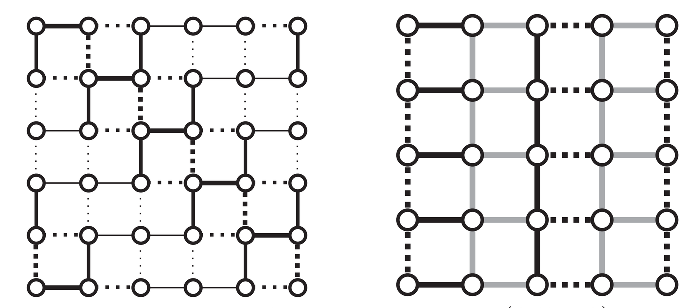
Lee et al., Nat. Phys. **10**, 883 (2014)
Ishii et al., Nat. Commun. **5**, 3714 (2014)
Ishii et al., Phys. Rev. B **96**, 115148 (2017)
Greco, HY, Bejas, Commun. Phys. **2**, 3 (2019)

l dependence in LCCO

M. Hepting et al., Nature **563**, 374 (2018)

d-wave bond-charge order

Relevant to electron-doped cuprates



$\mathbf{q} = (0.8\pi, 0.8\pi)$ $\mathbf{q} = (0.5\pi, 0)$

$$\Delta(\mathbf{q}) = \sum_{\mathbf{k}\,p} \gamma(\mathbf{k}) \langle f^\dagger_{\mathbf{k}-\frac{\mathbf{q}}{2}p} f_{\mathbf{k}+\frac{\mathbf{q}}{2}p} \rangle$$

$\gamma(\mathbf{k}) = (\cos k_x - \cos k_y)/2$

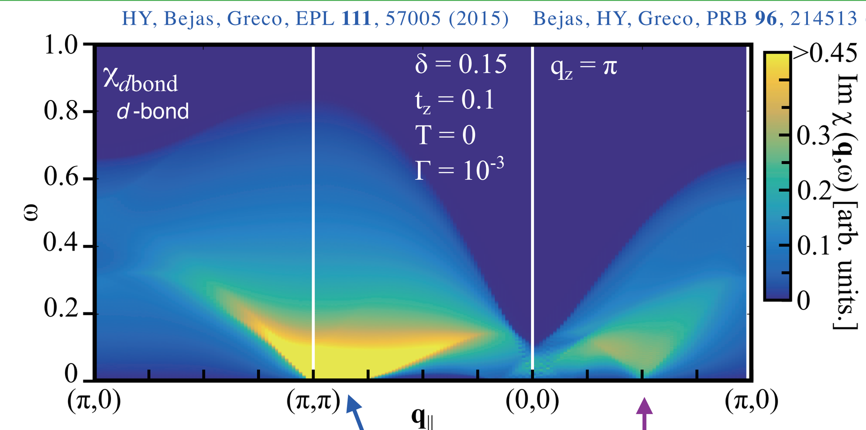
bond : Cu-Cu

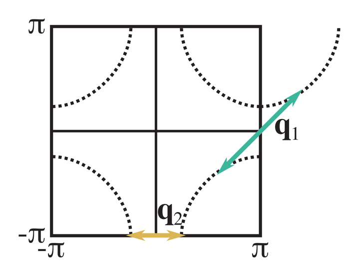
bond order : charge-density wave at oxygen sites

Bejas, Greco, H.Y., NJP **16**, 123002 (2014)
H.Y., Bejas, Greco, EPL **111**, 57005 (2015)

Excitation spectrum of *d*-bond

HY, Bejas, Greco, EPL **111**, 57005 (2015) Bejas, HY, Greco, PRB **96**, 214513 (2017)



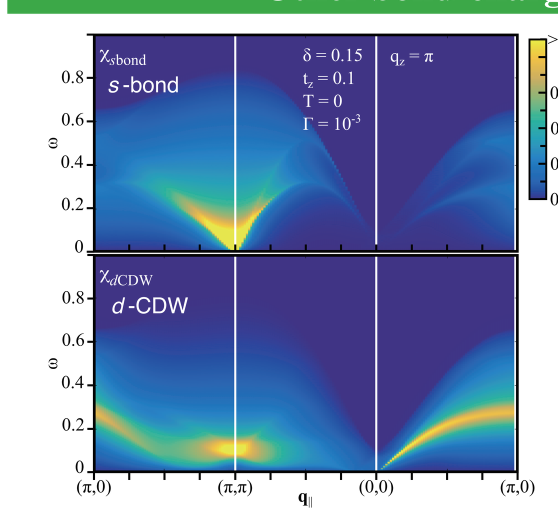


$\mathbf{q}_1 \approx 0.8(\pi,\pi)$ — prediction

$\mathbf{q}_2 \approx 0.5(\pi,0)$ — explains the RXS data in electron-doped cuprates
da Silva Neto *et al.*, Science **347**, 282 (2015)

Other bond-charge excitations

Bejas, HY, Greco, PRB **96**, 214513 (2017)



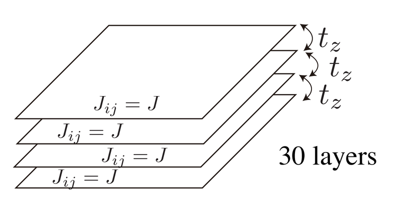
large low-energy weight around $\mathbf{q} = (\pi,\pi)$

large low-energy weight around $\mathbf{q} = (\pi,\pi)$
gapless dispersion along $(0,0)-(\pi,0)$ direction
essentially no qz dependence

Layered *t-J* model with long-range Coulomb

t-J-V model

$$H = -\sum_{i,j,\sigma} t_{ij}\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma} + \sum_{\langle i,j\rangle} J_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}n_i n_j\right) + \frac{1}{2}\sum_{i,j} V_{ij} n_i n_j$$



long-range Coulomb interaction V_{ij}

$\nabla\phi(\mathbf{r}) = -\rho(\mathbf{r})/\epsilon$

$$\epsilon_\parallel\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right) + \epsilon_\perp \frac{\partial^2\phi}{\partial z^2} = -\rho(\mathbf{r})$$

$$\frac{1}{2}\sum_{ij} V_{ij} n_i n_j = \frac{1}{2}\sum_{\mathbf{q}} V(\mathbf{q}) n_{\mathbf{q}} n_{-\mathbf{q}}$$

$$V(\mathbf{q}) = \frac{V_c}{A(q_x,q_y) - \cos q_z} \qquad V_c = e^2 d (2\epsilon_\perp a^2)^{-1}$$

$$A(q_x,q_y) = \frac{\tilde{\epsilon}}{(a/d)^2}(2 - \cos q_x - \cos q_y) + 1 \qquad \tilde{\epsilon} = \epsilon_\parallel/\epsilon_\perp$$

Becca et al., PRB **54**, 12443 (1996)

Path integral representation for Hubbard operators

Hubbard operators — Foussats et al., PRB **70**, 205123 (2004)

$$\tilde{c}^\dagger_{i\sigma} = X_i^{\sigma 0} \quad \tilde{c}_{i\sigma} = X_i^{0\sigma} \quad S_i^+ = X_i^{\uparrow\downarrow} \quad S_i^- = X_i^{\downarrow\uparrow} \quad n_i = X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow}$$

spin: *N* channels

$$H = -\frac{1}{N}\sum_{i,j,p} t_{ij} X_i^{p0} X_j^{0p} + \frac{J}{2N}\sum_{\langle i,j\rangle,pp'}\left(X_i^{pp'}X_j^{p'p} - X_i^{pp}X_j^{p'p'}\right) + \frac{1}{N}\sum_{\langle i,j\rangle,pp'} V_{ij} X_i^{pp} X_j^{p'p'} - \mu\sum_{i,p} X_i^{pp}$$

Path integral

$$L_E = \frac{1}{2}\sum_{i,p}\frac{\left(\dot{X}_i^{0p} X_i^{p0} + \dot{X}_i^{p0} X_i^{0p}\right)}{X_i^{00}} + H$$

$$X_i^{00} + \sum_p X_i^{pp} - \frac{N}{2} = 0 \qquad X_i^{pp'} - \frac{X_i^{p0}X_i^{0p'}}{X_i^{00}} = 0$$

Definition of bosonic fields

V-term: rewrite with X_i^{00}

eliminate $X_i^{pp'}$

three variables: $X_i^{00}, X_i^{p0}, X_i^{0p}$

$\lambda_i = \lambda_0 + \delta\lambda_i$

$X_i^{00} = N r_0 (1 + \delta R_i)$

$f^\dagger_{ip} = \frac{1}{\sqrt{N r_0}} X_i^{p0}$

$f_{ip} = \frac{1}{\sqrt{N r_0}} X_i^{0p}$

Lagrange multipliers

$$\frac{J}{2N}\sum_{\langle i,j\rangle,p,p'}\frac{f^\dagger_{ip}f_{jp'}}{1+\delta R_i}\frac{f^\dagger_{jp'}f_{ip}}{1+\delta R_j}$$

$$\Delta_{ij} = J\sum_p \frac{f^\dagger_{jp}f_{ip}}{\sqrt{(1+\delta R_i)(1+\delta R_j)}} = \Delta(1 + r_i^\eta + i A_i^\eta)$$

$$\delta X^a = (\delta R,\ \delta\lambda,\ r^x,\ r^y,\ A^x,\ A^y)$$

6 bosonic fields: onsite charge (δR, $\delta\lambda$); Re(bond charge) (r^x, r^y); Im(bond charge) (A^x, A^y)

$$D^{(0)}_{ab}(\mathbf{q}, i\omega_n) = \frac{1}{N}\begin{pmatrix} \frac{\delta^2}{2}(V(\mathbf{q}) - J(\mathbf{q})) & \frac{\delta}{2} & 0 & 0 & 0 & 0 \\ \frac{\delta}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{4\Delta^2}{J} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{4\Delta^2}{J} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{4\Delta^2}{J} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{4\Delta^2}{J} \end{pmatrix}^{-1} \qquad J(\mathbf{q}) = \frac{J}{2}(\cos q_x + \cos q_y)$$

Physical meaning

When *J*=0,
$\delta X^a = (\delta R, \delta\lambda)$
on-site charge fluctuations only → plasmons!

When $J \neq 0$
bond-charge fluctuations become active

on-site charge: charge-density wave at copper sites
bond charge: charge-density wave at oxygen sites

Large-*N* expansion

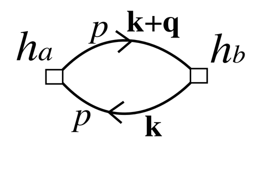
fermionic field f_{ip} — fermi-bose interactions

$$G(\mathbf{k}, i\nu_n) = \frac{1}{i\nu_n - \varepsilon_{\mathbf{k}}} = O(1)$$

At leading order

$$D^{-1}_{ab}(\mathbf{q}, i\omega_n) = [D^{(0)}_{ab}(\mathbf{q}, i\omega_n)]^{-1} - \Pi_{ab}(\mathbf{q}, i\omega_n)$$

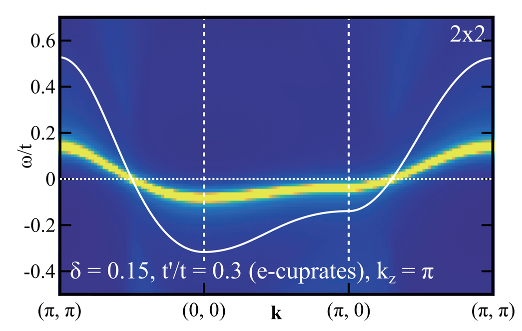
$O(N)$ $O(N)$



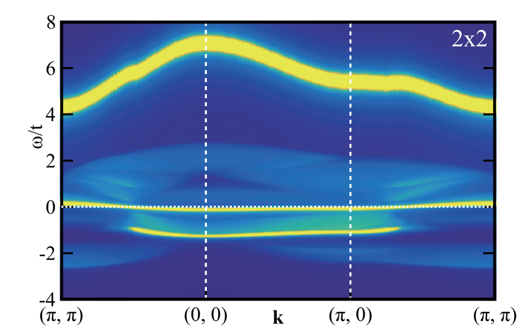
favoring collective charge fluctuations

Electron self-energy from charge fluctuations

HY, Bejas, Greco, PRB **104**, 045141 (2021)



isotropic suppression of the QP band width
QP residue Z=0.2-0.3



Mainly two emergent bands
band around $\omega/t \approx -1$ due to plasmons around $\mathbf{q} \approx \mathbf{0}$

Effect of plasmons is dominant
Effect of bond-charge is very weak on electron self-energy

Summary

Charge dynamics in cuprates
Study of layered *t-J* model with long-range Coulomb interaction

	electron-doped cuprates	hole-doped cuprates
low energy (< *J*=0.3*t*)	• *d*-wave bond-charge order near $\mathbf{q} = 0.5(\pi,0)$ explain experimental data • various bond-charge orders near $\mathbf{q} = (\pi,\pi)$ prediction	*Controversial. Bond-charge?*
high energy (> *J*=0.3*t*)	plasmons: gapped V-shaped dispersion around **q**=(0,0) explain experimental data	plasmons: gapped V-shaped dispersion around **q**=(0,0) explain experimental data

Dual structure of charge dynamics in energy space
Big self-energy corrections from plasmons

contact: yamase.hiroyuki@nims.go.jp