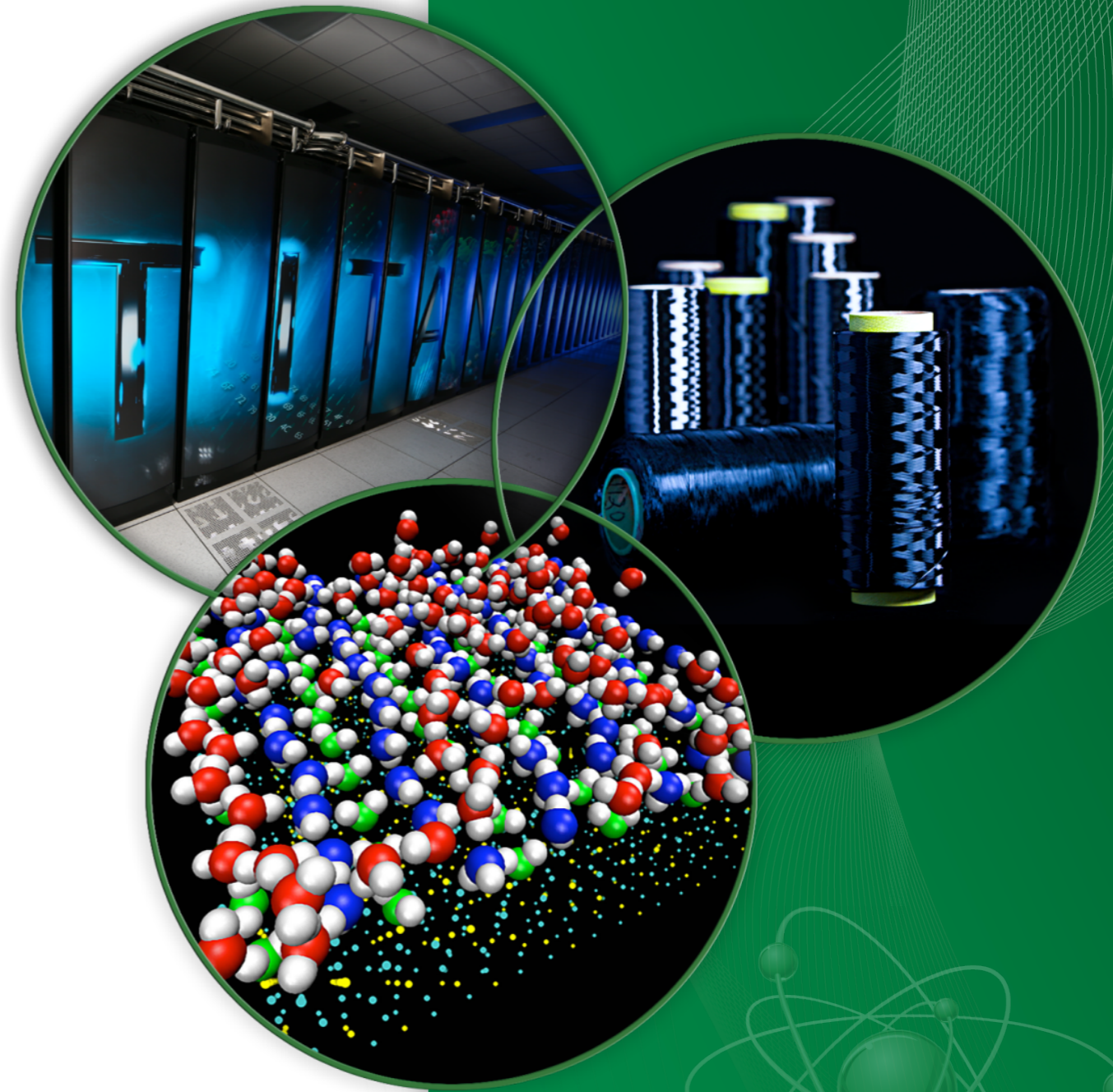


Pairing interaction near a nematic instability

Thomas A. Maier – ORNL
with Doug Scalapino – UCSB



Supported by the Center for Nanophase Materials Sciences at ORNL

ORNL is managed by UT-Battelle
for the US Department of Energy

Outline

- **Underdoped cuprates have charge and nematic order**
- **3-band Hubbard model has a nematic instability**
- **Nematic charge fluctuations contribute to *d*-wave pairing**

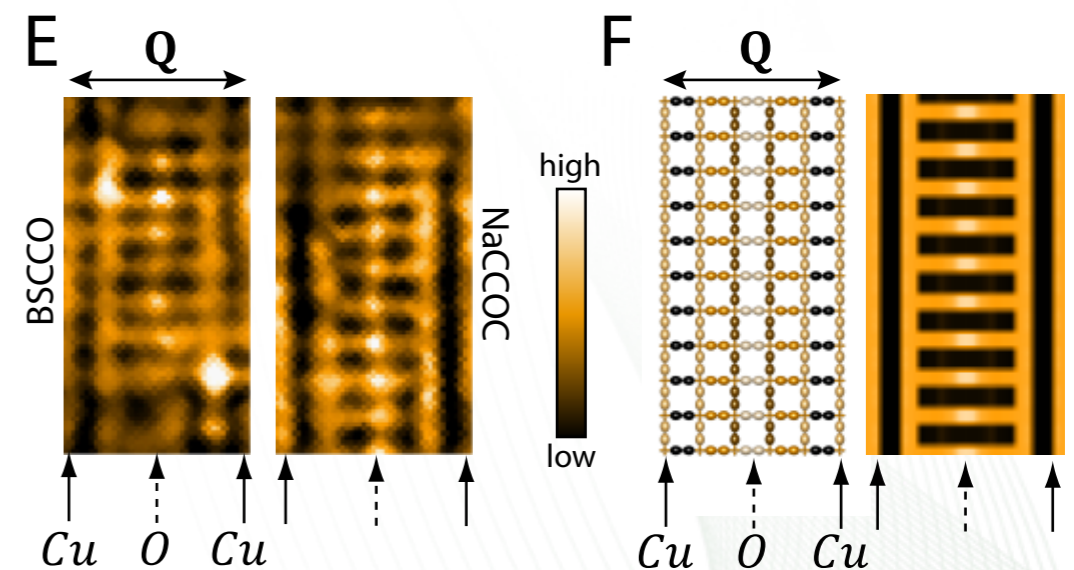
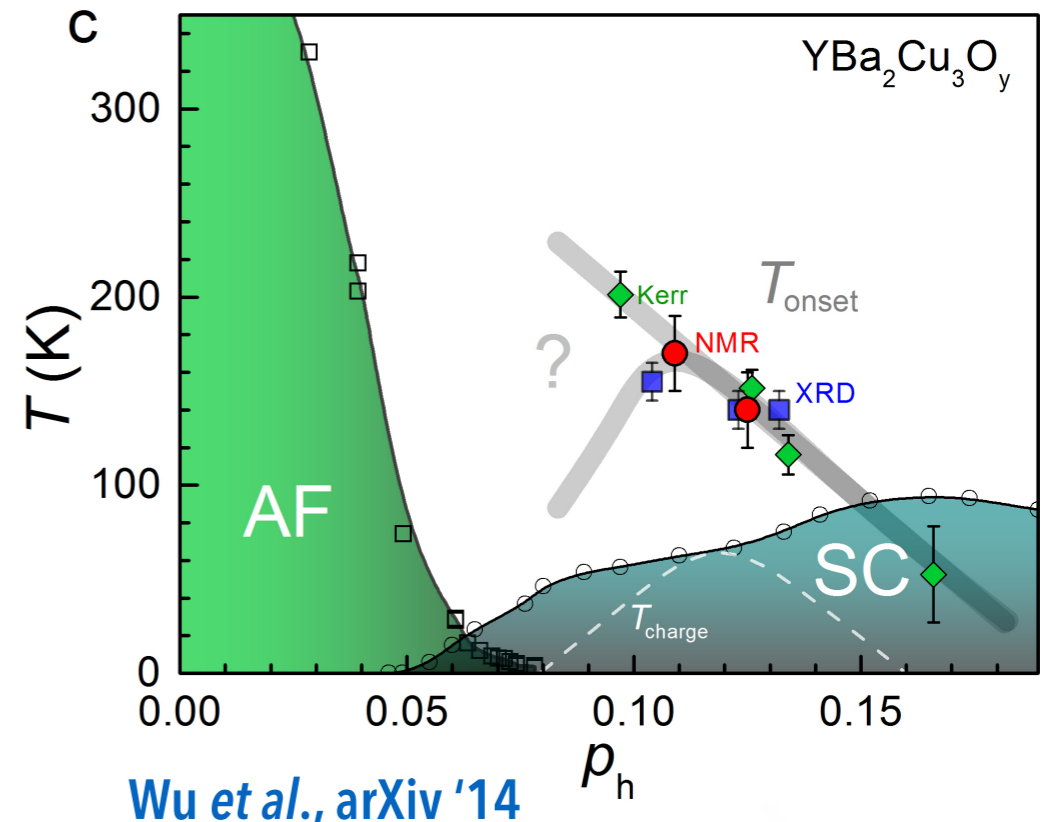
Maier & Scalapino, arXiv:1405.5238
see also: Lederer *et al.*, arXiv:1406.1193

Charge order and nematicity in the cuprates

Broken symmetries in underdoped cuprates

- Evidence for static, but short-ranged charge order from NMR, XRD, STM, ...
- Charge order accompanied by intra-unit-cell nematic order
- d -form factor density wave

Sachdev & La Placa, PRL '13



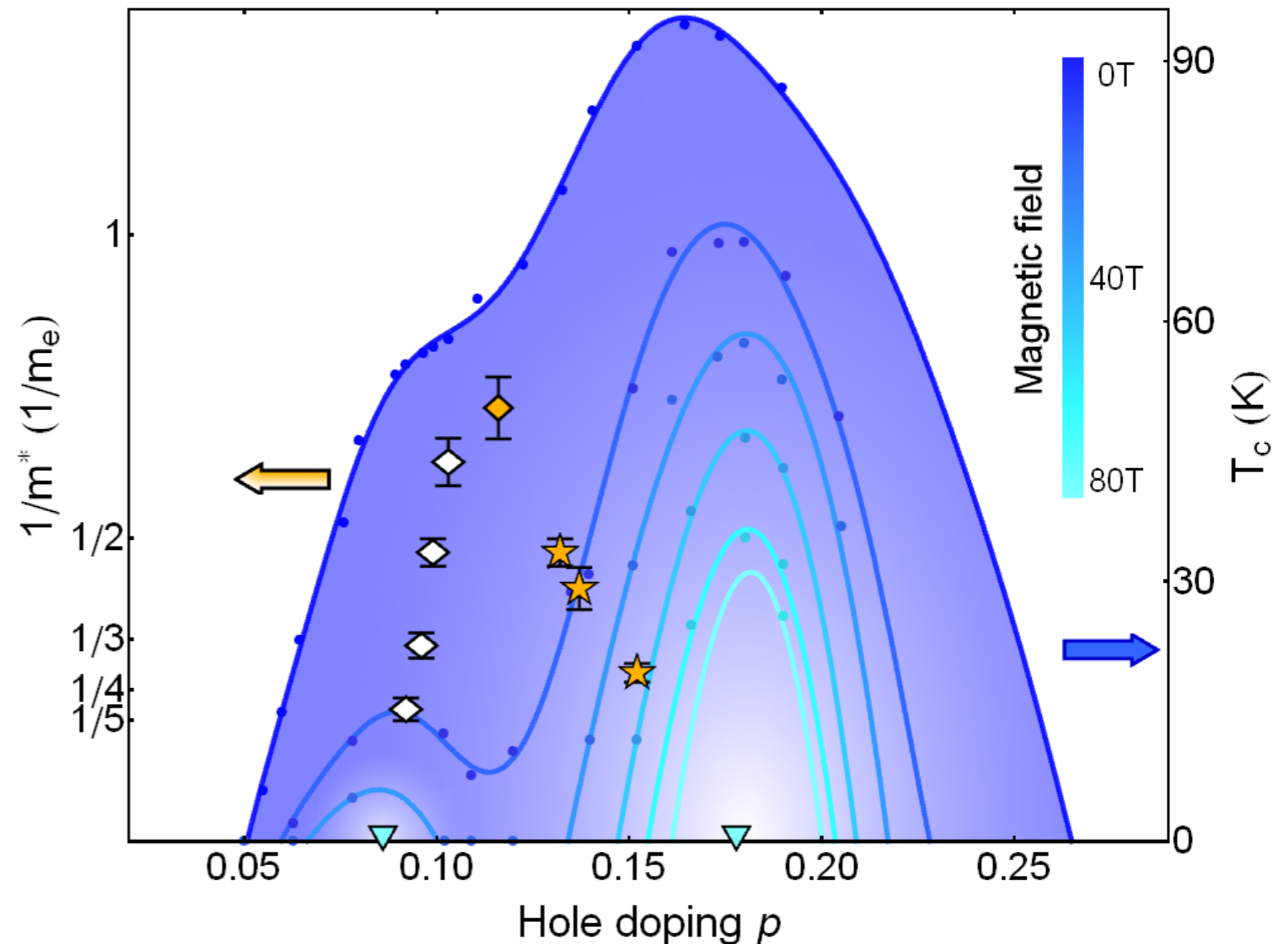
Fujita *et al.*, PNAS '14

Pseudogap quantum critical fluctuations and pairing

Quantum oscillations:

Ramshaw *et al.*, arXiv '14

- $m^* \rightarrow \infty$ identifies QCP at $p_c = 0.18$ where $T^*(p) \rightarrow 0$
- Magnetic field needed to suppress superconductivity peaked at p_c
- Pseudogap quantum critical fluctuations involved in pairing



Ramshaw *et al.*, arXiv '14

Pairing near a nematic QCP: Theory

Doped Mott insulator

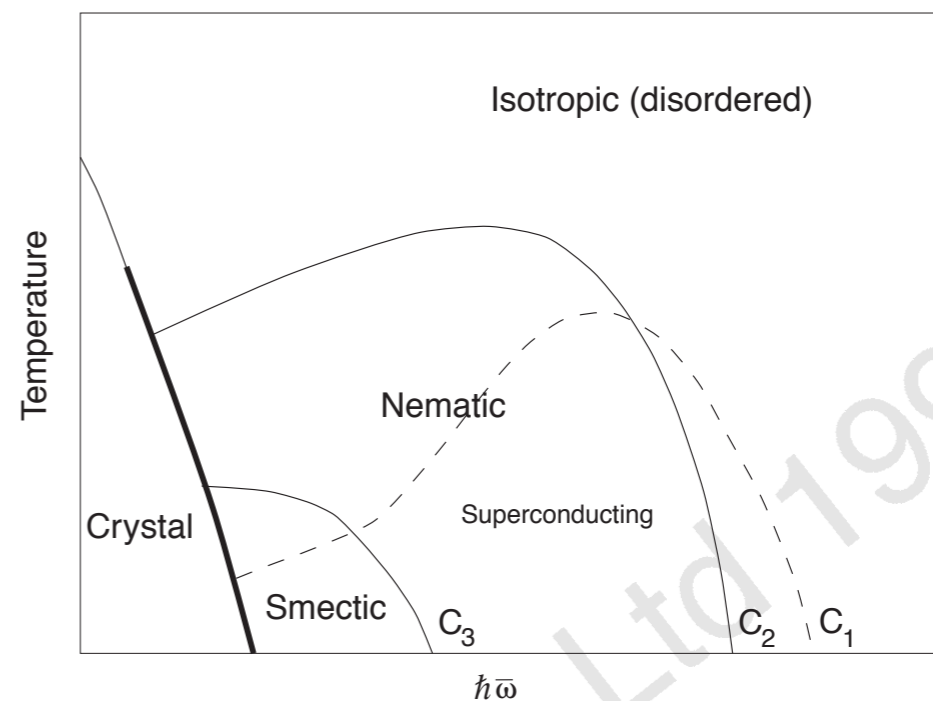
Kivelson, Fradkin, Emery, Nature '89

- Nematic QCP just beyond optimal doping

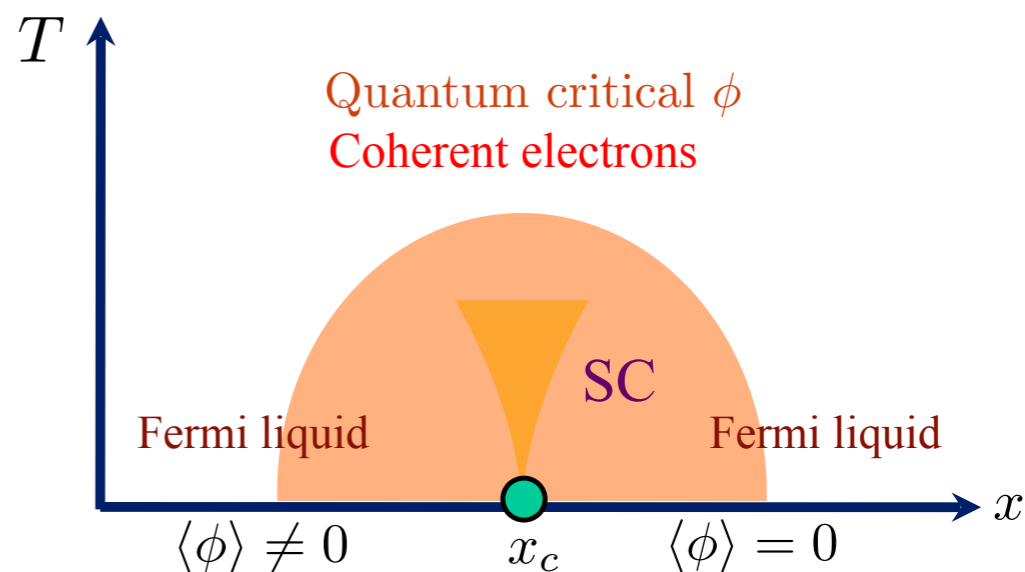
Pairing near nematic QCP

Metlitski *et al.*, NJP '10; arXiv '14

- Nematic charge (bond) ordered phase near SDW
- Nematic fluctuations mediate attractive interaction



Kivelson, Fradkin, Emery, Nature '89

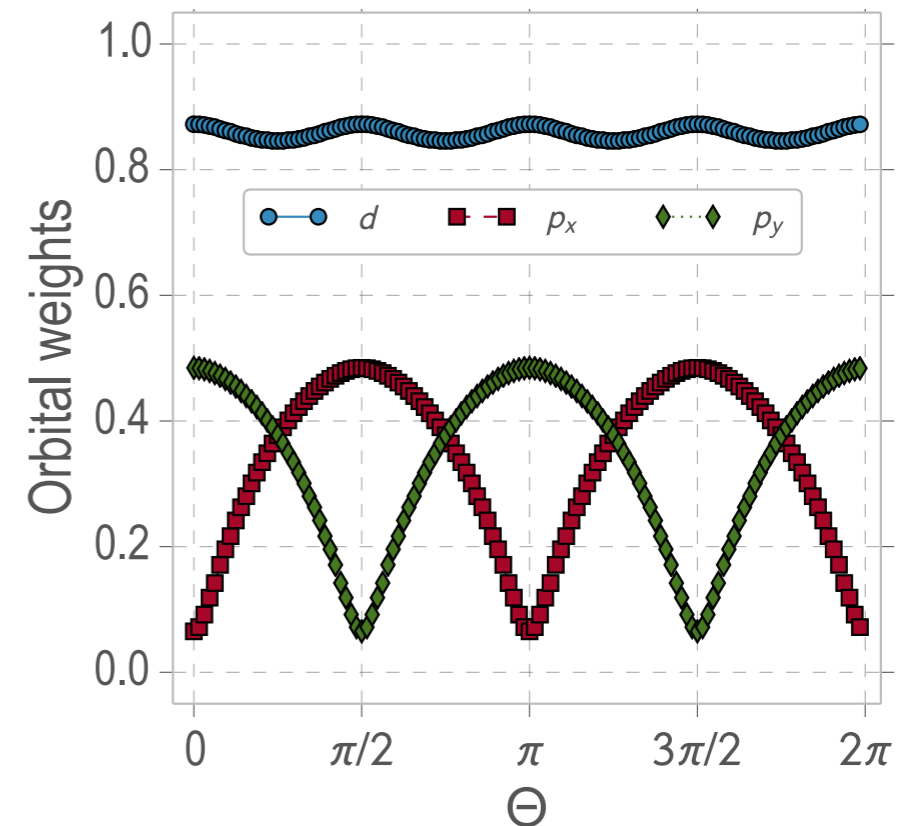
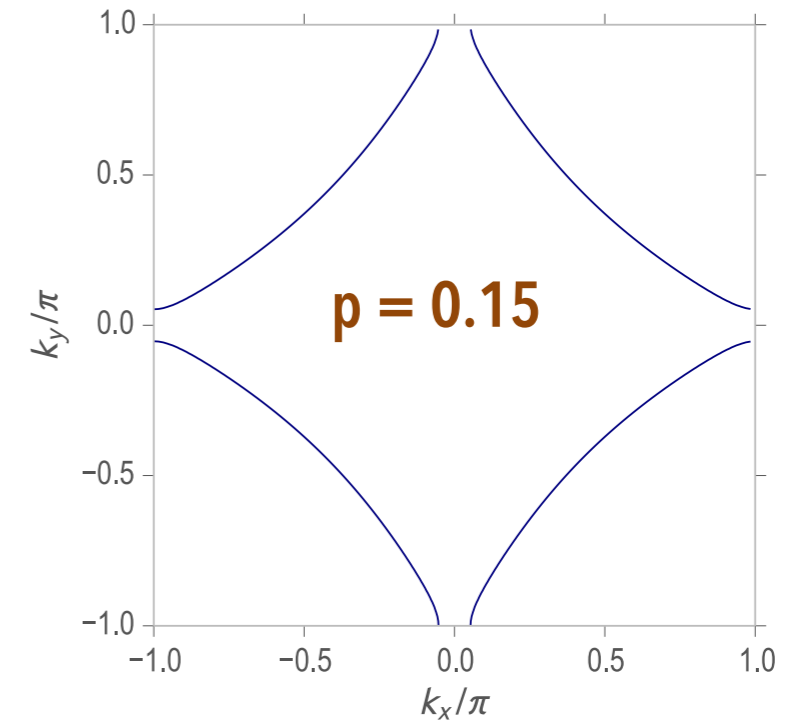
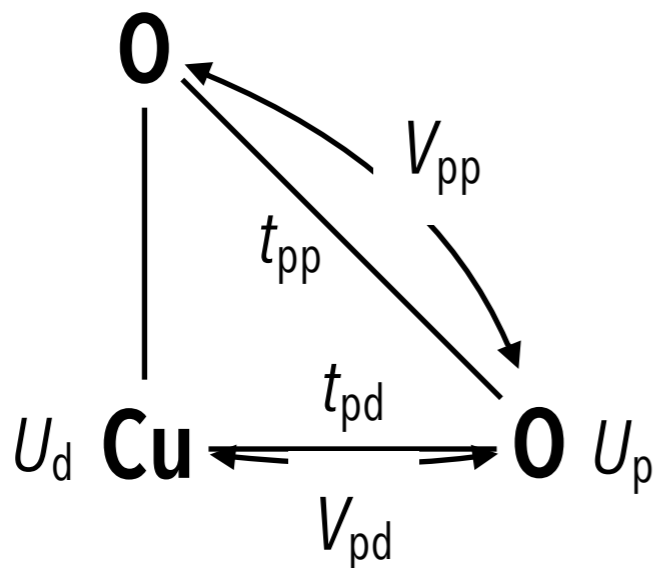


Metlitski *et al.*, arXiv '14

3-band Hubbard model for CuO₂

$$\varepsilon_d - \varepsilon_p = 2.5, t_{pd} = 1, t_{pp} = 0.5$$

$$\begin{aligned}
 H = & \sum_{i,\sigma} \varepsilon_d d_{i\sigma}^\dagger d_{i\sigma} + \sum_{j,\sigma} \varepsilon_p p_{i\sigma}^\dagger p_{i\sigma} \\
 & + \sum_{\langle ij \rangle} t_{pd} (d_{i\sigma}^\dagger p_{j\sigma} + h.c.) + \sum_{\langle jj' \rangle} t_{pp} p_{j\sigma}^\dagger p_{j'\sigma} \\
 & + \sum_i U_d n_{i\uparrow}^d n_{i\downarrow}^d + \sum_j U_p n_{j\uparrow}^p n_{j\downarrow}^p \\
 & + \sum_{\langle ij \rangle} V_{pd} n_i^d n_j^p + \sum_{\langle jj' \rangle} V_{pp} n_j^p n_{j'}^p
 \end{aligned}$$



Nematicity in 3-band model: RPA

Bulut, Atkinson & Kampf, PRB '13
Mean-field: Fischer & Kim, PRB '11

PHYSICAL REVIEW B **88**, 155132 (2013)

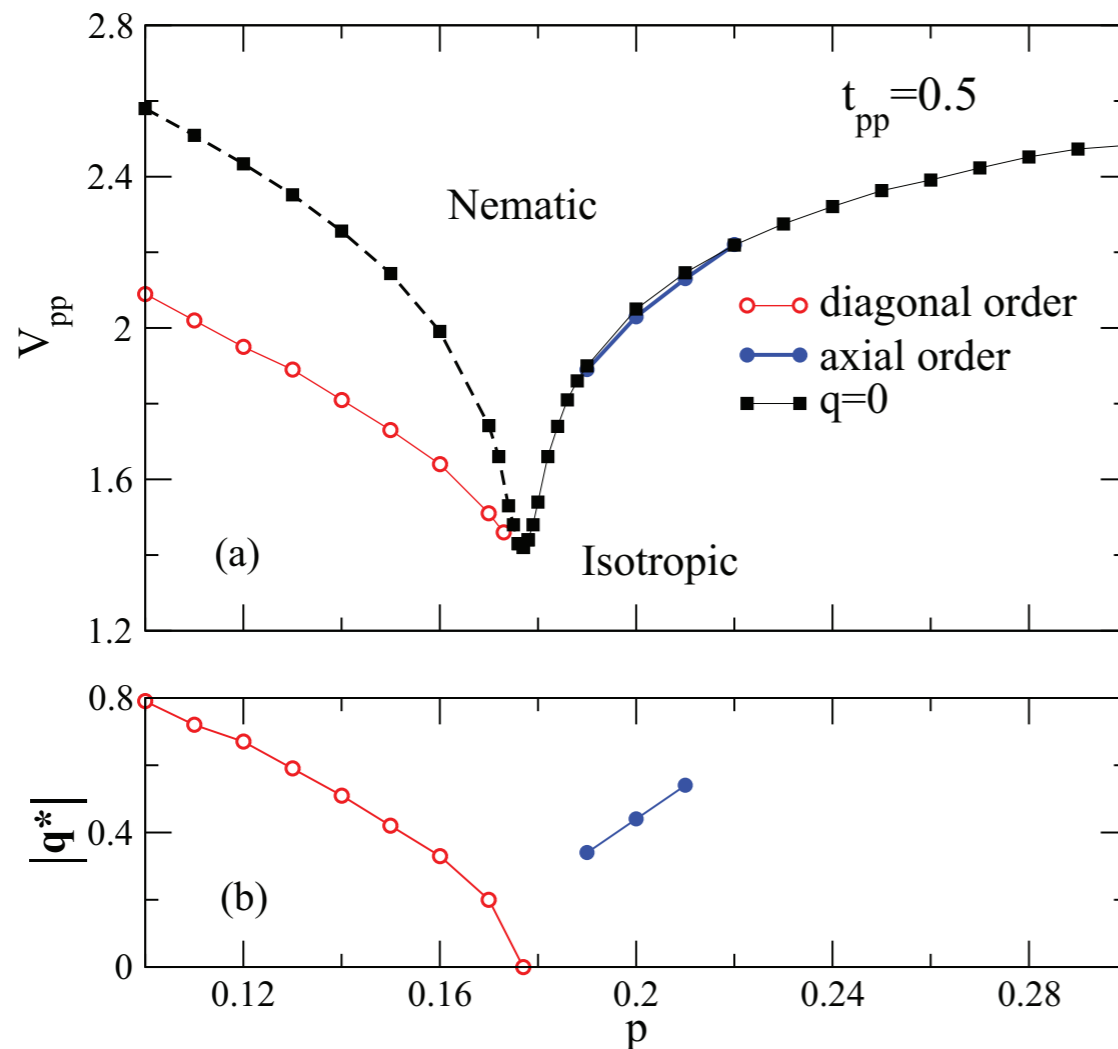
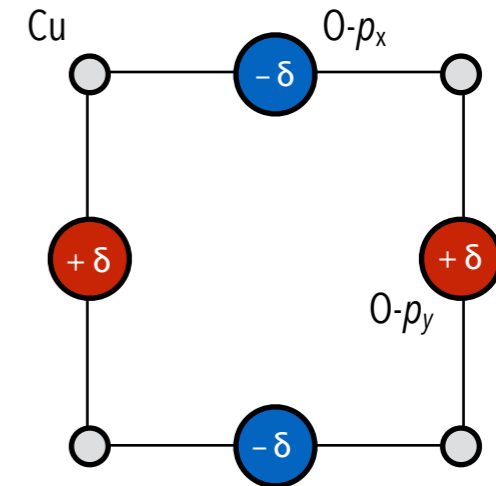
Spatially modulated electronic nematicity in the three-band model of cuprate superconductors

S. Bulut,^{1,2} W. A. Atkinson,^{1,*} and A. P. Kampf³

¹Department of Physics and Astronomy, Trent University, Peterborough Ontario, Canada, K9J 7B8

²Department of Physics, Queen's University, Kingston Ontario, Canada, K7L 3N6

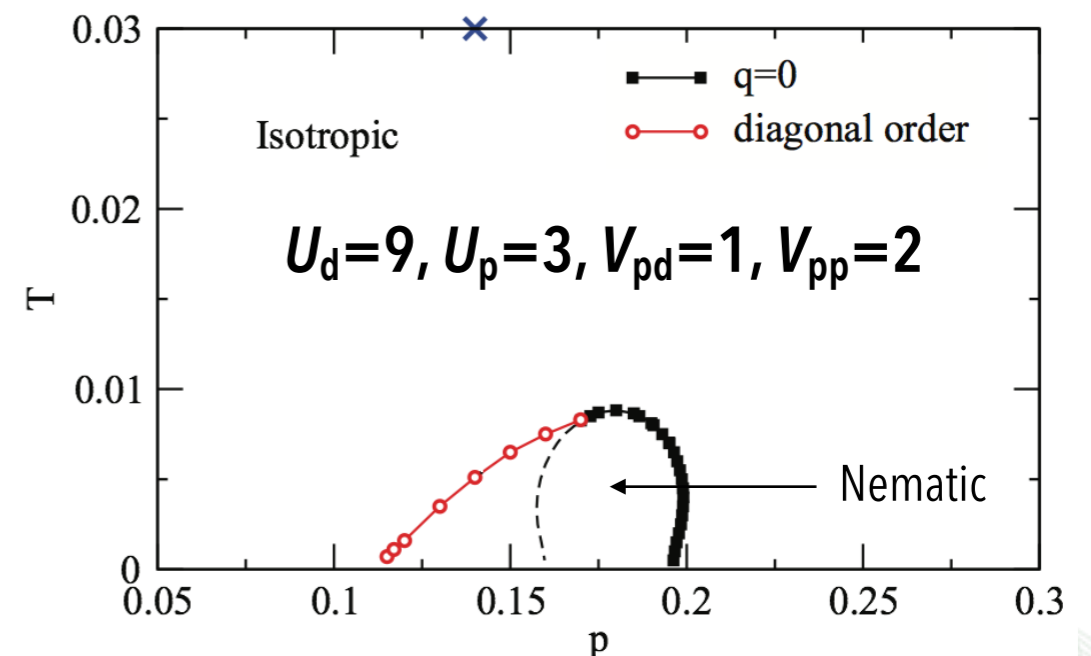
³Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany



Nematic charge susceptibility:

$$\chi_N(q) = \chi_{xx}(q) + \chi_{yy}(q) - \chi_{xy}(q) - \chi_{yx}(q)$$

$$\chi_{\ell_1 \ell_2} = \int_0^\beta d\tau \langle \mathcal{T} n_{\ell_1}(q, \tau) n_{\ell_2}(q, 0) \rangle$$



From Bulut, Atkinson & Kampf, PRB '13

What is the nature of the pairing interaction associated with these nematic fluctuations?

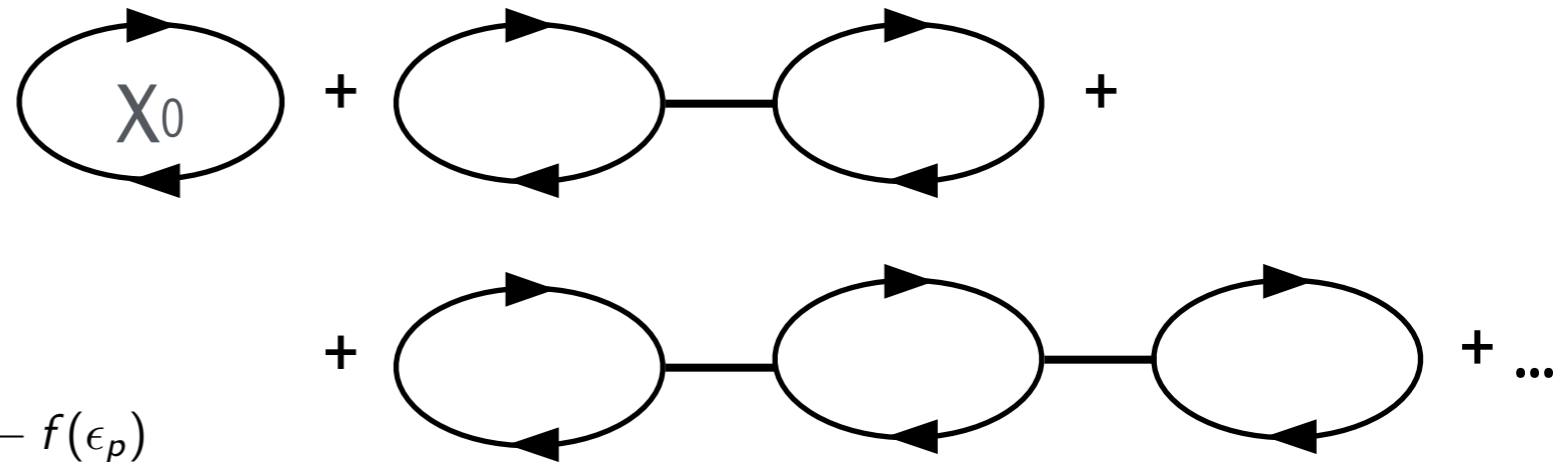
Random phase approximation

For 3-band model see Littlewood, PRB '90;
Bulut, Atkinson & Kampf, PRB '13

Spin/Charge Susceptibility

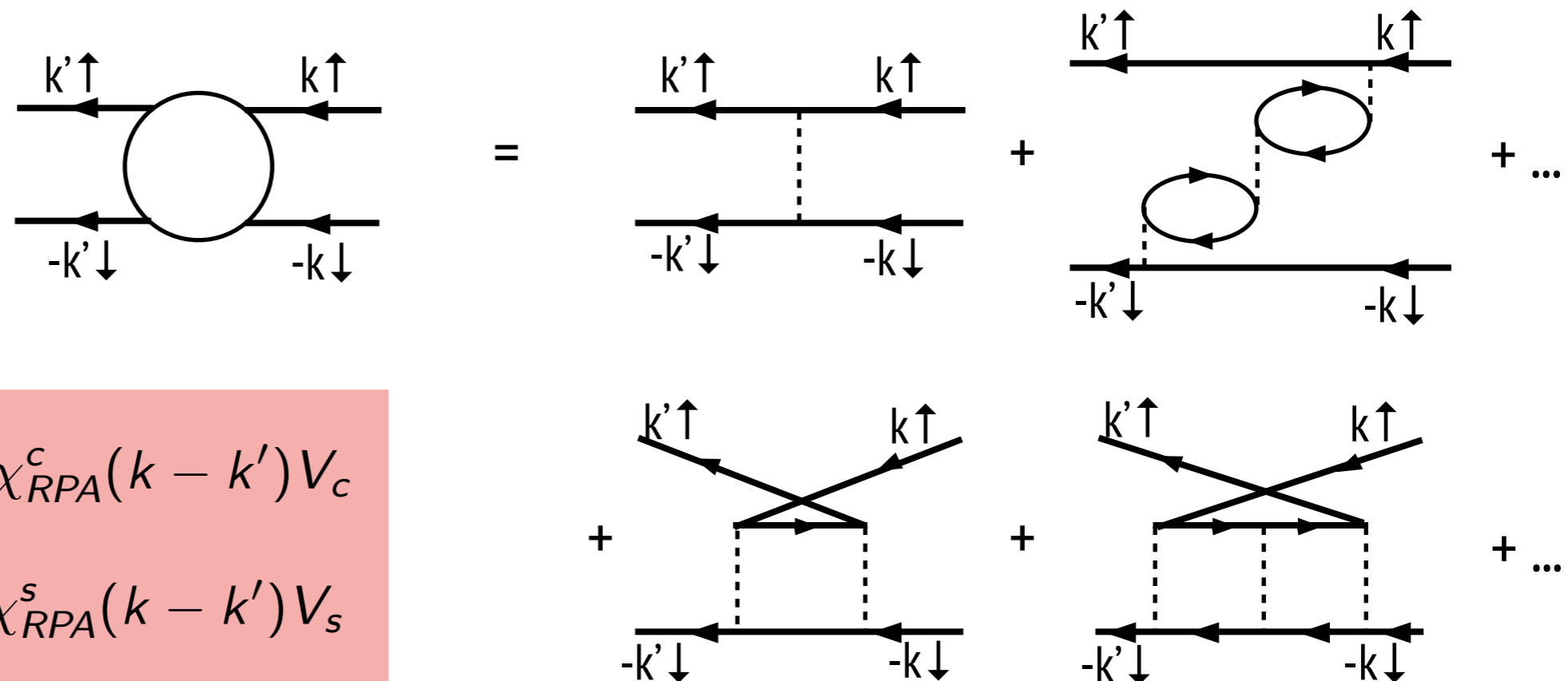
$$\chi_{RPA}(q, \omega) = \frac{\chi_0(q, \omega)}{1 \pm U\chi_0(q, \omega)}$$

$$\chi_0(q, \omega) = \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{p+q}) - f(\epsilon_p)}{\omega - (\epsilon_{p+q} - \epsilon_p) + i\delta}$$



Pairing interaction

Berk, Schrieffer 1966

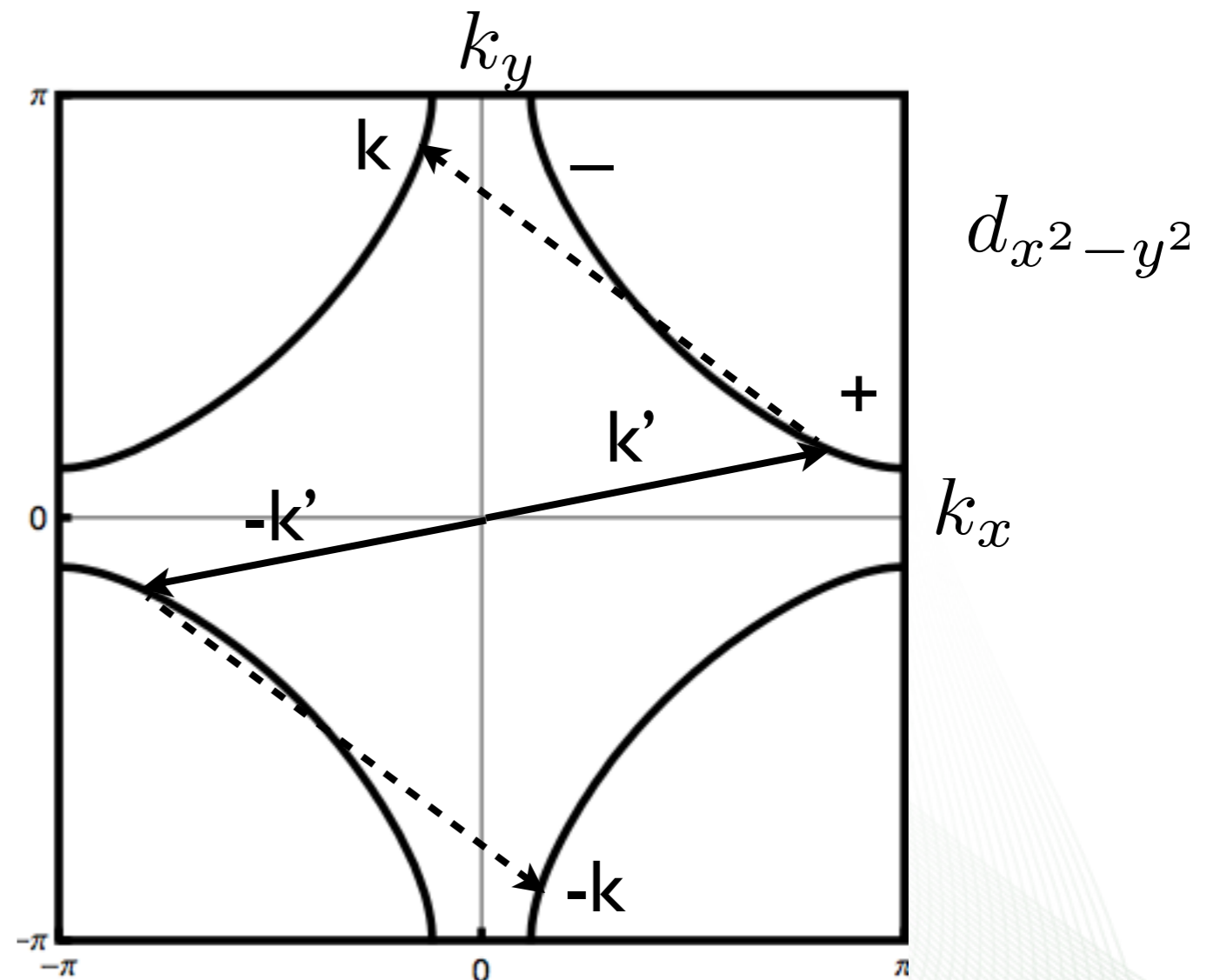


$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c + \frac{V_s}{2} + \frac{3}{2} V_s \chi_{RPA}^s(k - k') V_s$$

d-wave pairing near $Q=(\pi,\pi)$ SDW

$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

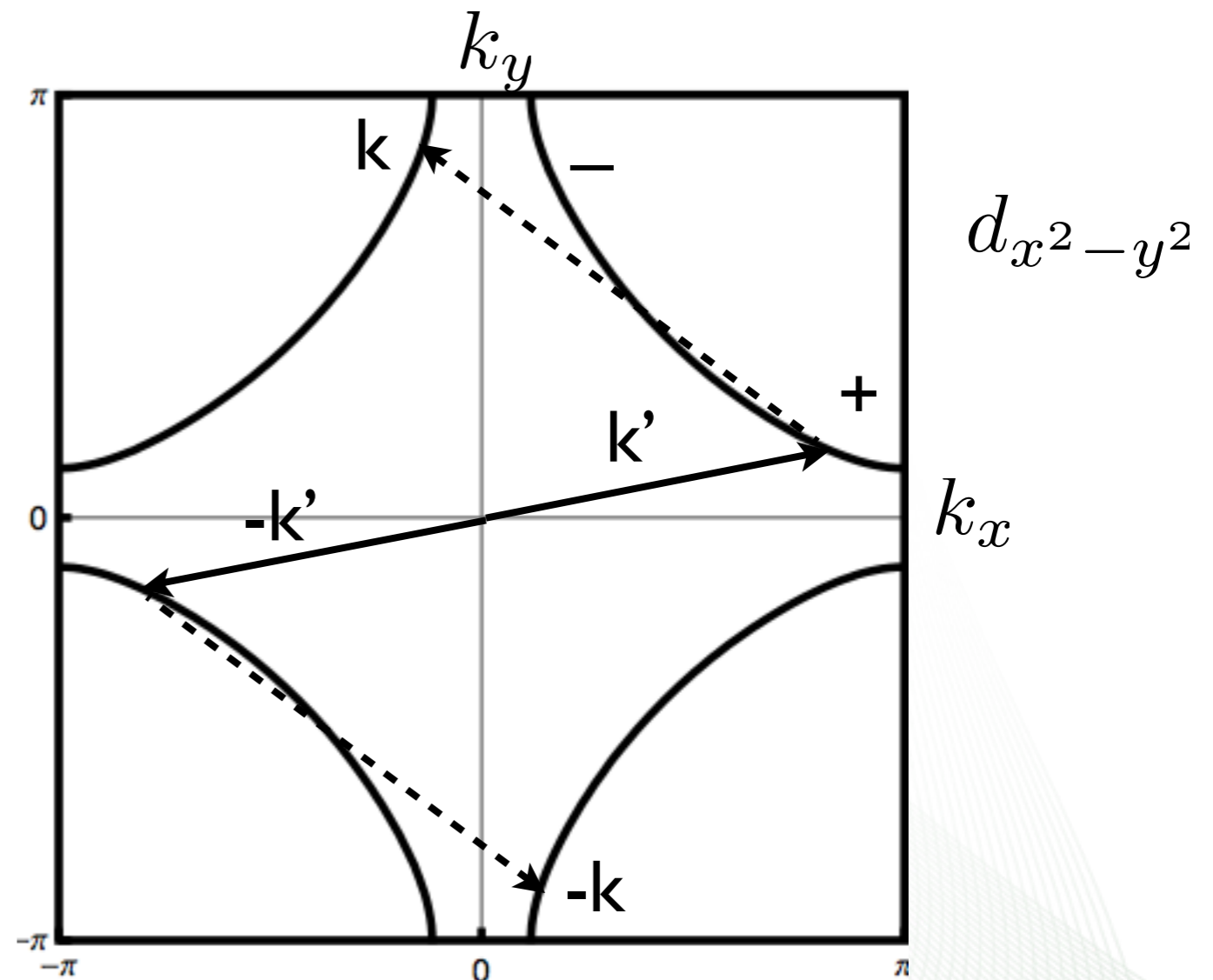
$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c + \frac{V_s}{2} + \frac{3}{2} V_s \chi_{RPA}^s(k - k') V_s$$



d-wave pairing near $Q=(\pi,\pi)$ SDW

$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

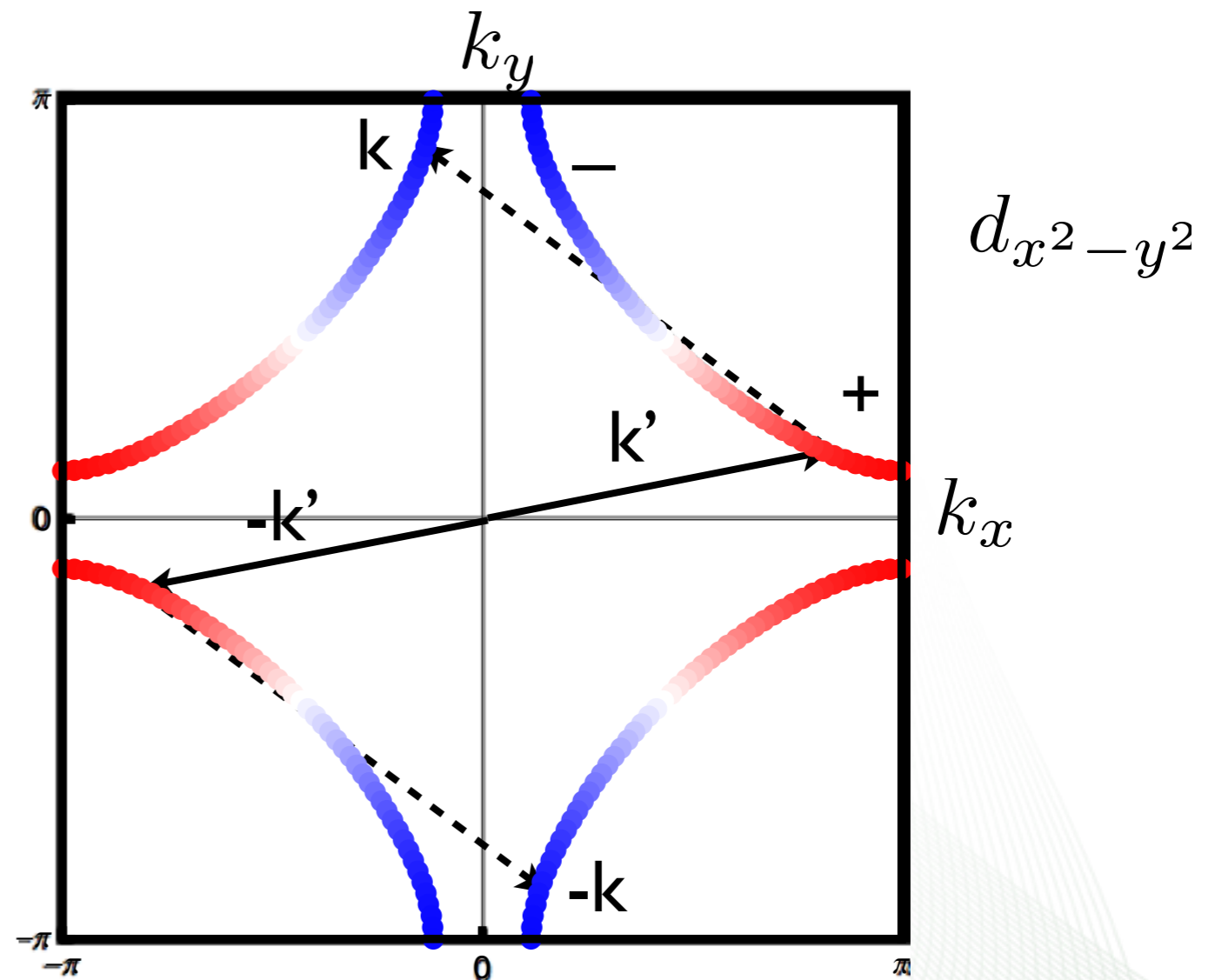
$$\Gamma(k, k') = + \frac{V_s}{2} + \frac{3}{2} V_s \chi_{RPA}^s(k - k') V_s$$



d-wave pairing near $Q=(\pi,\pi)$ SDW

$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

$$\Gamma(k, k') = + \frac{V_s}{2} + \frac{3}{2} V_s \chi_{RPA}^s(k - k') V_s$$



Charge fluctuations and pairing

$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

$$\begin{aligned} \Gamma(k, k') = & \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c \\ & + \frac{V_s}{2} + \frac{3}{2} V_s \chi_{RPA}^s(k - k') V_s \end{aligned}$$

Charge fluctuations and pairing

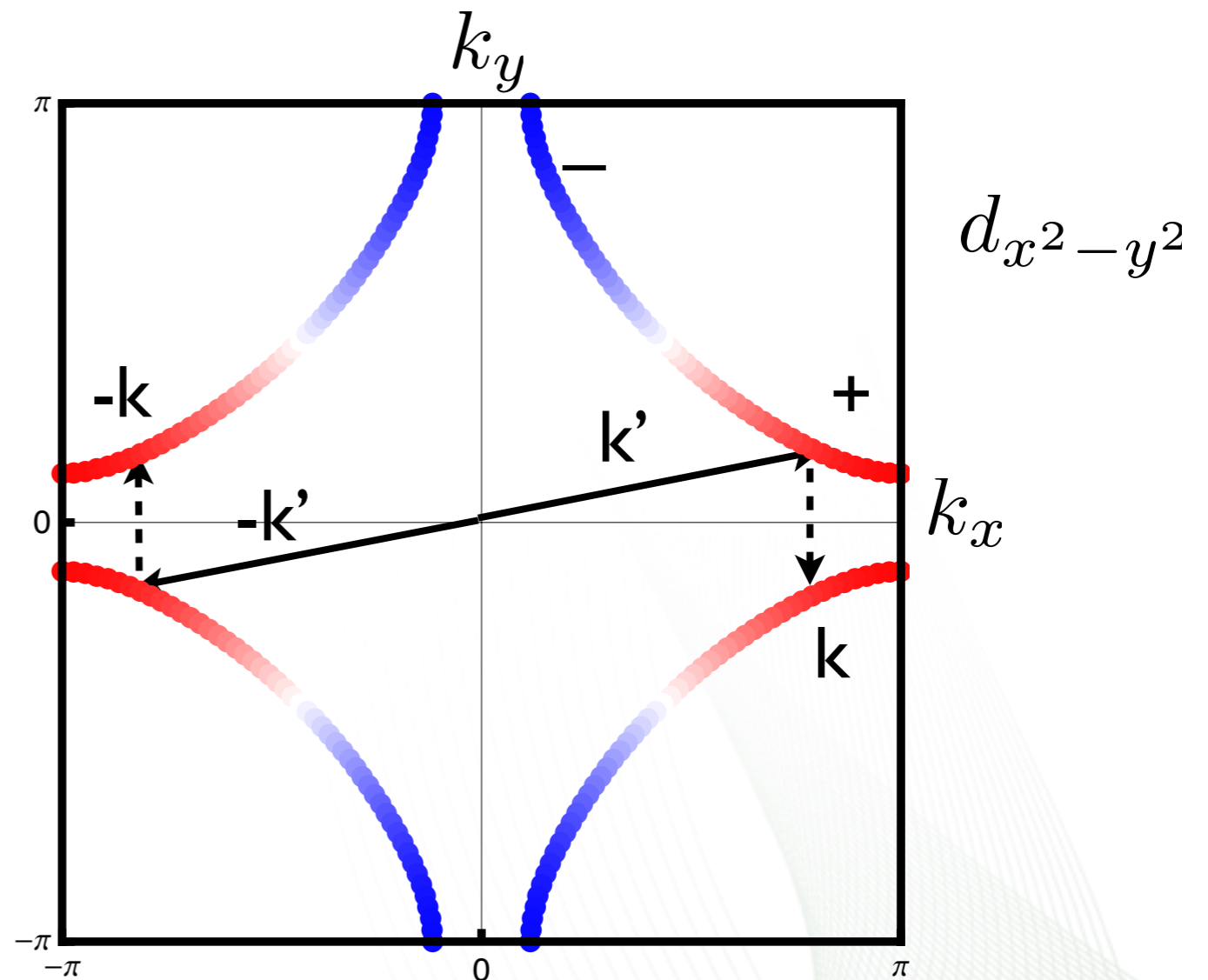
$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$

Charge fluctuations and pairing

$$\Delta(k) = - \sum_{k'} \frac{\Gamma^{pp}(k - k') \Delta(k')}{E(k')}$$

$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$

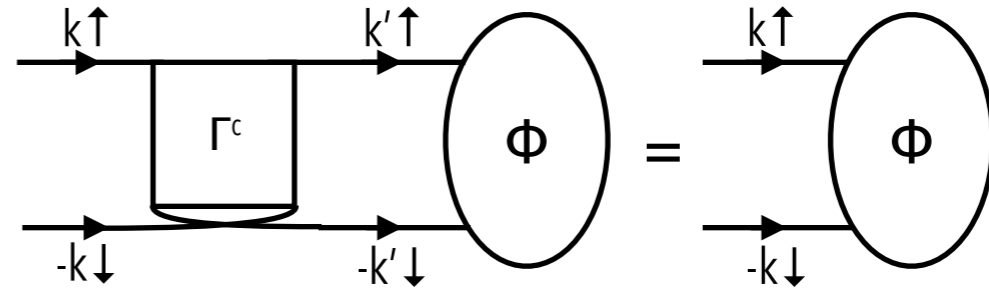


Pairing from charge fluctuations in 3-band model

— Consider only charge part of the interaction and neglect spin

interaction:
$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$

— Solve linearized gap equation:



$$\oint \frac{dk'_{\parallel}}{2\pi v_F(k'_{\parallel})} \Gamma_c(k, k') \Phi_{\alpha}(k') = \lambda_{\alpha} \Phi_{\alpha}(k)$$

with

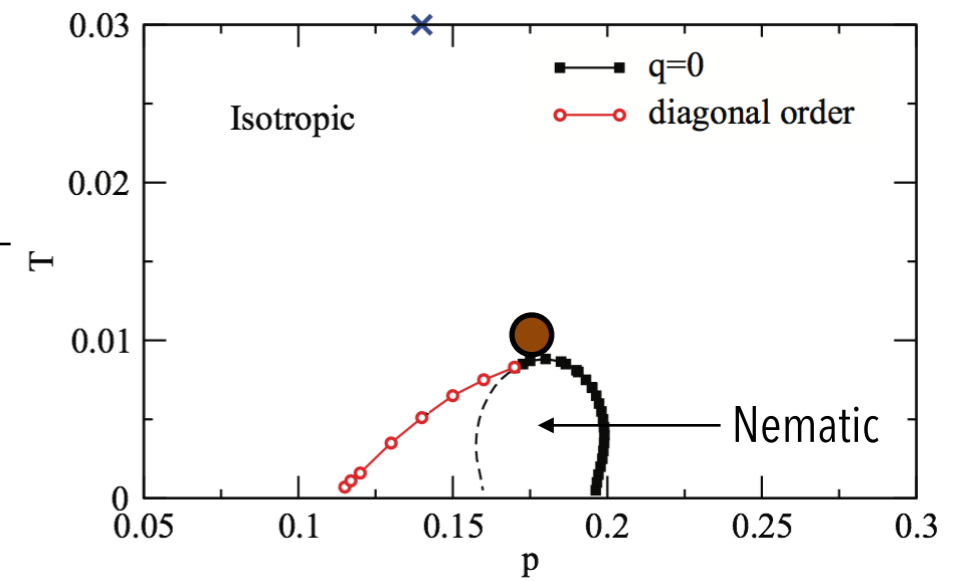
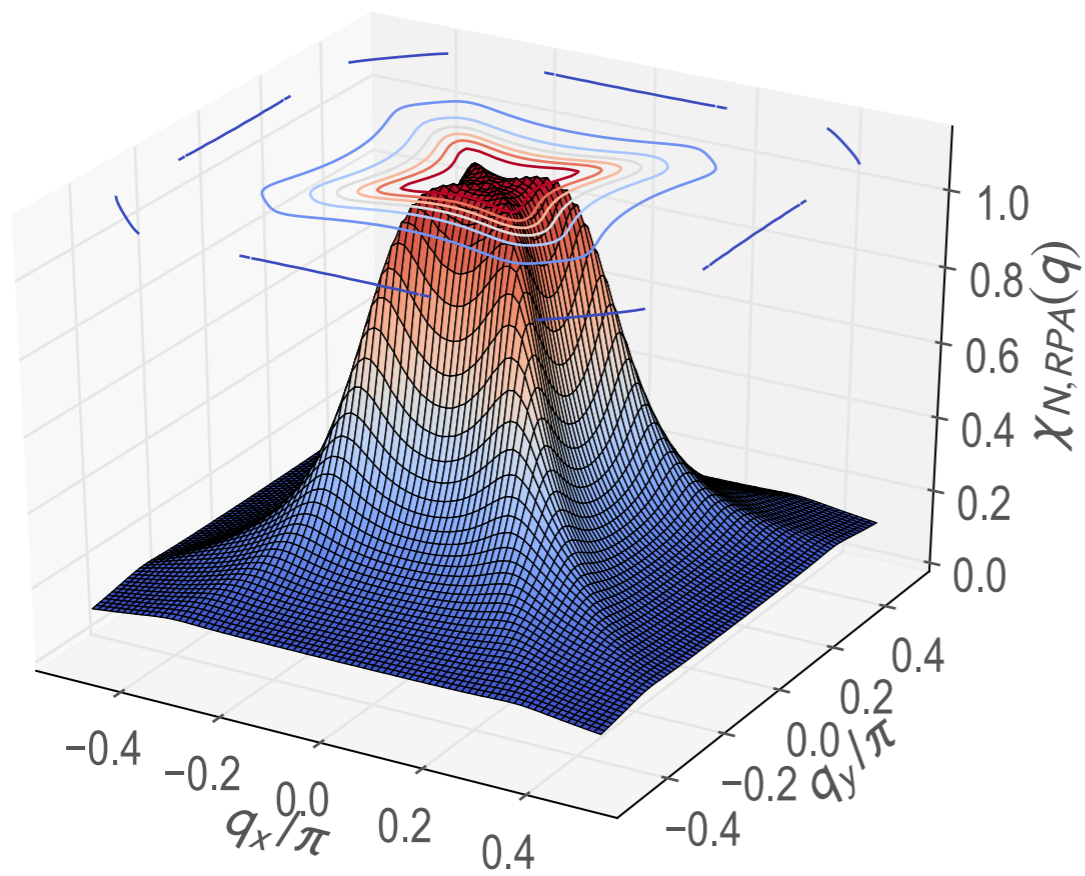
$$\Gamma_c(k, k') = \sum_{l_1, l_2, l_3, l_4} a_{\nu}^{l_1*}(k) a_{\nu}^{l_4*}(-k) \Gamma_{l_1 l_2 l_3 l_4}(k, k') a_{\mu}^{l_2}(k') a_{\mu}^{l_3}(-k')$$

$$U_d=9, U_p=3, V_{pd}=1, V_{pp}=2$$

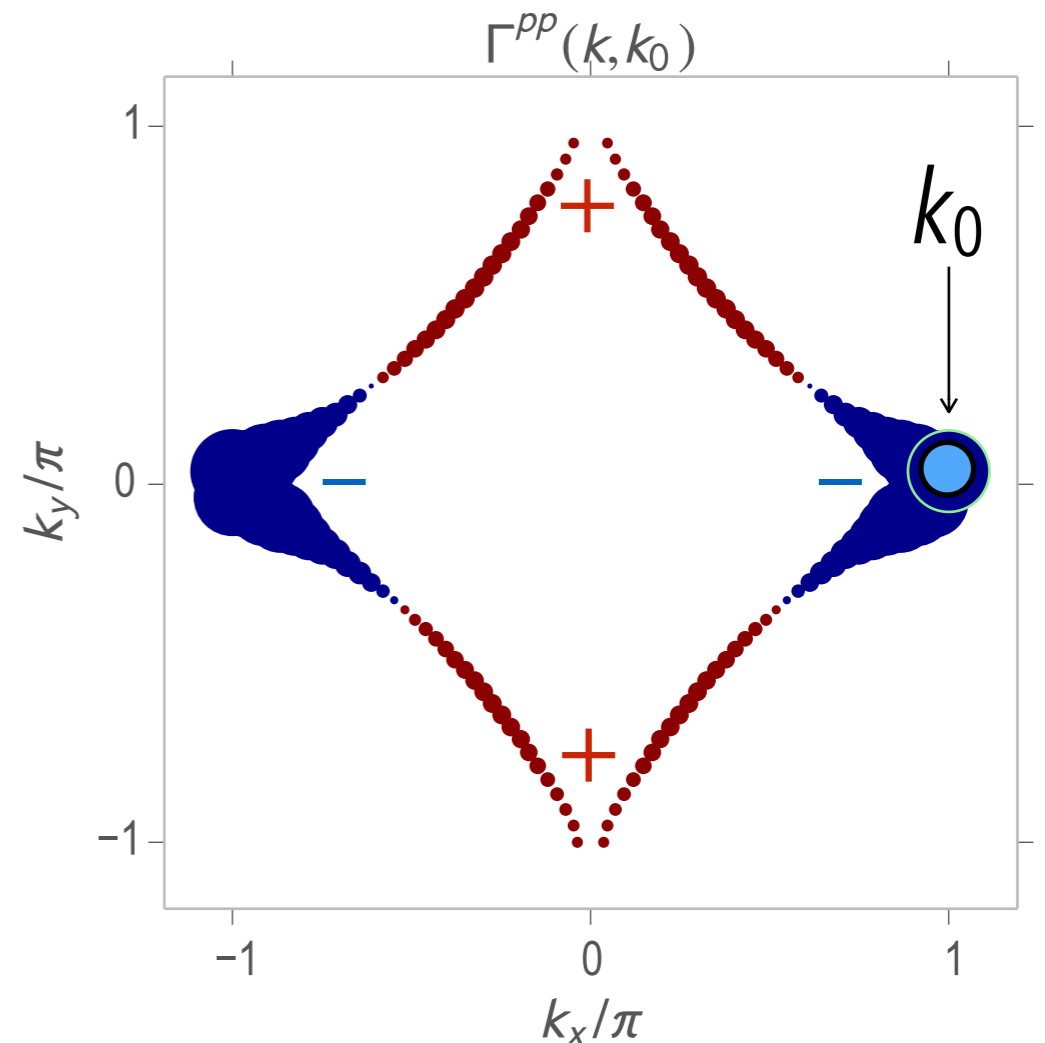
RPA pairing interaction from nematic $q=0$ charge fluctuations

$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$

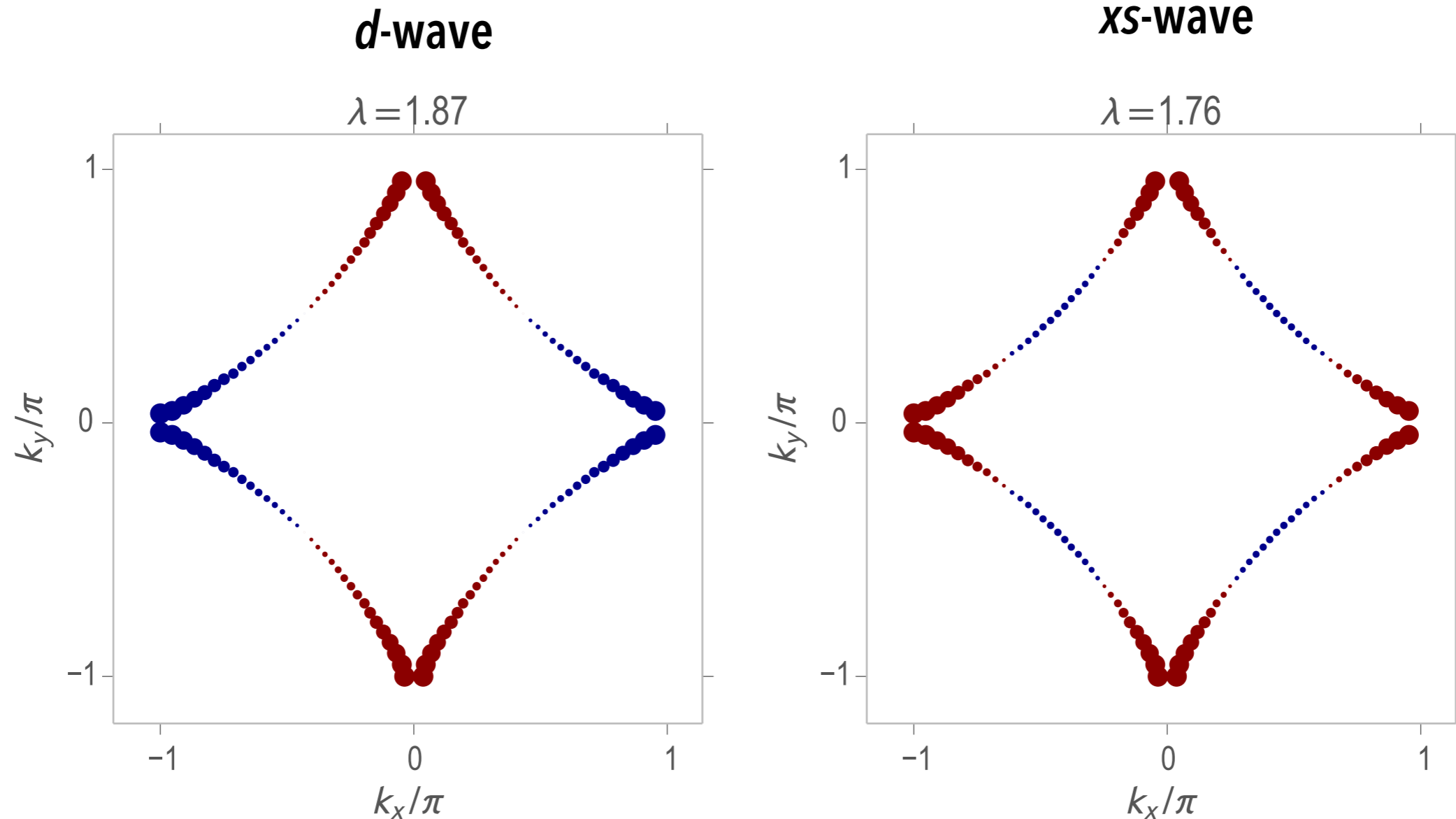
Nematic charge susceptibility



Pairing interaction



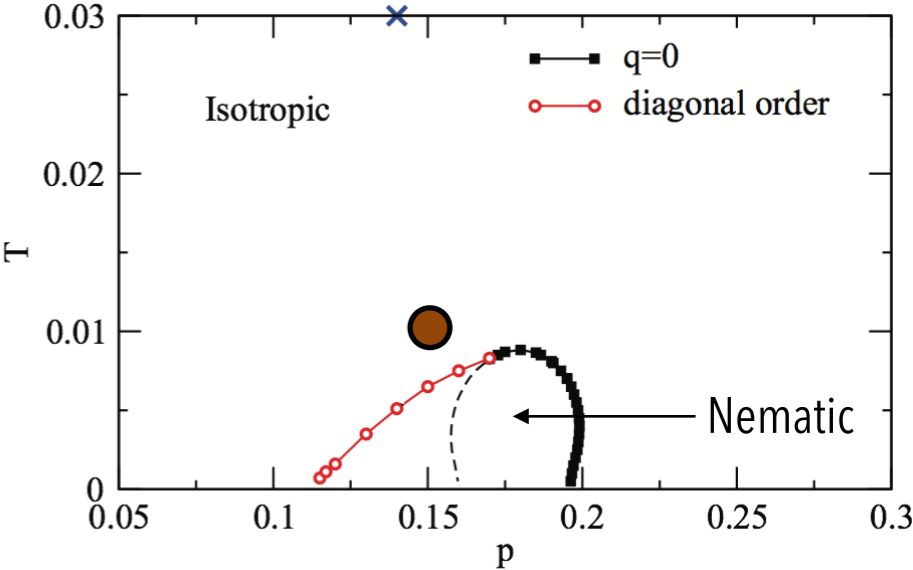
Leading gap structures



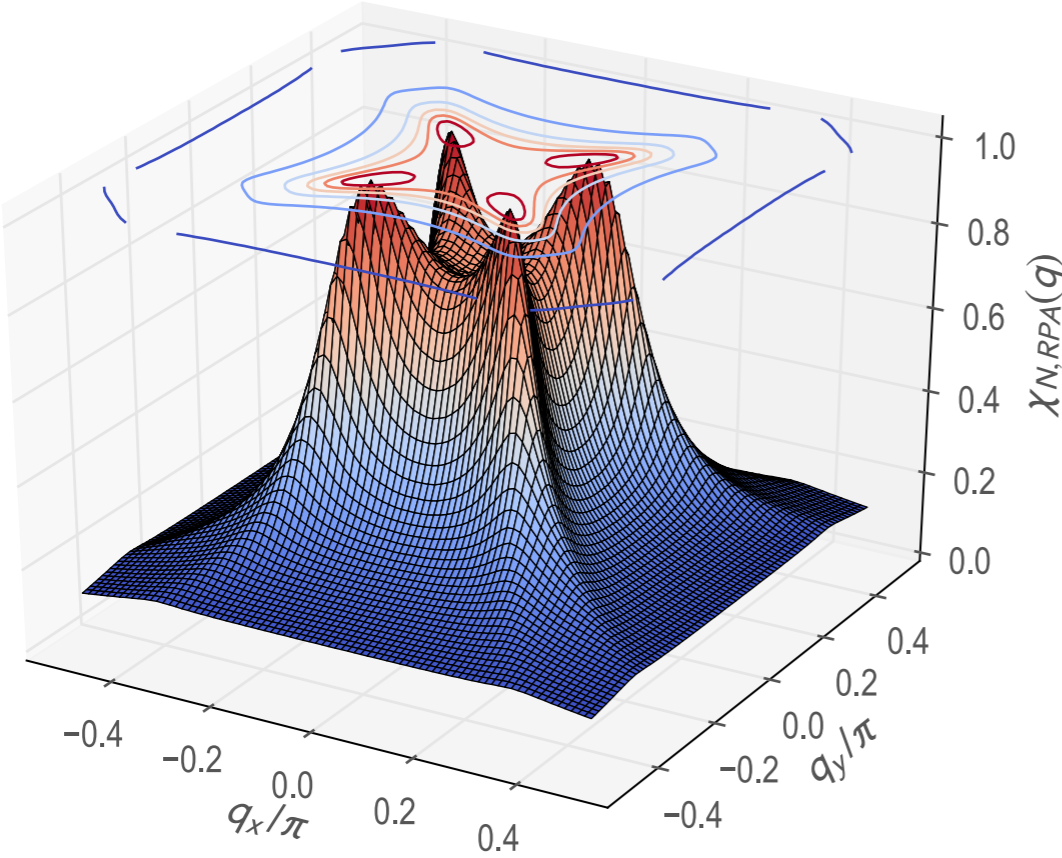
Nematic pairing interaction attractive in d -wave and xs -wave channels

RPA pairing interaction from nematic $q^*=(q_0, q_0)$ fluctuations

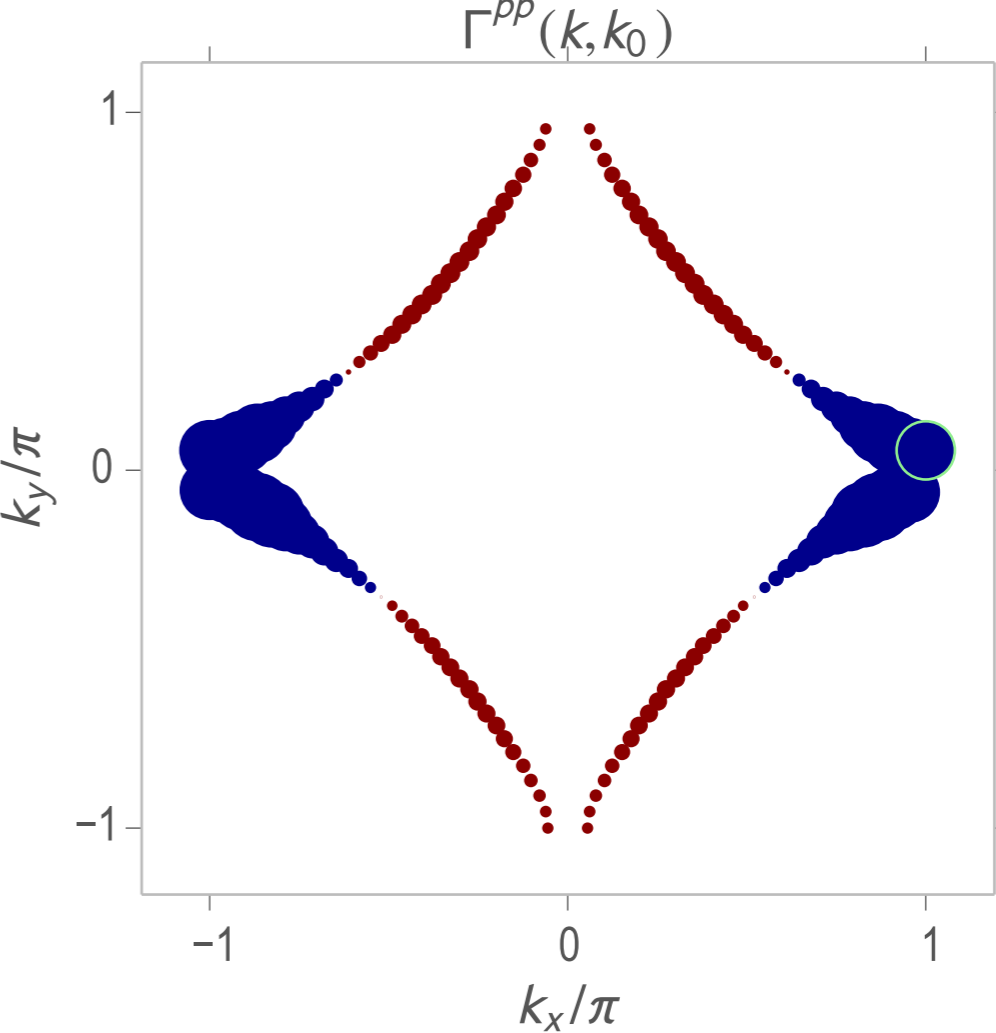
$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$



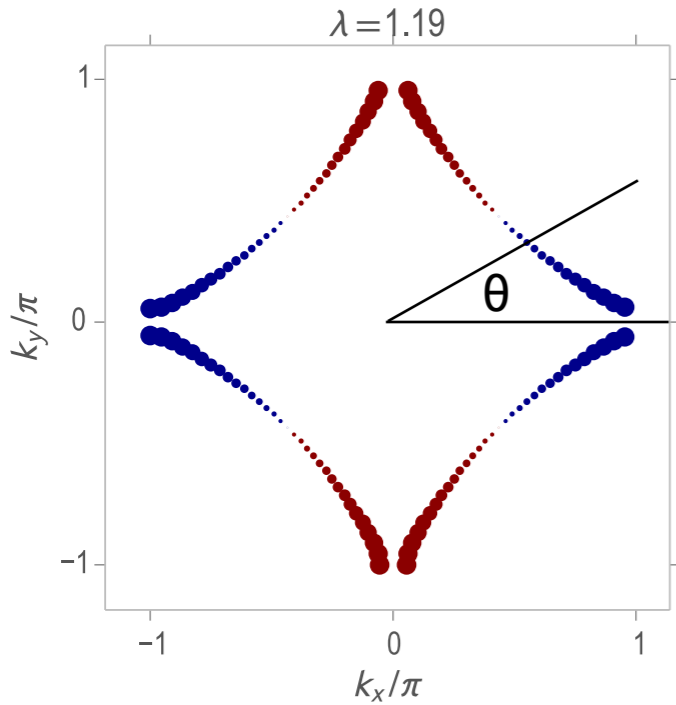
nematic charge susceptibility



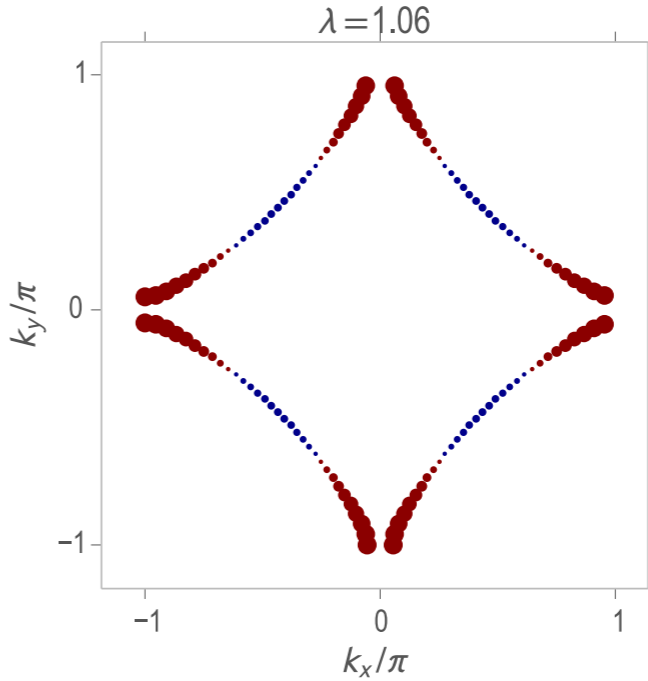
pairing interaction



Leading gap structures

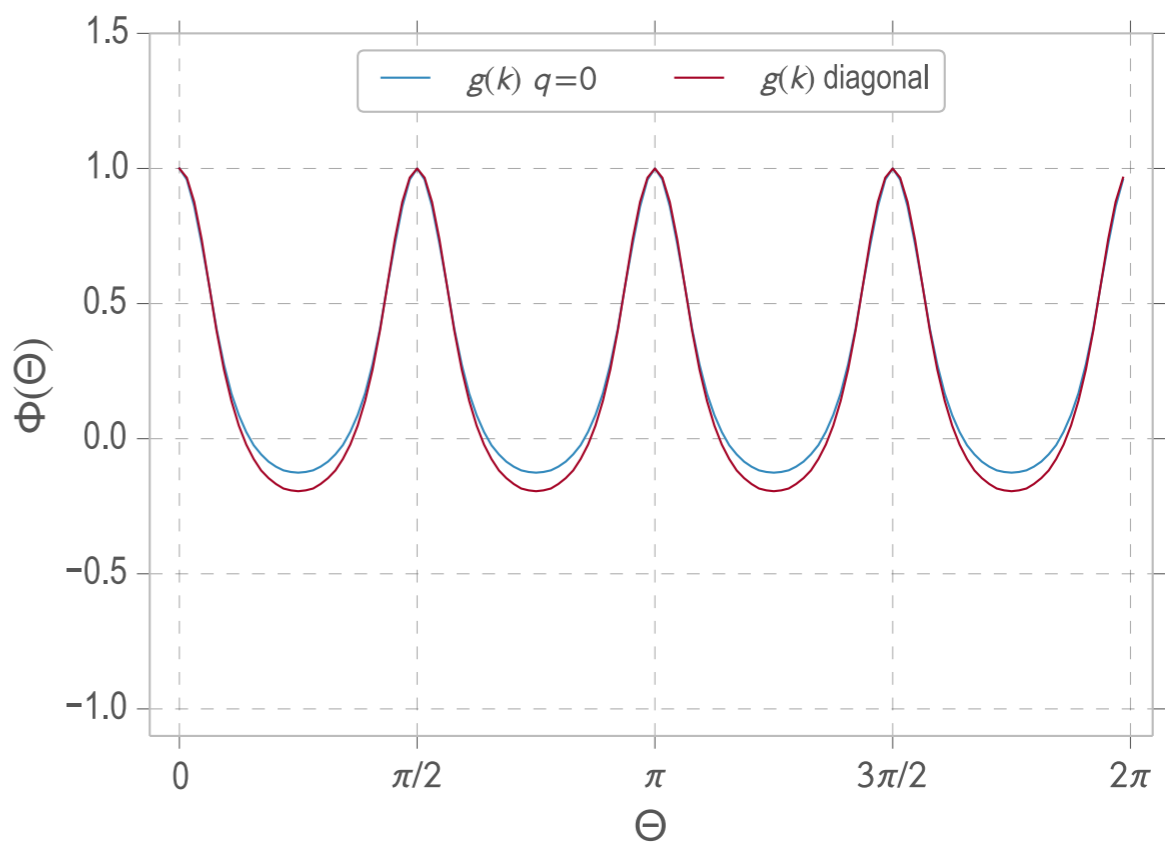
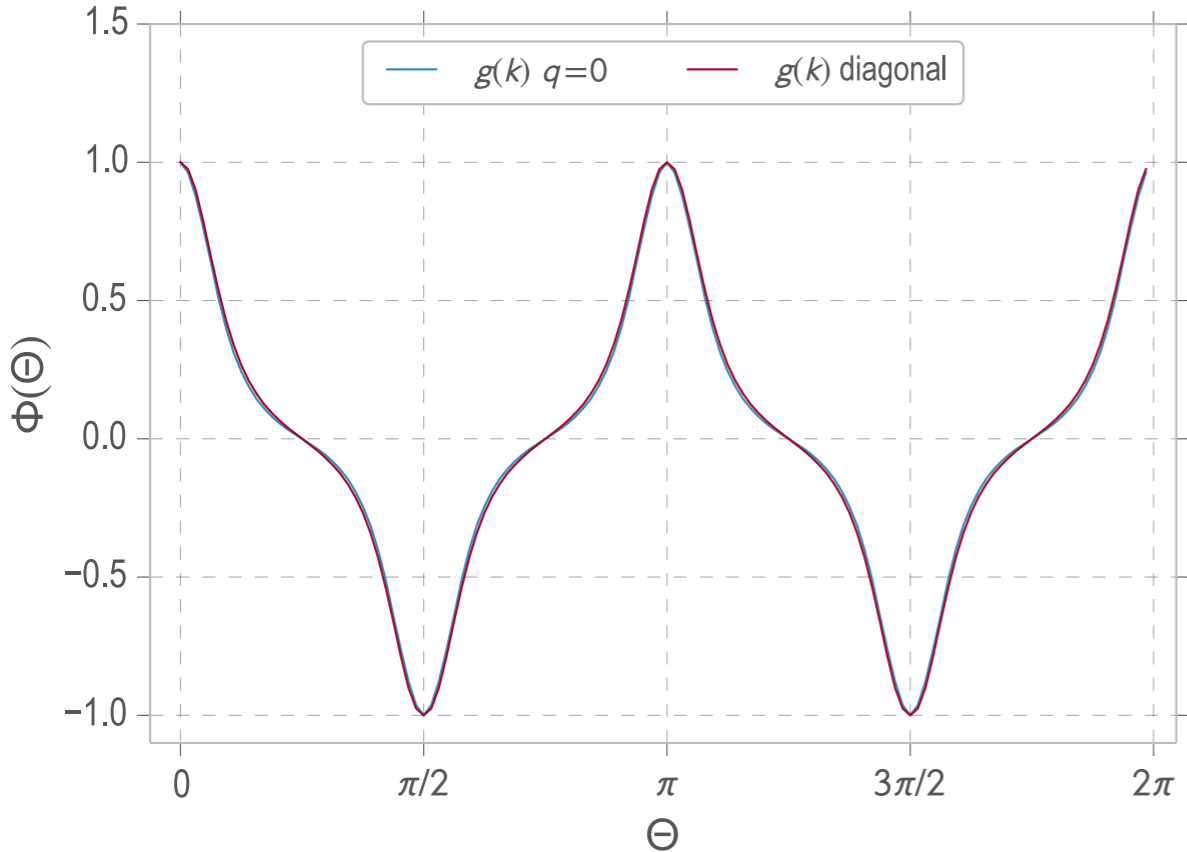


d-wave
 $\lambda_d = 1.2$

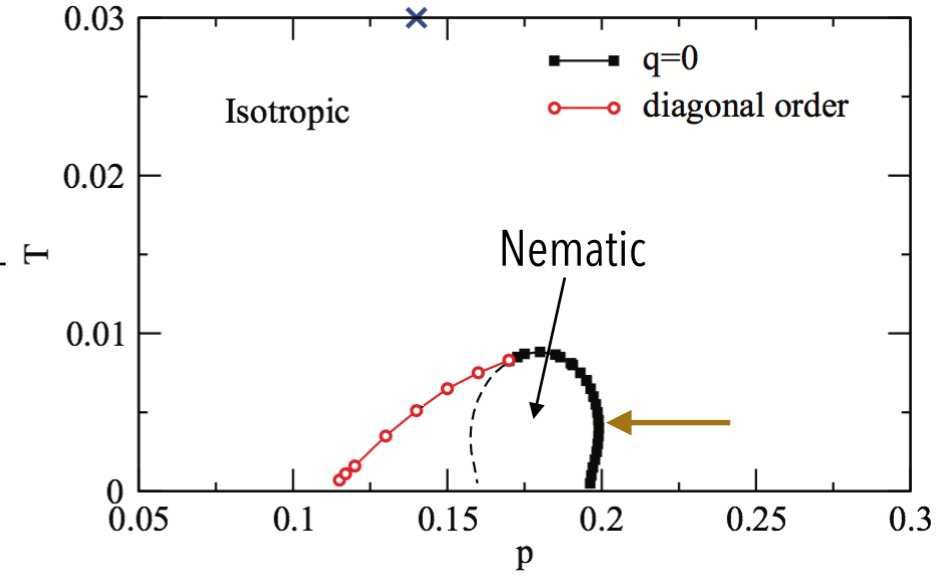


xs-wave
 $\lambda_s = 1.1$

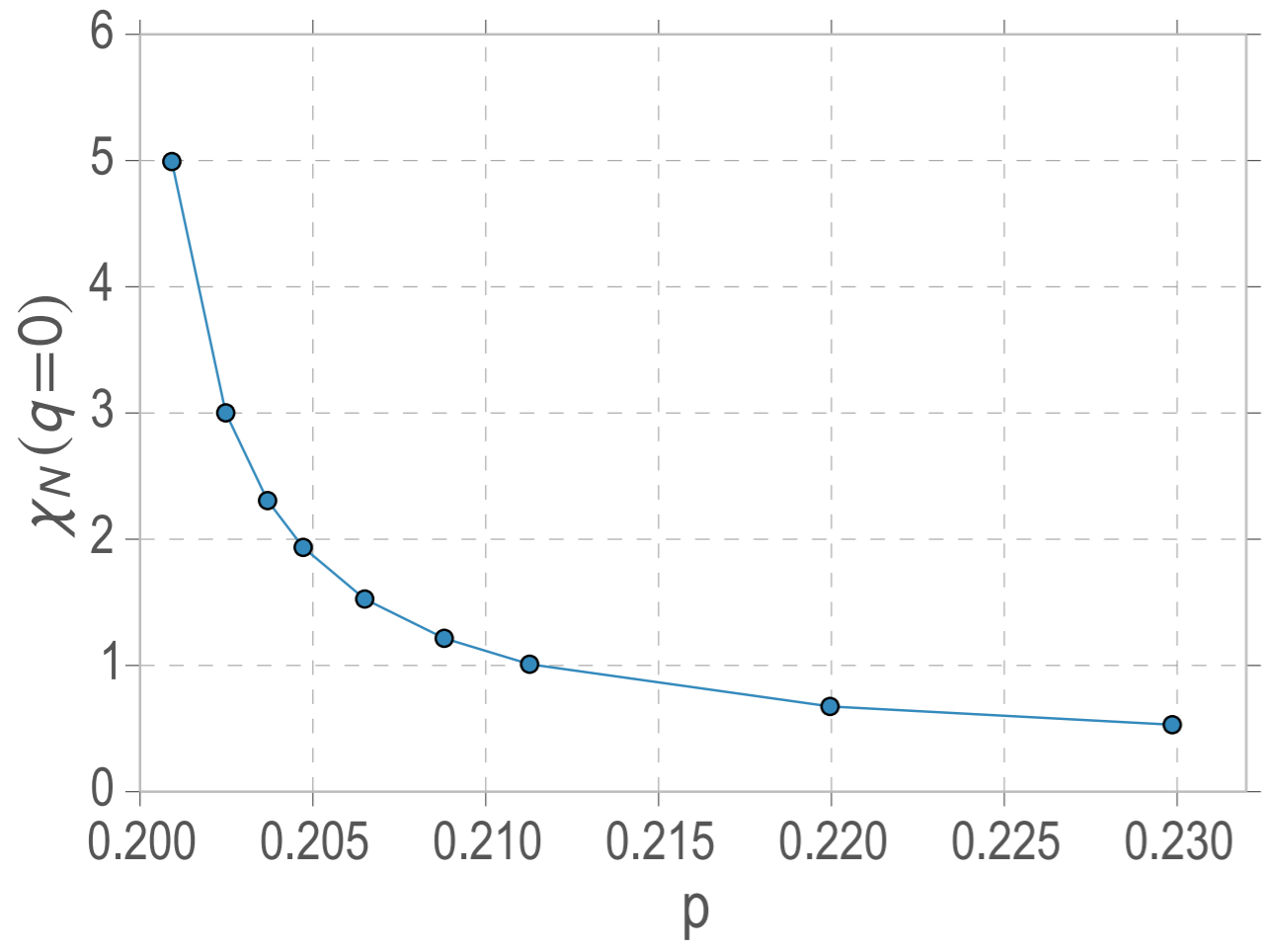
Compared to case with $q^* = 0$



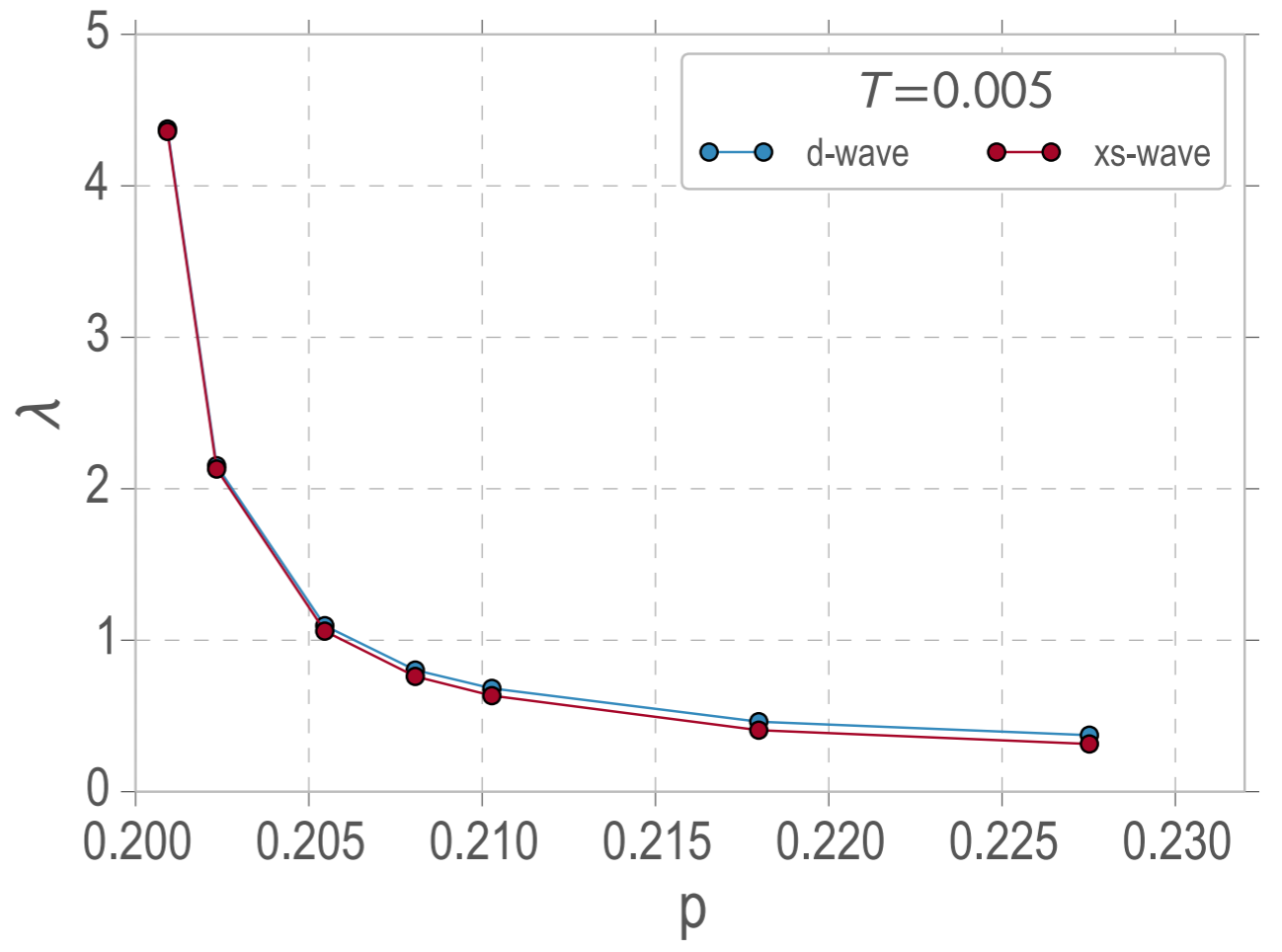
Approaching the QCP



$q = 0$ nematic susceptibility vs. doping



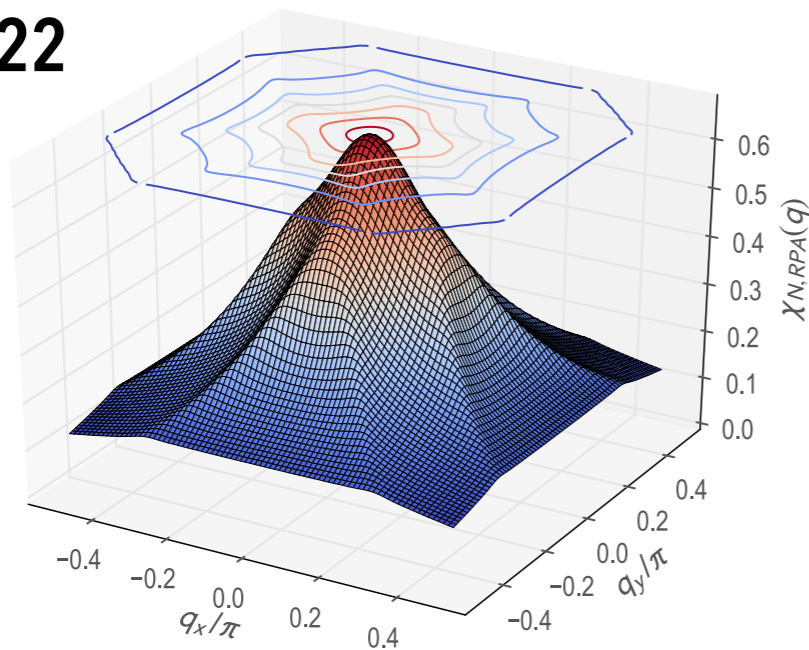
pairing strength λ vs. doping



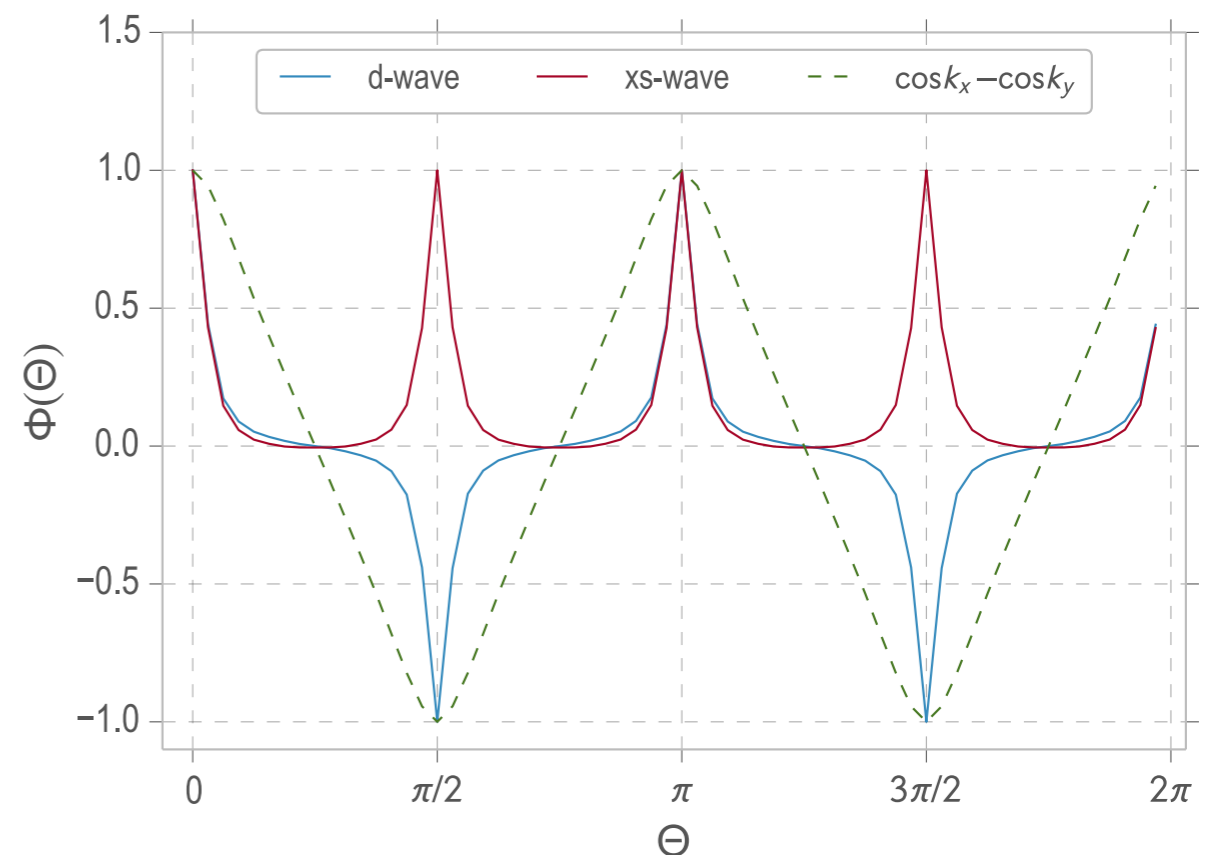
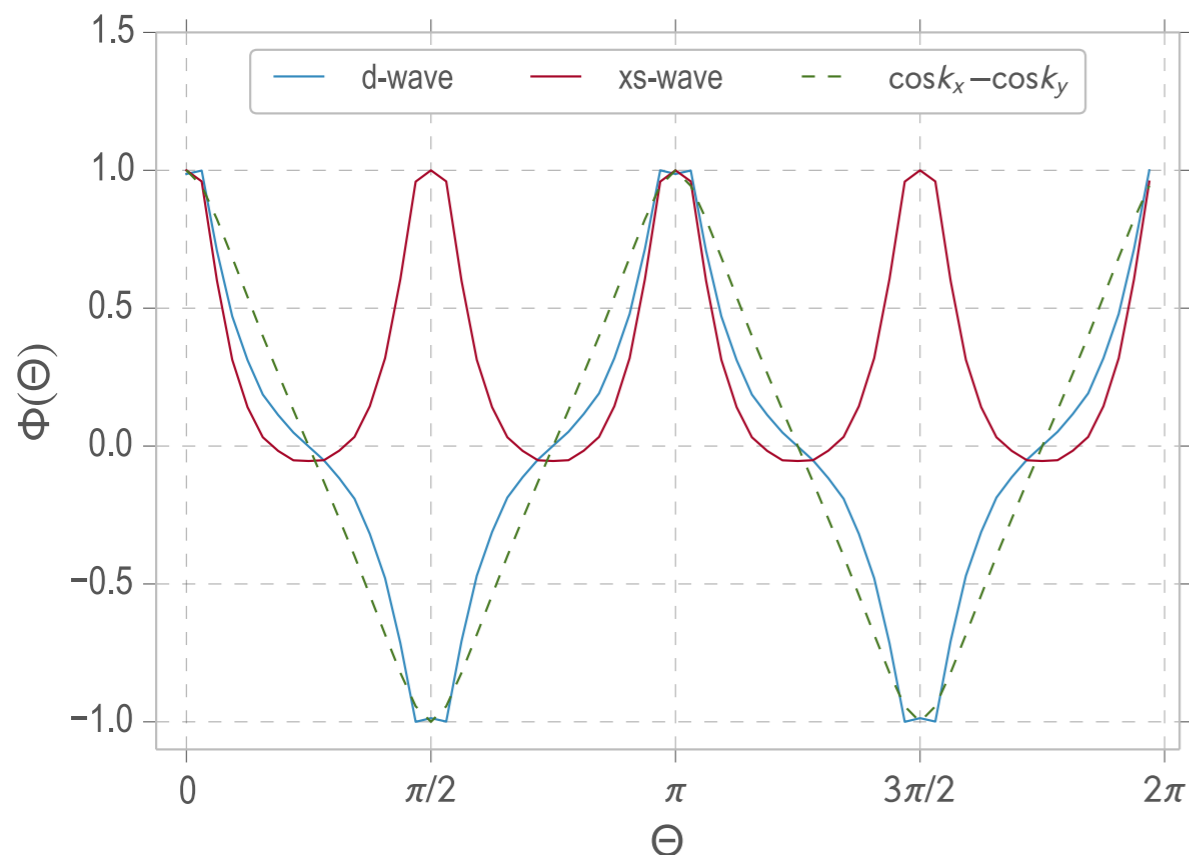
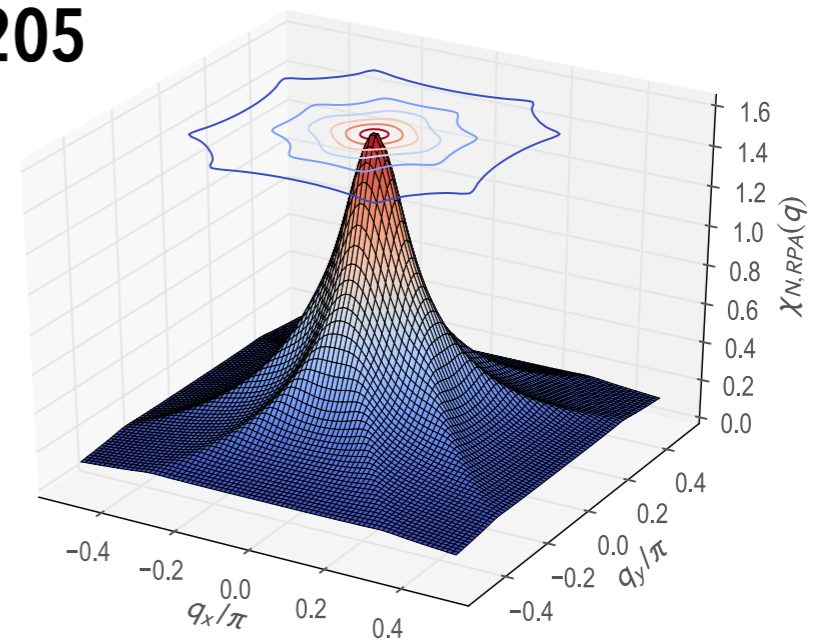
Pairing strength increases as nematic QCP is approached

Gap momentum structure on approaching the QCP

$\rho = 0.22$



$\rho = 0.205$

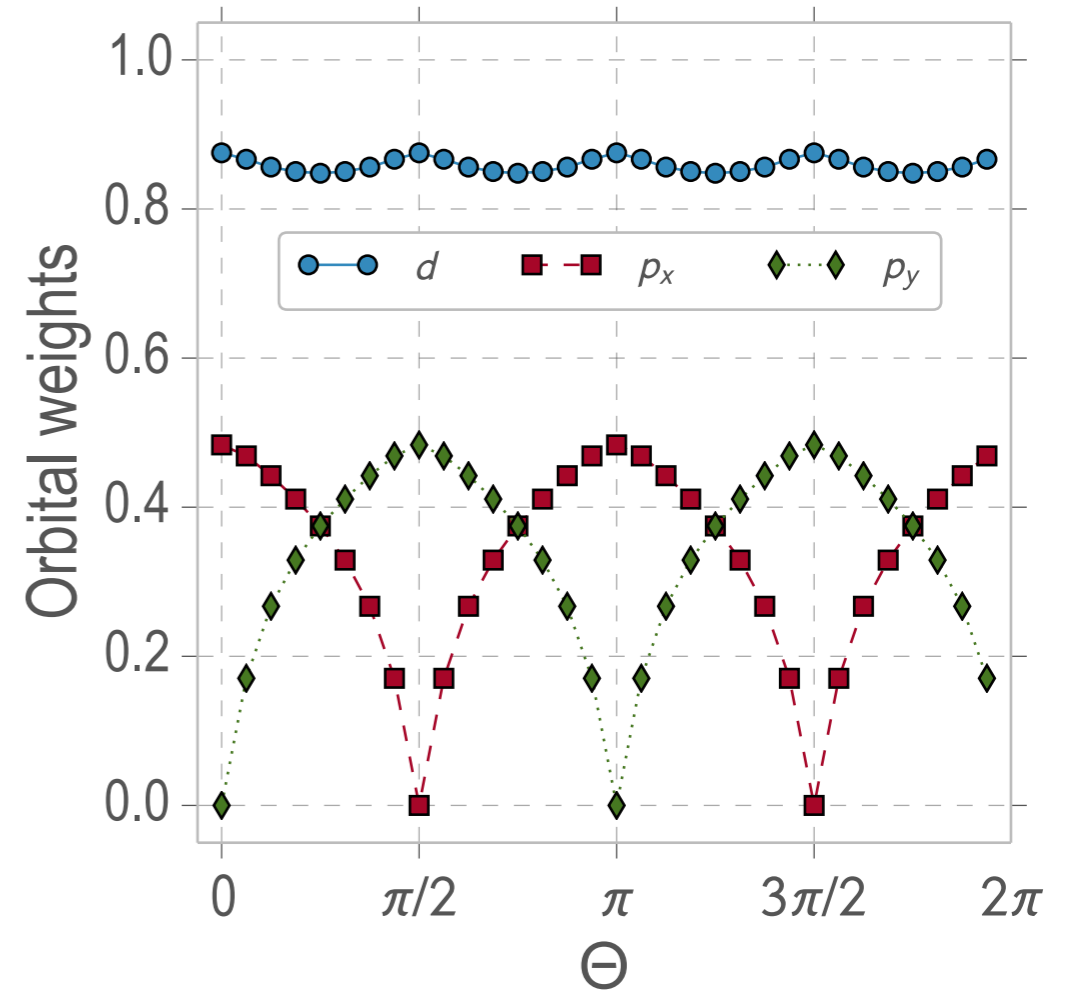
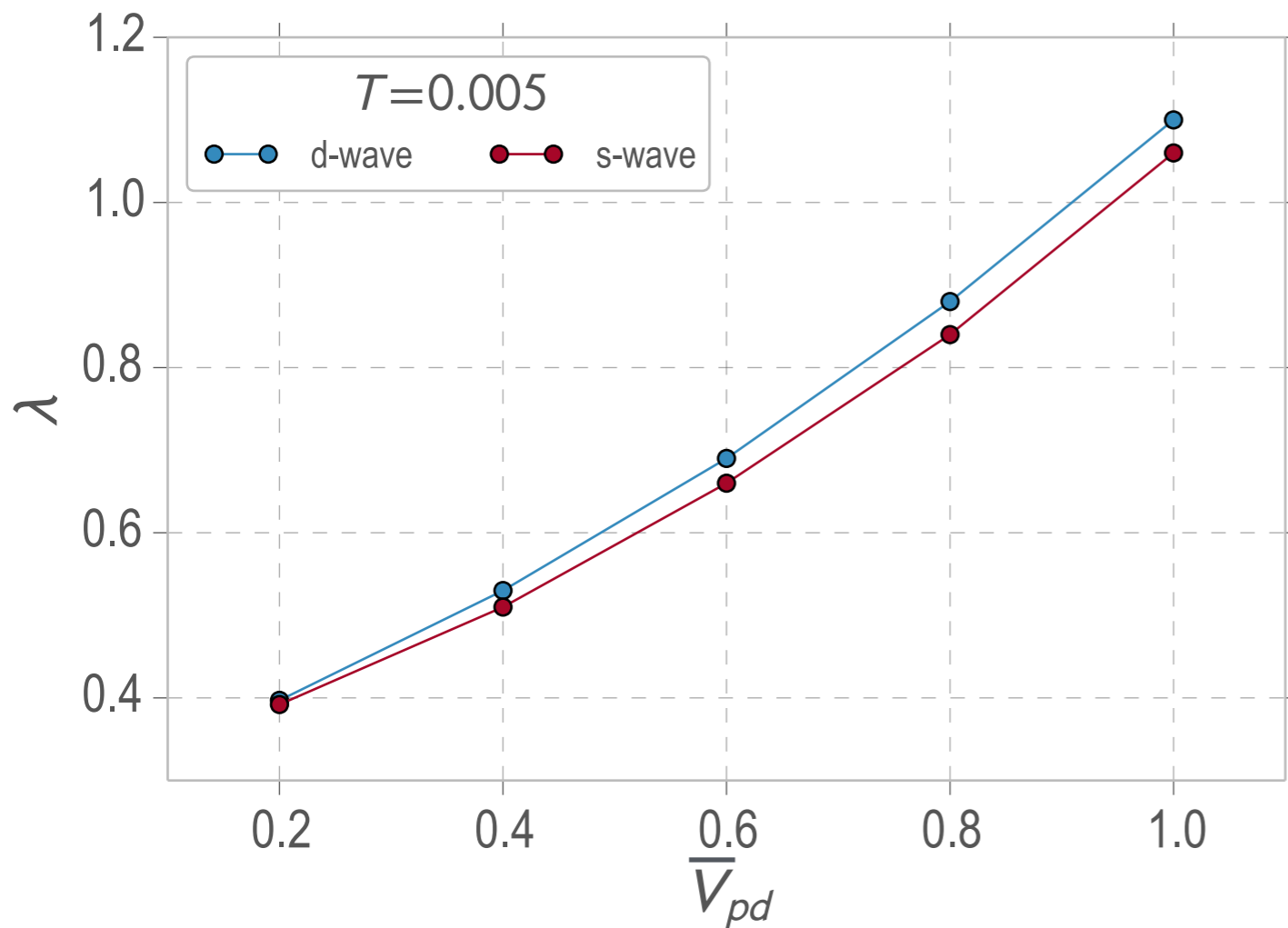


Longer ranged interaction reflected in higher *d*-wave harmonics

The role of V_{pd}

$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} \bar{V}_c \chi_{RPA}^c(k - k') \bar{V}_c$$

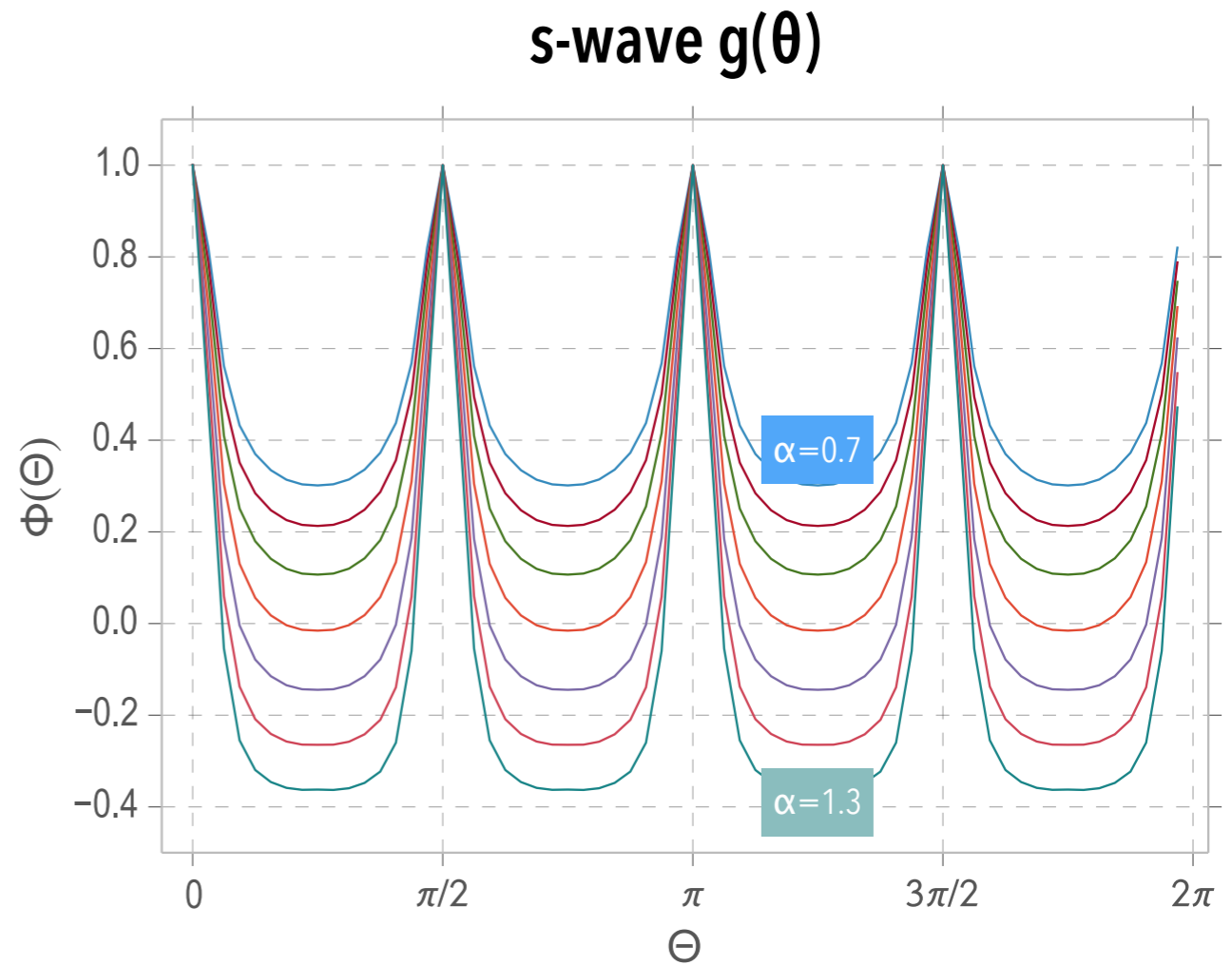
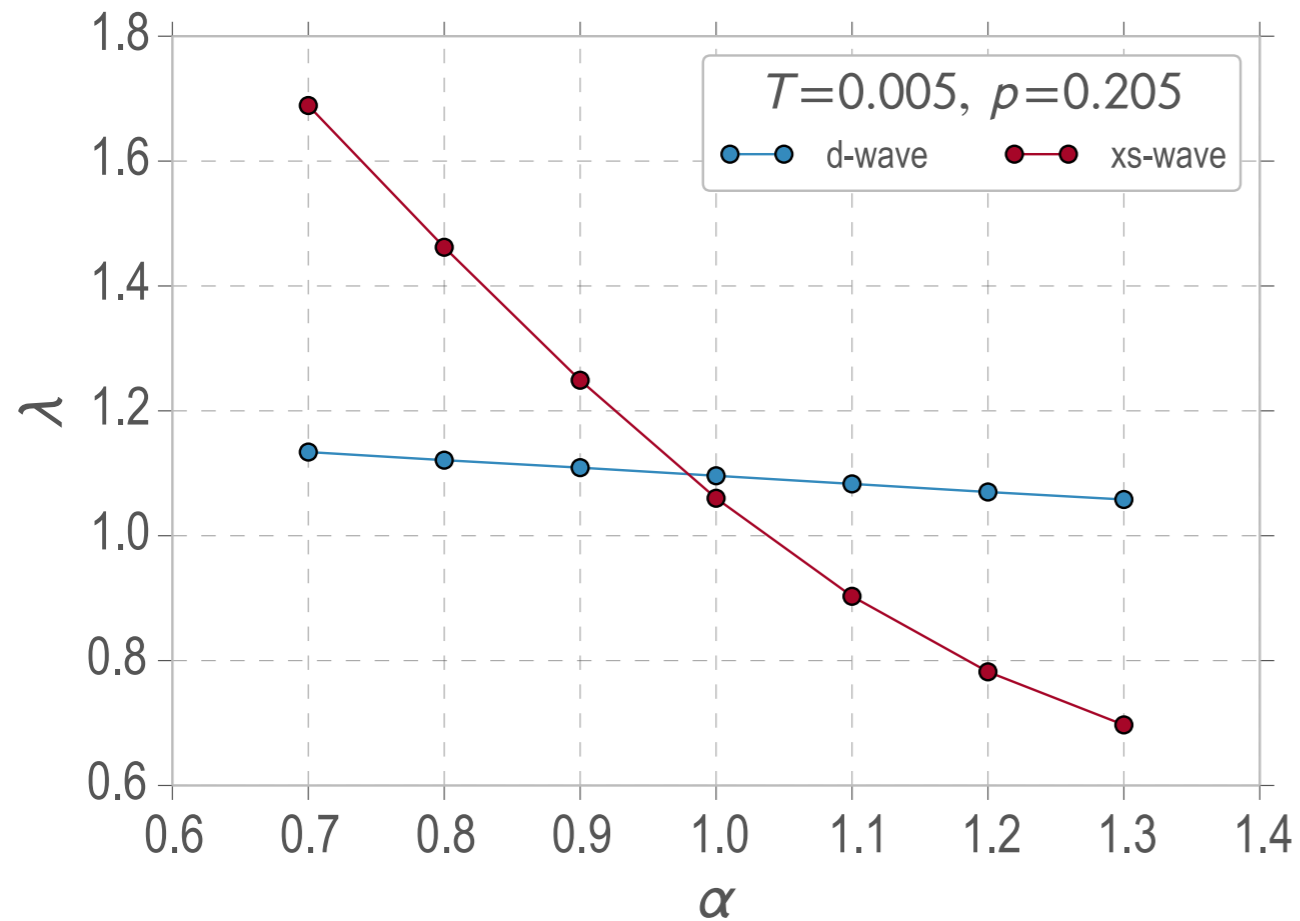
$$\Gamma_c(k, k') = \sum_{l_1, l_2, l_3, l_4} a_\nu^{l_1^*}(k) a_\nu^{l_4^*}(-k) \Gamma_{l_1 l_2 l_3 l_4}(k, k') a_\mu^{l_2}(k') a_\mu^{l_3}(-k')$$



V_{pd} couples d -band to nematic fluctuations on p -orbitals

The role of the repulsive static interaction

$$\Gamma(k, k') = \alpha \frac{V_c}{2} - \frac{1}{2} V_c \chi_{RPA}^c(k - k') V_c$$

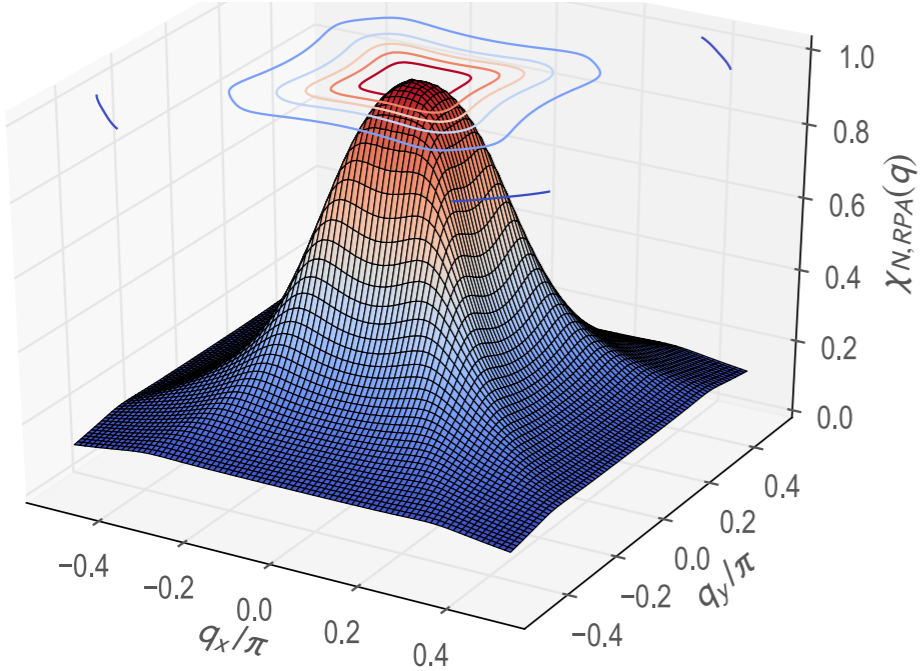


Who is the main player: Charge or spin?

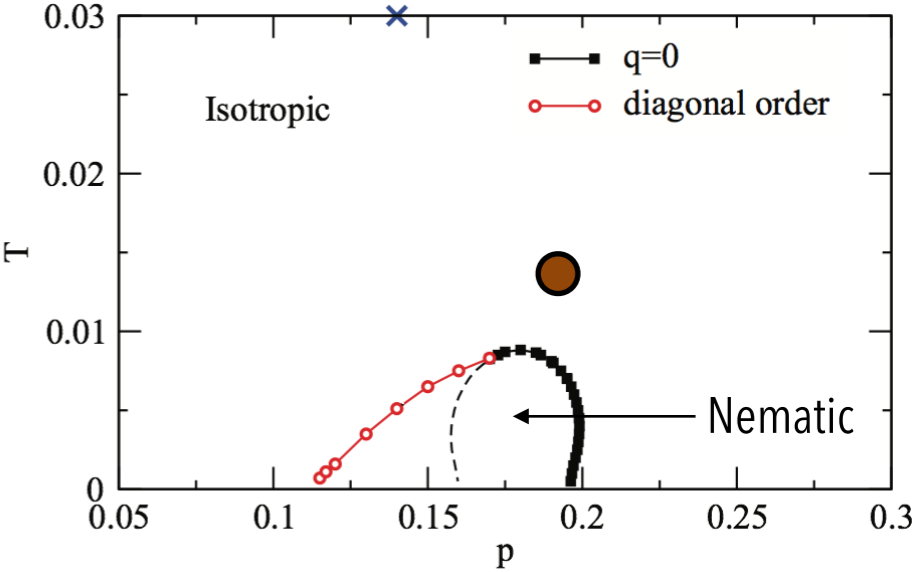
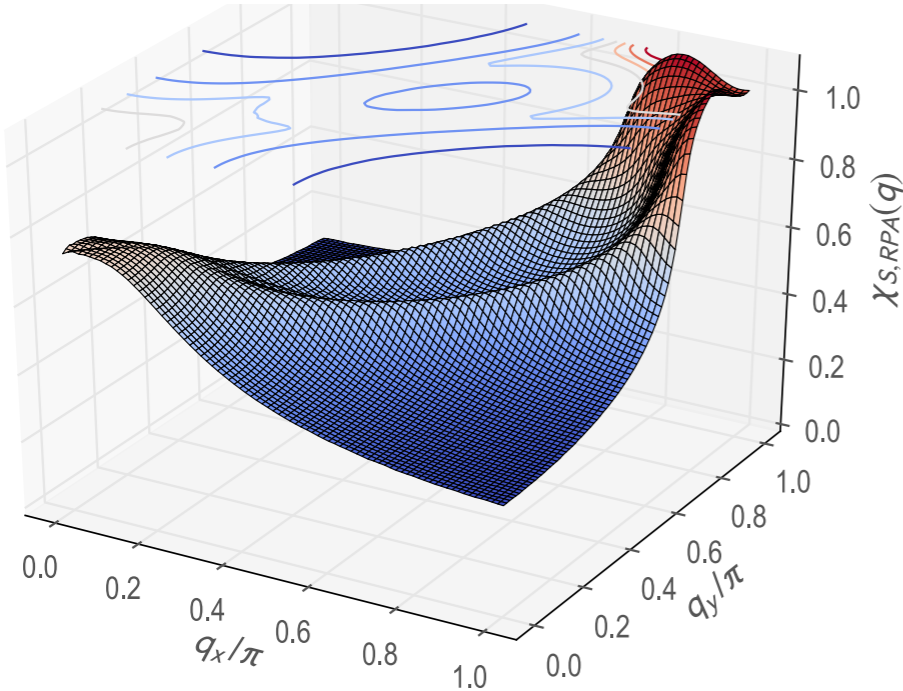
$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} \bar{V}_c \chi_{RPA}^c(k - k') \bar{V}_c$$
$$+ \frac{V_s}{2} + \frac{3}{2} \bar{V}_s \chi_{RPA}^s(k - k') \bar{V}_s$$

Charge vs. Spin

Charge susceptibility ($U_d=9, U_p=3, V_{pd}=1, V_{pp}=2$)



Spin susceptibility ($U_d=0.7, U_p=0.2, V_{pd}=0.1, V_{pp}=0.1$)



$$\Gamma(k, k') = \frac{V_c}{2} - \frac{1}{2} \bar{V}_c \chi_{RPA}^c(k - k') \bar{V}_c + \frac{V_s}{2} + \frac{3}{2} \bar{V}_s \chi_{RPA}^s(k - k') \bar{V}_s$$

$$\bar{U}_d = 4, \bar{U}_p = 1, \bar{V}_{pd} = 0.8, \bar{V}_{pp} = 0.6$$

Pairing strength from *charge* interaction: $\lambda_d = 0.76$
 Pairing strength from *spin* interaction: $\lambda_d = 16$

Conclusions

Maier & Scalapino, arXiv:1405.5238
see also: Lederer *et al.*, arXiv:1406.1193

- The nematic pairing interaction is attractive for small momentum transfer
- Nematic charge fluctuations contribute to the d-wave pairing interaction with increasing strength as the nematic QCP is approached.
- It can cooperate with the repulsive, large momentum transfer spin fluctuation interaction so that both the spin and the charge channel contribute to the d-wave pairing strength.