The electronic structure within the norm-conserving cluster perturbation theory

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СИБИРСКИЙ ФЕДЕРАЛЬНЫЙ УНИВЕРСИТЕТ
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Grants NSh-1044.2012.2, and MK-1168.2012.2

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→ **GTB**

→ **DCA**

→ **CPT**

→ **CDMFT**

→ **V-CPT**

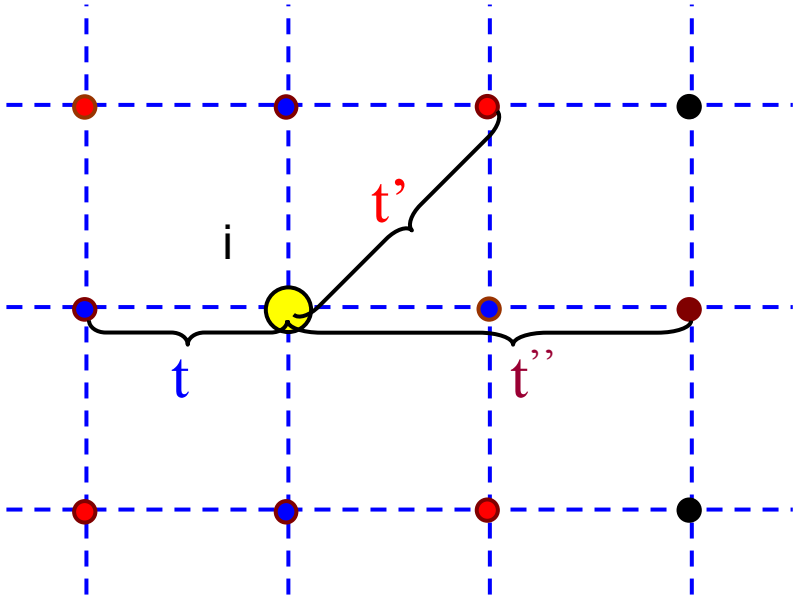
The Hubbard model

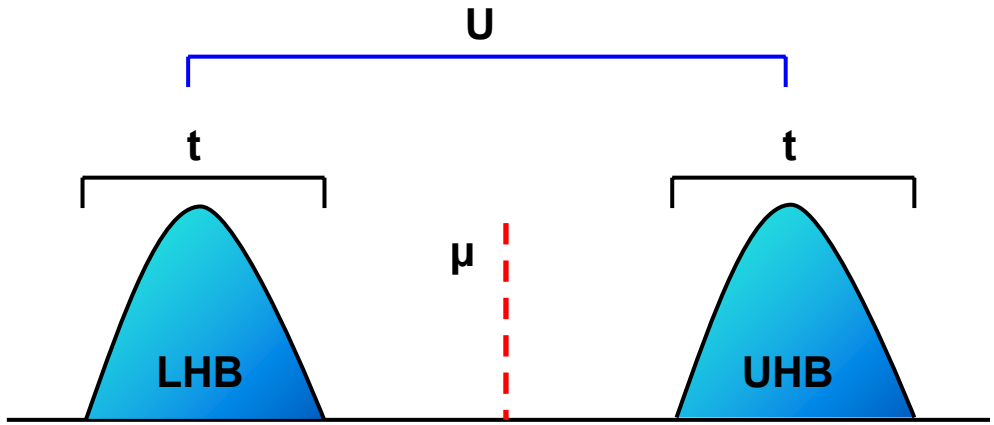
The one-band two-dimensional Hubbard model

$$H = H_0 + H_1, \tag{1}$$

$$H_0 = \sum_{i\sigma} \left\{ (\varepsilon - \mu) n_{i\sigma} + \frac{U}{2} n_{i\sigma} n_{i\bar{\sigma}} \right\}, \tag{2}$$

$$H_1 = \sum_{i \neq j, \sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma}. \tag{3}$$



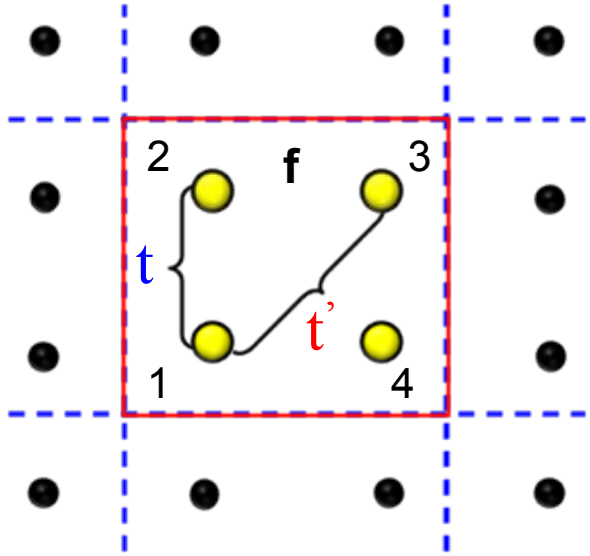


The Hubbard model for cluster 2x2

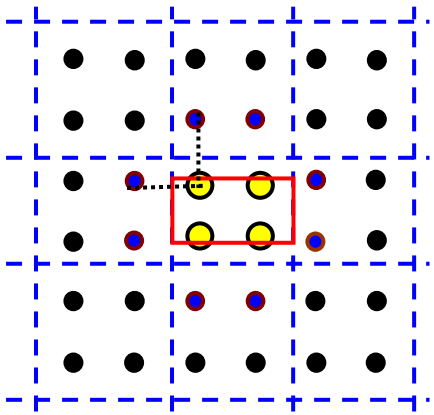
$$H = \sum_f H_0^c(f) + \sum_{f \neq g} H_1^c(f,g), \quad (4)$$

$$H_1^c = H_t^c + H_{t'}^c + H_{t''}^c,$$

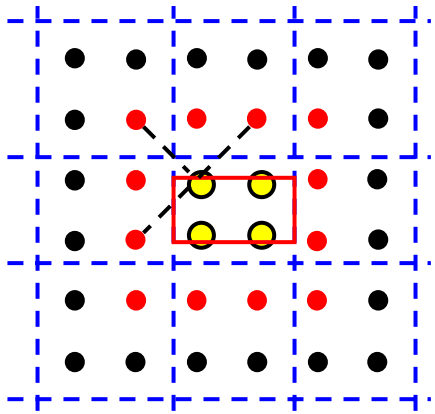
H_0^c ⇒



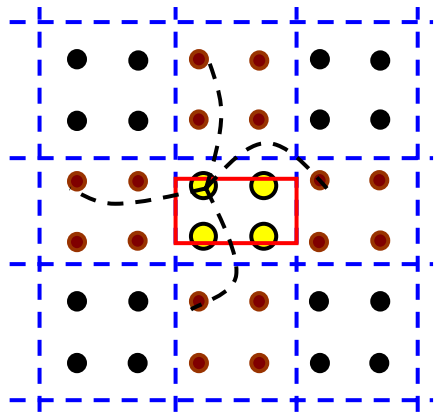
H_t^c



$H_{t'}^c$



$H_{t''}^c$



Exact diagonalization

$$H_0^c(f) \rightarrow \left\{\varepsilon_p, |p\rangle \equiv |m, N_e\rangle\right\}$$

$$|p\rangle = \sum_n C_n |\varphi_n\rangle \quad (5)$$

Hubbard X-operators

$$X_f^\alpha \equiv X_f^{pq} = |p><q| = |m, N_e><m', N_e'| \quad (6)$$

$$a_{f\sigma i} = \sum_\alpha \gamma_{i\sigma}(\alpha) X_f^\alpha, \qquad \gamma_{i\sigma}(\alpha) = \langle m', N_e - 1 | a_{i\sigma} | m, N_e \rangle \quad (7)$$

where f is the cluster index, i is the site index (1, 2, 3, 4), σ is an electron spin at site.

The sum rule

$$[a_{f\sigma i}, a_{f\sigma i}^+]_+ = 1$$

$$\sum_\alpha |\gamma_{i\sigma}(\alpha)|^2 F(\alpha) \equiv f, \quad \Longrightarrow \quad f > 0.99$$

$$F(\alpha) = \langle X^{pp} \rangle + \langle X^{qq} \rangle$$

Hubbard-I $\Longrightarrow$

$$D^{-1}\left(\tilde{k},\omega\right)=\left(D^{0}(\omega)\right)^{-1}-T\left(\tilde{k}\right) \tag{8}$$

$$D_{nm}\left(\tilde{k},\omega\right)=\langle\langle X^{n}_{\tilde{k}} \mid X^{m+}_{\tilde{k}}\rangle\rangle_{\omega}$$

$$D^{0}_{nm}(\omega)=\frac{F_{n}}{\omega-\Omega_{n}}\delta_{n,m}$$

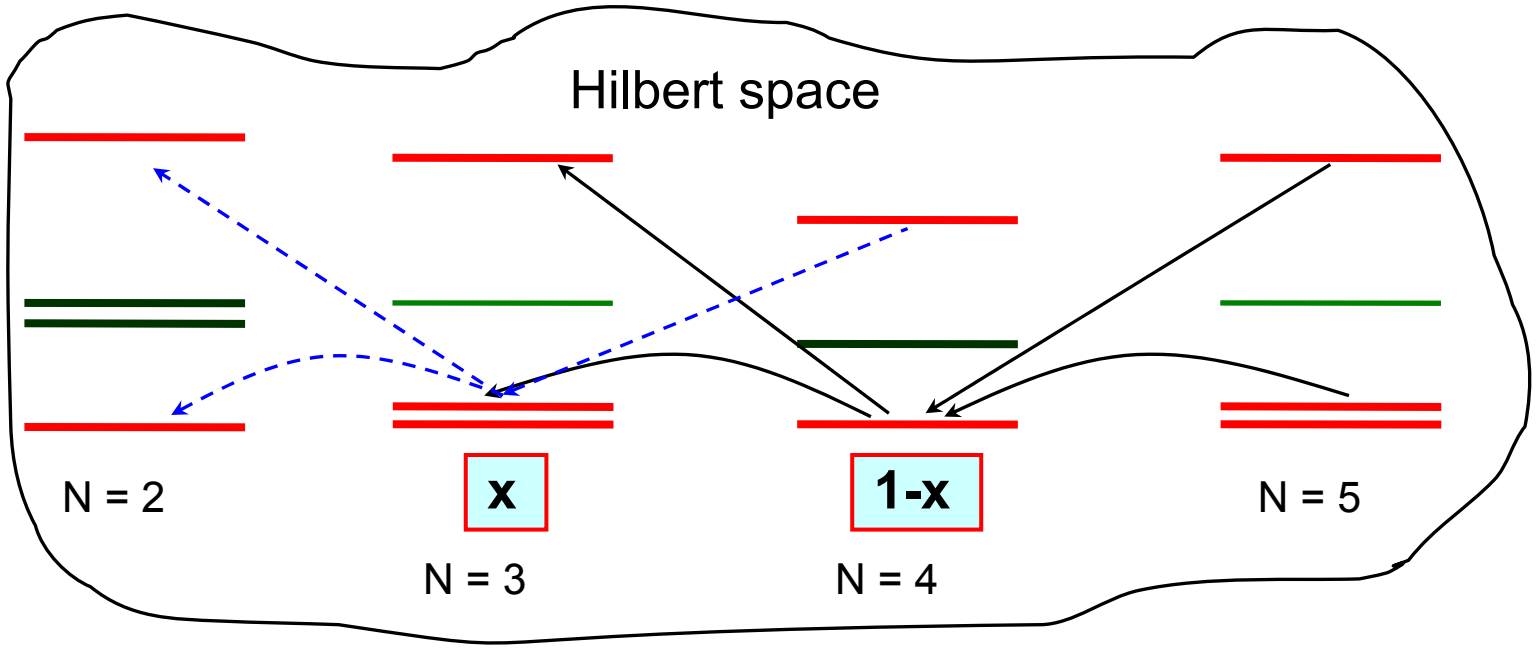
$$F_{n}\equiv F(pq)=\langle X^{pp}\rangle+\langle X^{qq}\rangle$$

$$G_{\sigma}(\boldsymbol{k},\omega)=\frac{1}{N_{c}}\sum_{nm}\sum_{i,j=1}^{N_{c}}\gamma_{\sigma i}(n)\gamma_{\sigma j}(m)\,e^{-i\boldsymbol{k}(\boldsymbol{r}_{i}-\boldsymbol{r}_{j})}D_{nm}\left(\boldsymbol{k},\omega\right) \tag{9}$$

$$A_{\sigma}(k,\omega)=-\frac{1}{\pi}\lim_{\eta\to+0}\left(\mathrm{Im}\,G_{\sigma}(k,\omega+i\eta+\mu)\right) \tag{10}$$

$$\int d\omega\; A_{\sigma}\left(k,\omega\right)=\left\langle\left[a_{k\sigma},a^{+}_{k\sigma}\right]_{+}\right\rangle=f \tag{11}$$

The scheme of doping



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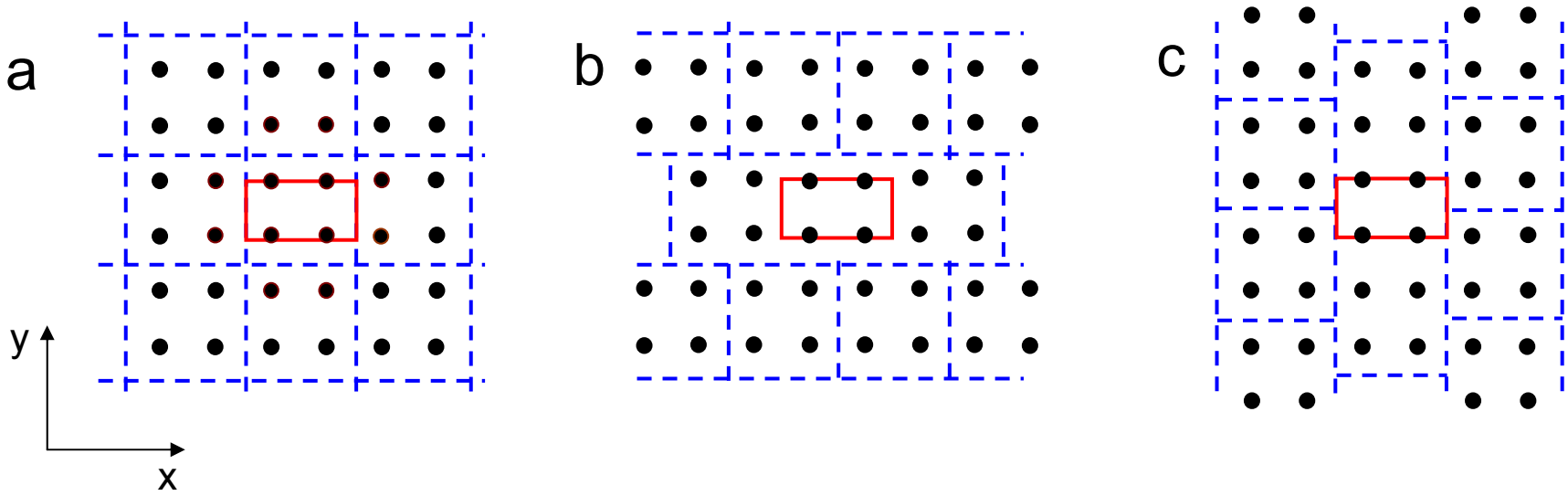
NC-CPT method: the tiling



$$T_{\alpha\beta}(\boldsymbol{k}) = \frac{1}{2}\left(T^{\mathrm{b}}_{\alpha\beta}(\boldsymbol{k}) + T^{\mathrm{c}}_{\alpha\beta}(\boldsymbol{k})\right), \qquad (12)$$

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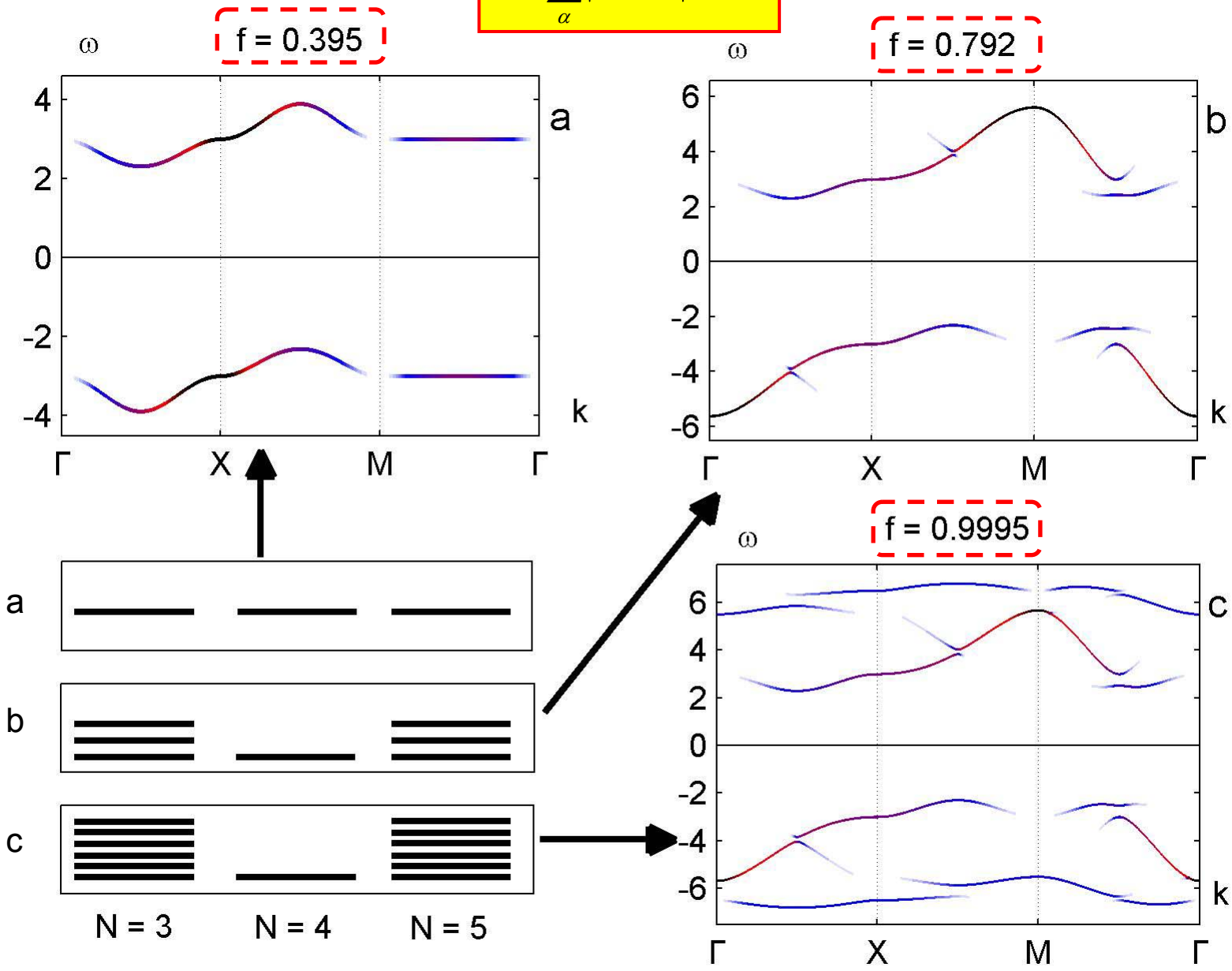
NC-CPT method: f-factor

$$f = \sum_{\alpha} |\gamma_{i\sigma}(\alpha)|^2 F(\alpha)$$



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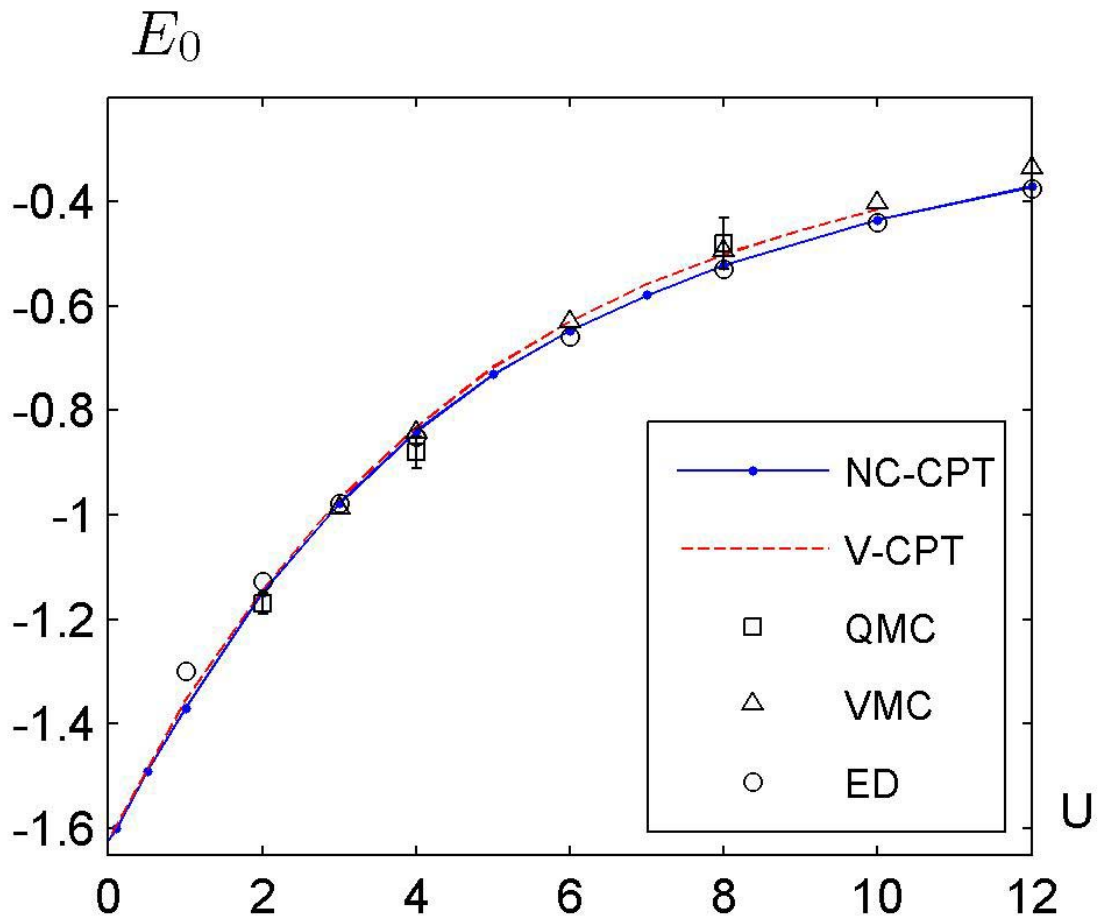
The ground state energy



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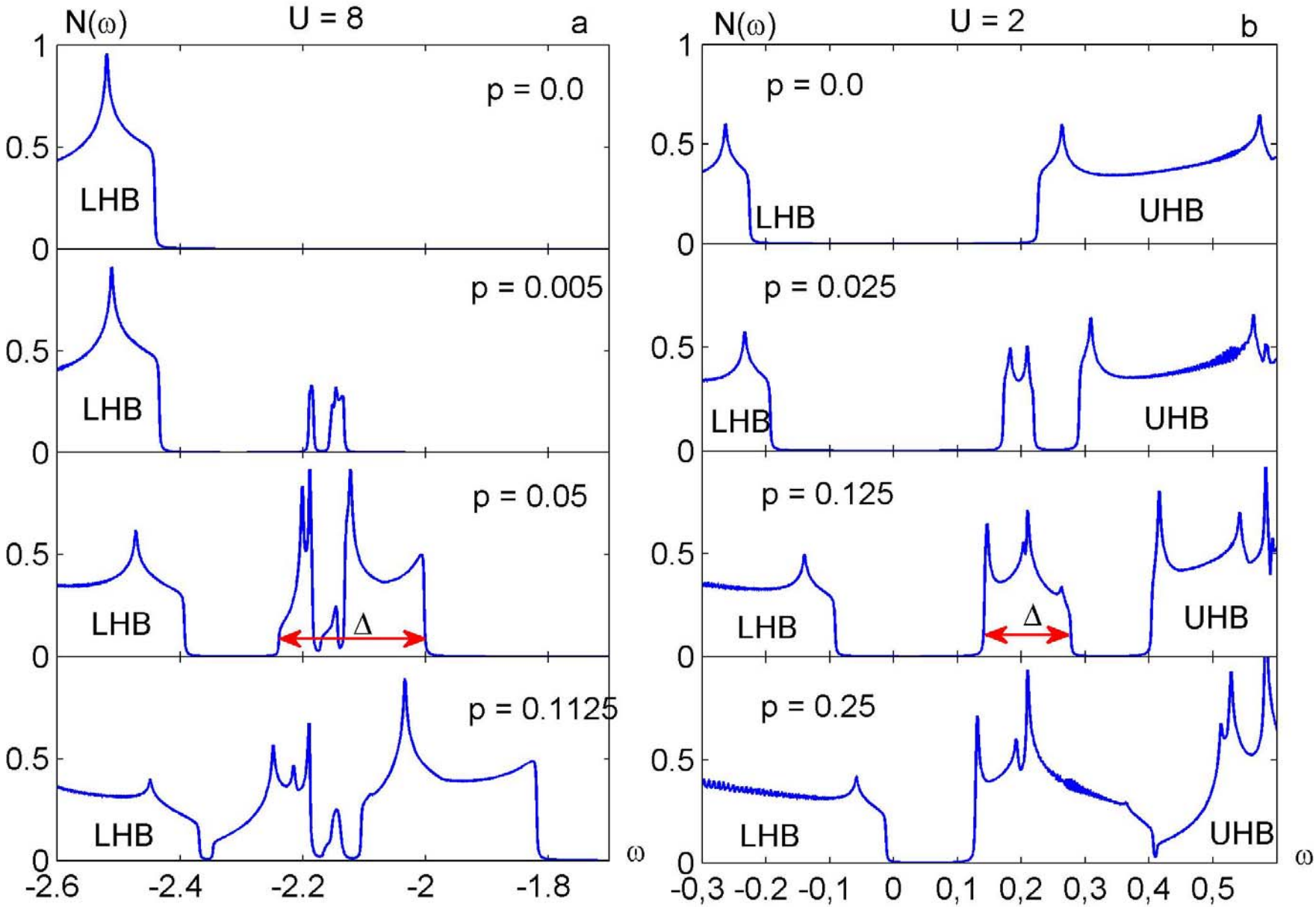
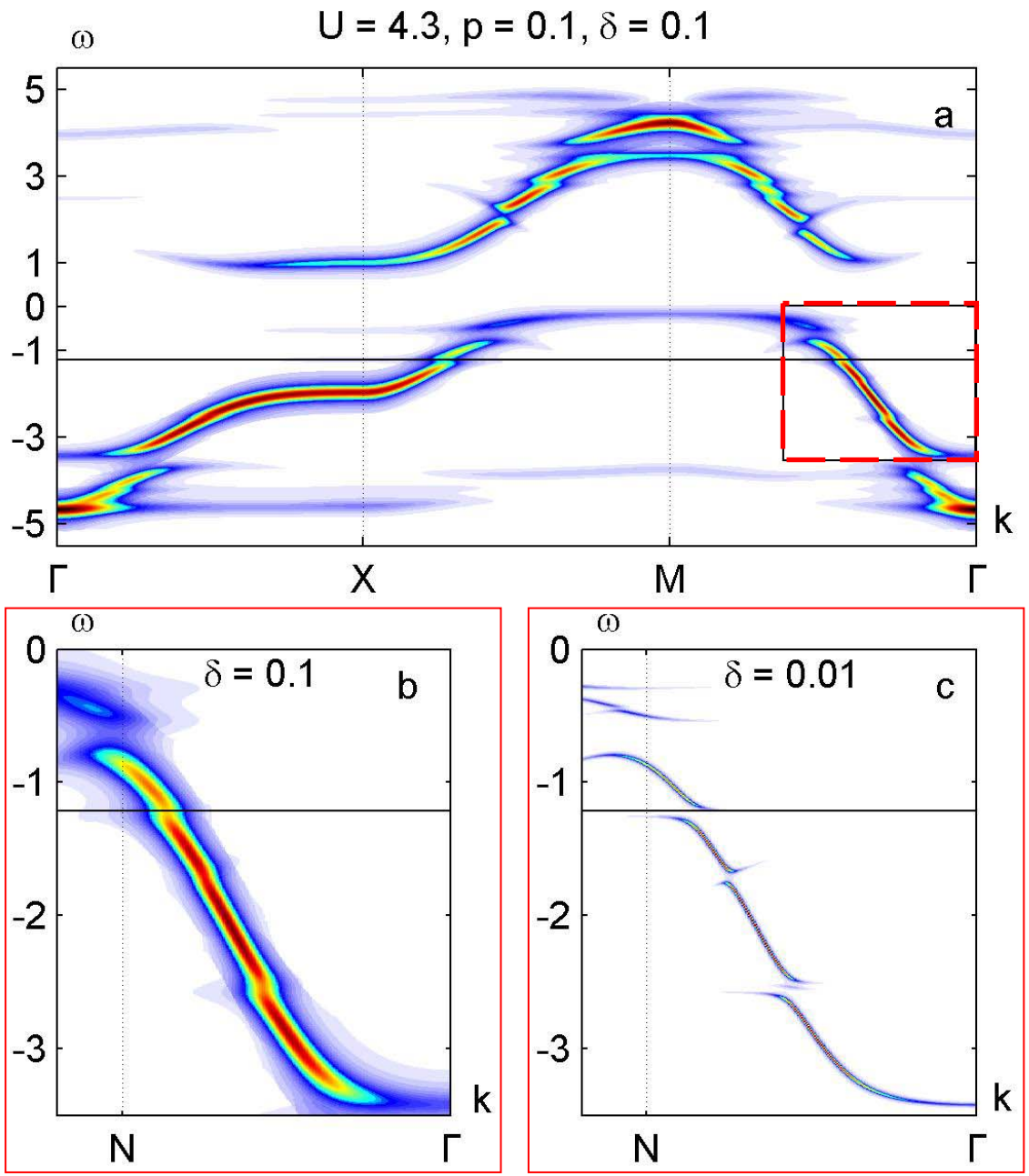
ED G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B 42, 6877 (1990)
QMC J. E. Hirsch, Phys. Rev. B 31, 4403 (1985)
V-CPT C. Dahnken, M. Aichhorn, W. Hanke and et al., Phys. Rev. B 70, 245110 (2004)

In-gap states. t'=t"=0



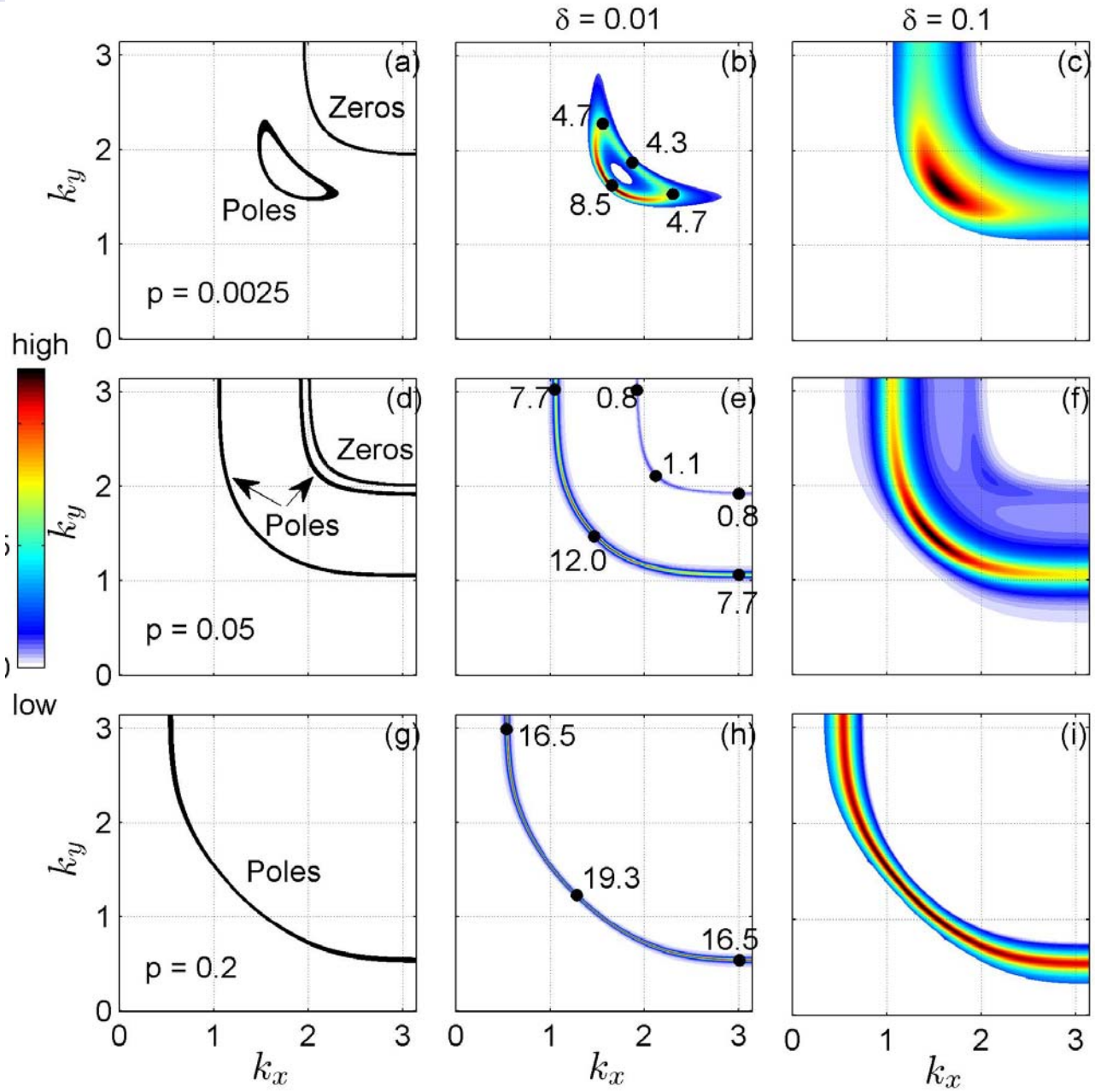
Dispersion for U = 4.3t, t' = 0.13t, t'' = -0.16t

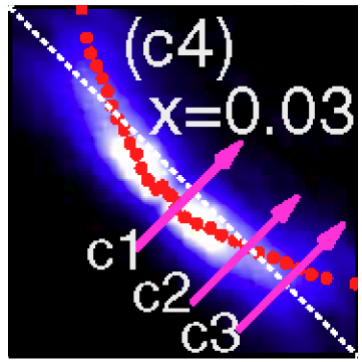


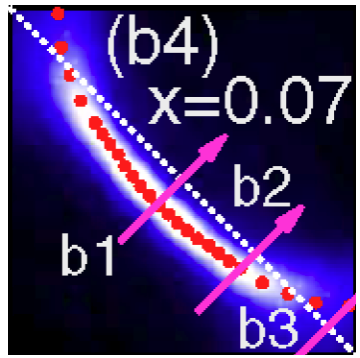
Spectral weight maps. U=4.3t, t'=0.13t, t"=-0.16t

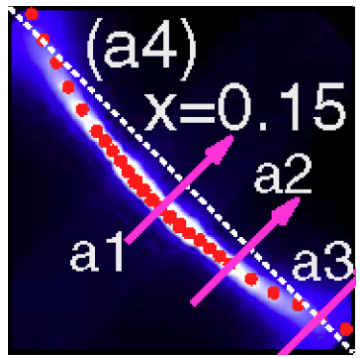
Yoshida T., PRL103, 037004 (2009)

δ = 20 meV / 250 = **0.08** t





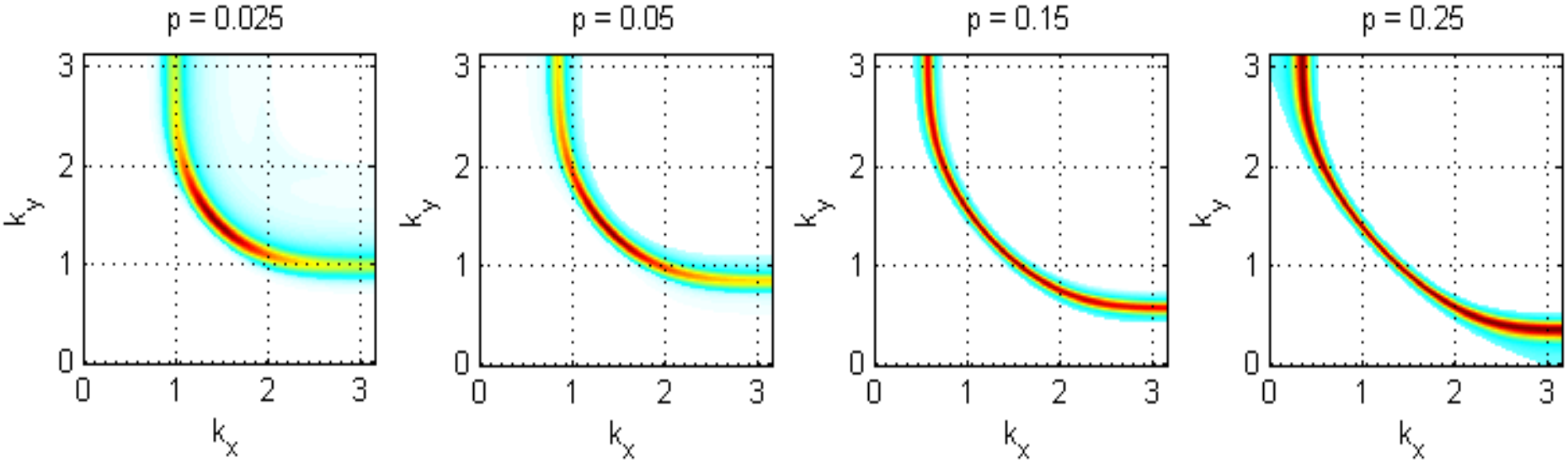


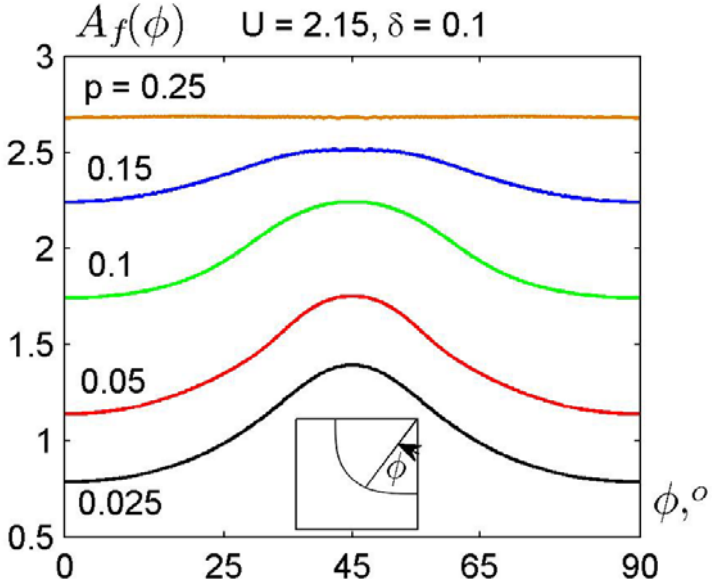


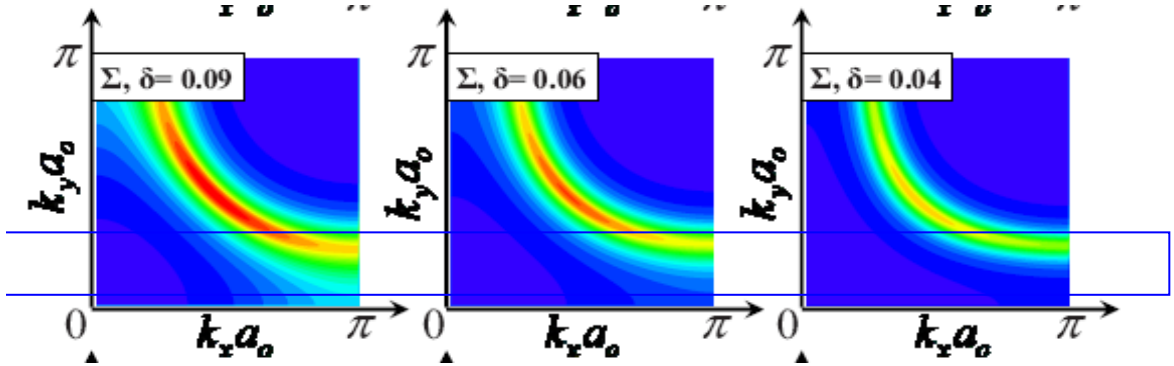
$La_{2-x}Sr_xCuO_4$

The Fermi surface. U = 2.15t, t' = 0.13t, t'' = -0.16t

$$\delta = 0.1$$



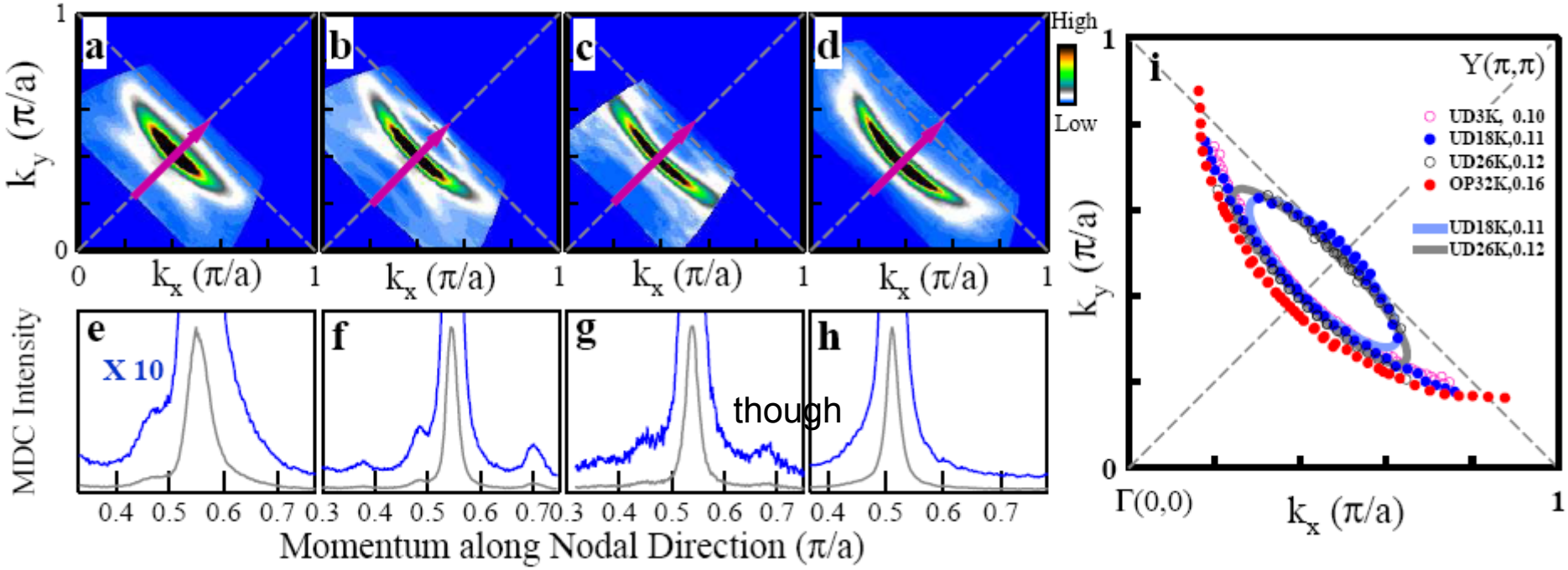




M. Civelli Phys.Rev.B **79**, 195113(2009)

CDMFT

Doping evolution of Fermi surface topology in La-Bi2201



(a-d) show Fermi surface mapping of UD3K (underdoped, Tc3 K), UD18K, UD26K (underdoped, Tc=26 K) and OP32K (optimally-doped, Tc=32 K) samples, respectively.

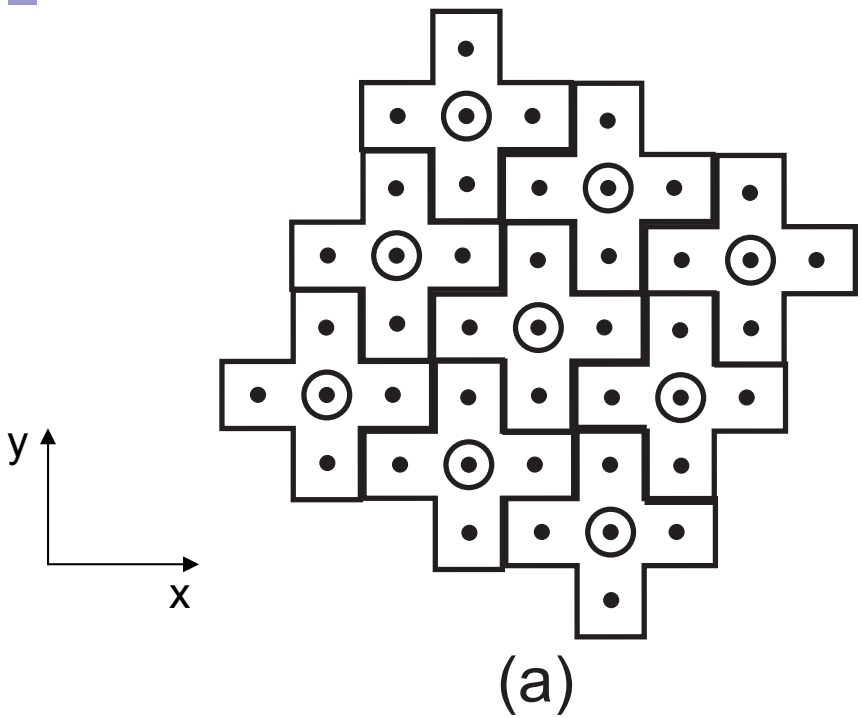
J. Meng, G. Liu, W. Zhang, and et al., Nature **462** (2009) 335

Main conclusion

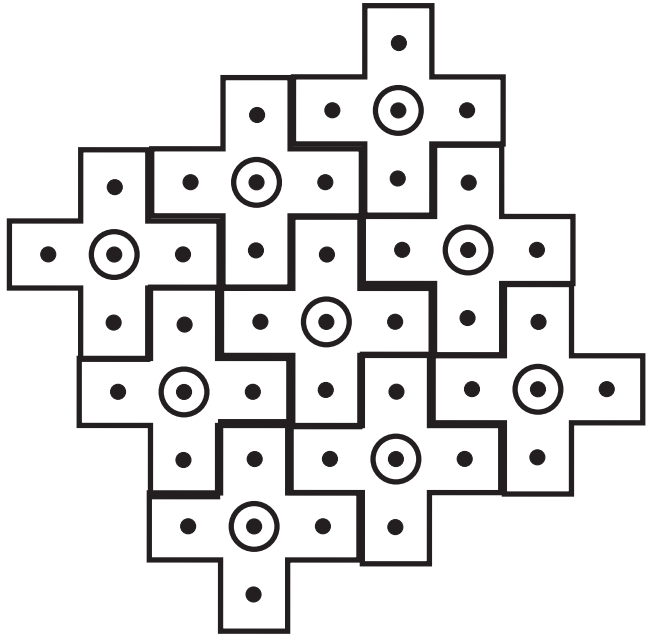
Our calculations of the spectral weight maps have found the strong dependence on the spectral line width (the broadening parameter) that is related to the experimental resolution. The spectral weight maps with better resolution can give full details about the Fermi surface

Thank you for your attention!

NC-CPT method



(a)



(b)

$$T_{nm}(\boldsymbol{k}) = \frac{1}{2}\left(T_{nm}^{(a)}(\boldsymbol{k}) + T_{nm}^{(b)}(\boldsymbol{k})\right)$$

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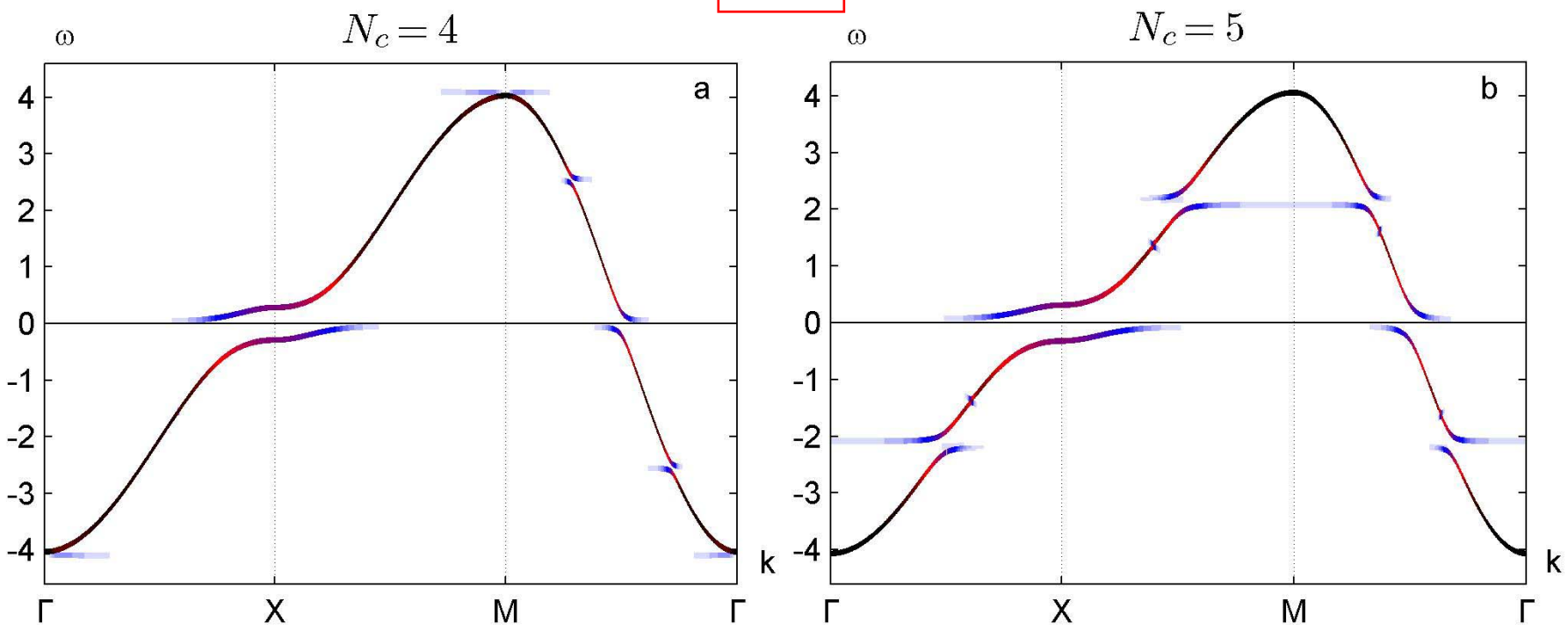
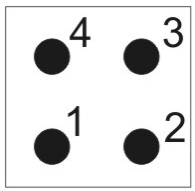
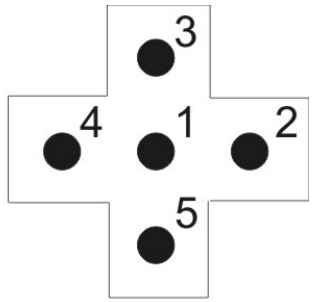
The band structure

U = 1

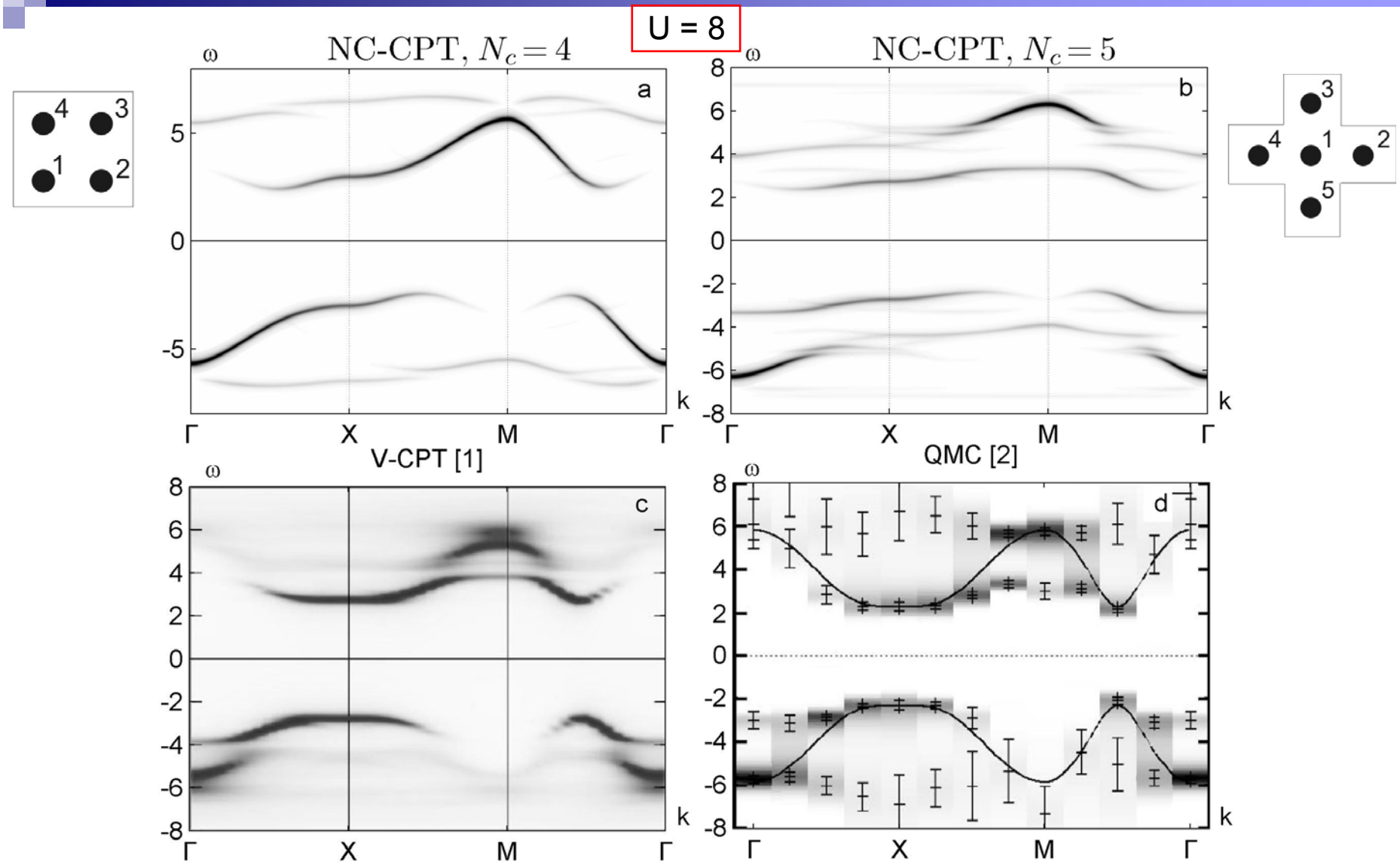




Size effect



The band structure



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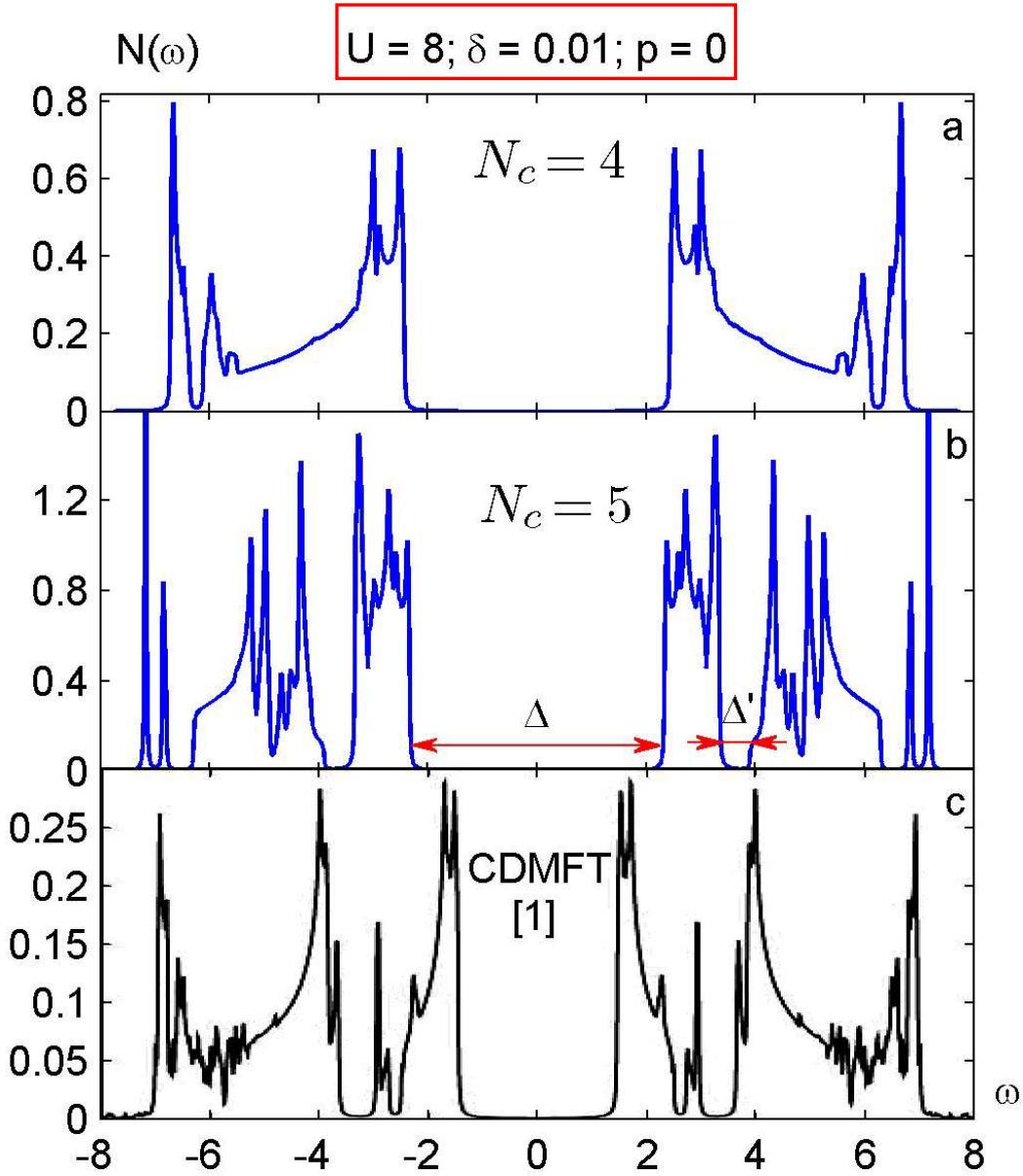
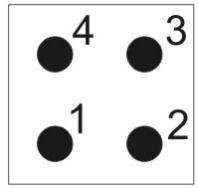
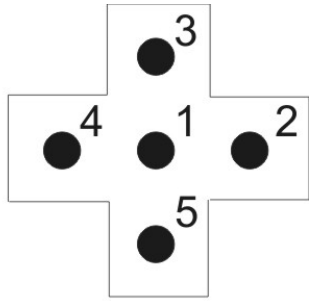
[2] C. Grober, R. Eder, and W. Hanke, Phys. Rev. B **62**, 4336 (2000)

The density of states







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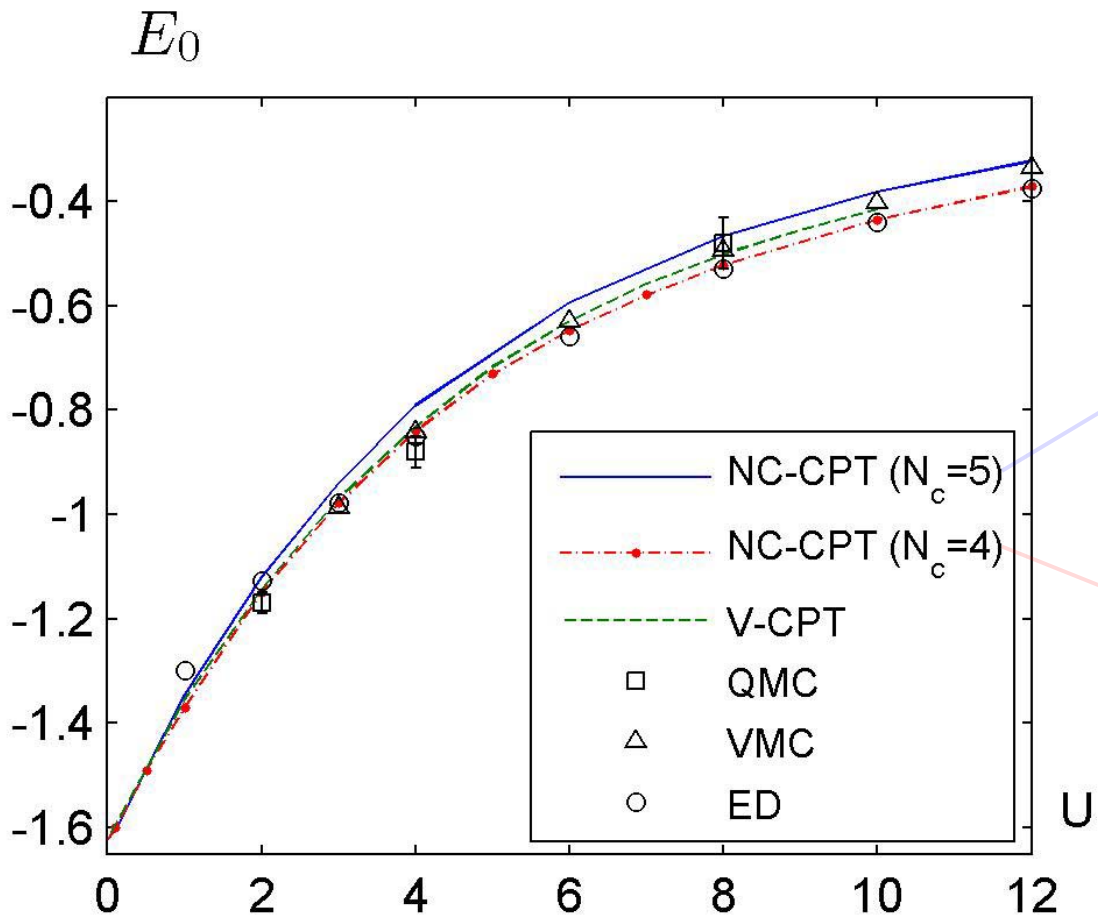
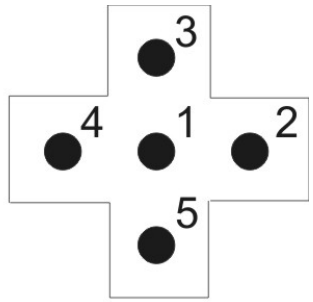
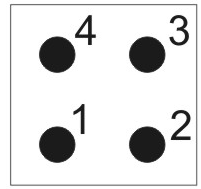
The ground state energy



$0.8C_1 + 0.8C_2 + 0.4C_3$



Shape effect



$1.0C_1 + 0.5C_2$

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V-CPT C. Dahnken, M. Aichhorn, W. Hanke and et al., Phys. Rev. B 70, 245110 (2004)

The doping transformation of the Fermi surface