Thoughts Concerning the Origins and Implications of Charge Order in Correlated Electron Fluids

S. Kivelson

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In more than 1D, CDW (*and SDW*) order is generically:

Not a weak-coupling instability

Not related to Fermi surface nesting

Not well described in the context of mean-field theory

Contrary to what has been widely assumed in the cuprates, the recently discovered CDW order:

Is not related to Fermi surface nesting

Does not much affect the quasi-particle spectrum

Is probably a parasitic order

Mean field theory
(single band example)

$$1 = V(\vec{Q})\chi(\vec{Q}, T_{\vec{Q}}) \qquad\qquad T_{cdw} = \text{ Max}\left[T_{\vec{Q}}\right]$$

Ordering $\vec{Q}$ determined by $\chi(\vec{Q})$ iff it is more peaked than $V(\vec{Q})$

Ordering requires $V(\vec{Q}) > 1/\chi(\vec{Q}, 0)$

Mean field theory
(single band example)

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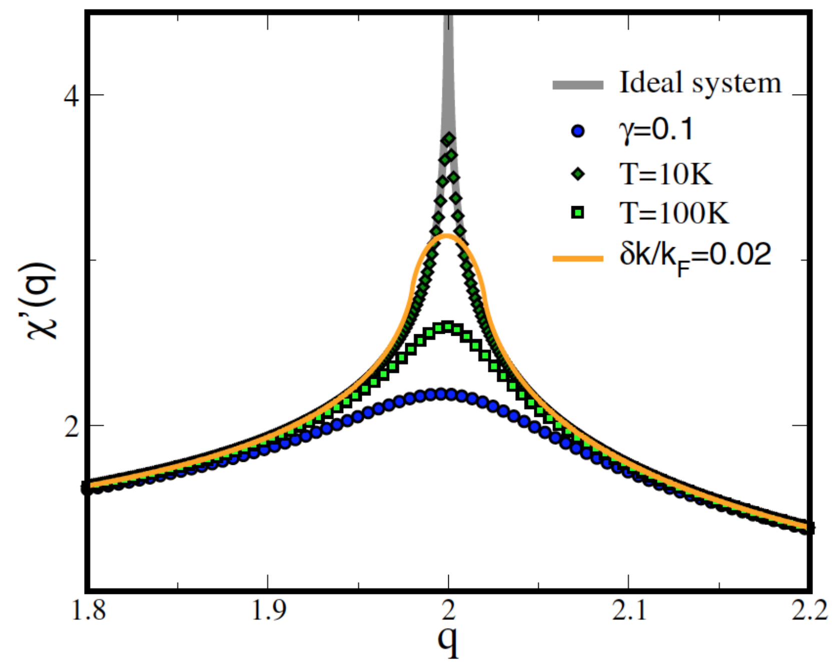
In 1D:

$$\chi(Q,0) \sim \rho(E_F)\log\left[\frac{2k_F}{|Q-2k_F|}\right]$$

$$\chi(2k_F,T) \sim \rho(E_F)\log\left[\frac{1}{\rho(E_F)T}\right]$$



from M.D. Johannes and I.I. Mazin, (2008) - $T_F \sim 10^4$K

Mean field theory
(single band example)

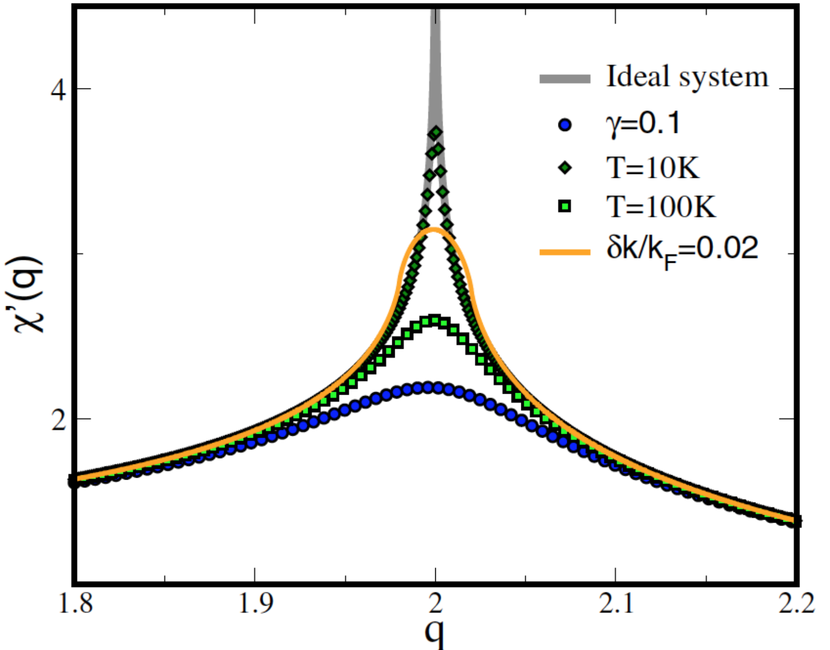
$$1 = V(\vec{Q})\chi(\vec{Q}, T_{\vec{Q}}) \qquad T_{cdw} = \text{Max}\left[T_{\vec{Q}}\right]$$

$$\text{In quasi} - \text{1D, divergence cut} - \text{off at}$$

$$T_{dim} \sim \rho(E_F)t_\perp^2 \;;\quad |\vec{Q} - 2\vec{k}_F| \sim 2k_F[\rho(E_F)t_\perp]^2$$

$$\text{In 2D}: \quad \chi(\vec{Q}, T=0) \approx \rho(E_F)$$

$$\text{In 3D}: \quad \chi(\vec{Q}, T=0) < \rho(E_F)$$



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Theory of stripes in quasi two dimensional rare-earth tritellurides, H. Yao, J.A. Robertson, E-A. Kim, and S.A.Kivelson, Phys. Rev. B **74**, 245126 (2006).

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$\text{Generally, for } D > 1 \;\; \chi(\vec{Q}) \text{ is not highly peaked}$

$$V(\vec{Q}) \text{ plays a large role in determining } \vec{Q}_{cdw}$$

$\text{Digression concerning ``Fermi surface nesting''}$

$$\text{Peak in } \chi''(\vec{Q}, \omega) \text{ vs } \chi'(\vec{Q}, \omega \to 0) \equiv \chi(\vec{Q})$$

This is important in the discussion of M.D. Johannes and I.I. Mazin, (2008)

Mean field theory
(single band example)

$$1 = V(\vec{Q})\chi(\vec{Q}, T_{\vec{Q}}) \qquad T_{cdw} = \text{ Max}\left[T_{\vec{Q}}\right]$$

Generally, for $D > 1$ $\chi(\vec{Q})$ is not highly peaked

$V(\vec{Q})$ plays a large role in determining $\vec{Q}_{cdw}$

and instability requires intermediate to strong $V(\vec{Q}) > E_F$

States near Fermi energy play no special role

Mean field theory breaks down

Local order and pseudo gaps persist above T_{cdw}

Emergence of coherence in the charge density wave state of 2H-NbSe$_2$, U. Chatterjee, J. Zhao, M. Lavarone, R. Di Capua, J. P. Castellan, G. Karapetrov,C. D. Malliakas , M. G. Kanatzidis, H. Claus, J. P. C. Ruff, F. Weber, J. Van Wezel, J. C. Campuzano, R. Osborn, M. Randeria, N. Trivedi, M. R. Norman, and S. Rosenkranz, unpublished.

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(single band example)

$$1 = V(\vec{Q})\chi(\vec{Q}, T_{\vec{Q}}) \qquad\qquad T_{cdw} = \text{ Max}\left[T_{\vec{Q}}\right]$$

There exist non generic situations in which $\chi(\vec{Q})$ is peaked

2D system with quadratic band touching

"Hidden" quasi – 1D band – structure e.g. $\mathrm{CeTe_3}$ (like $\mathrm{Sr_2RuO_4}$)

Topological Insulators and Nematic Phases from Spontaneous Symmetry Breaking in 2D Fermi Systems with a Quadratic Band Crossing, K. Sun, H. Yao, E. Fradkin, and S. A. Kivelson, Phys. Rev. Lett. **103**, 046811 (2009).

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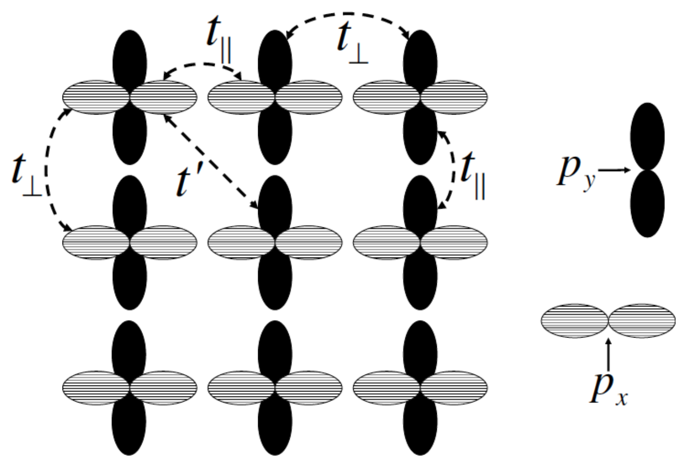

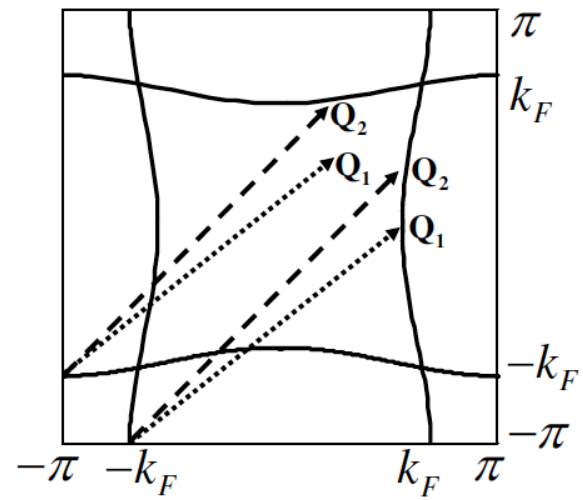

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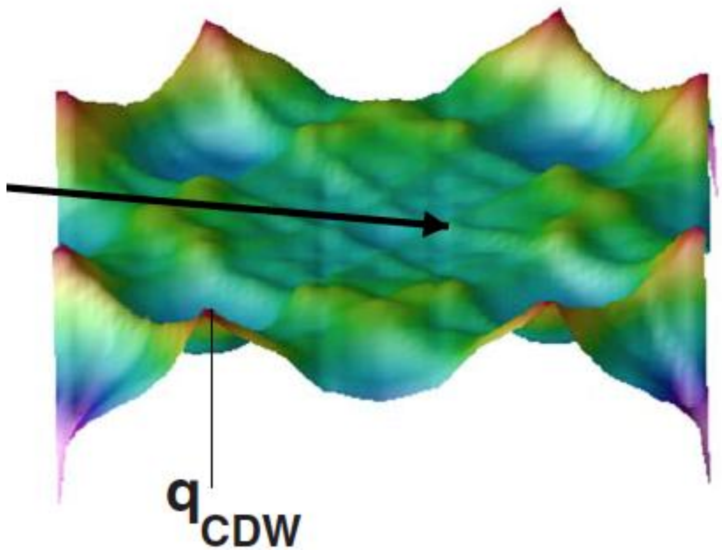
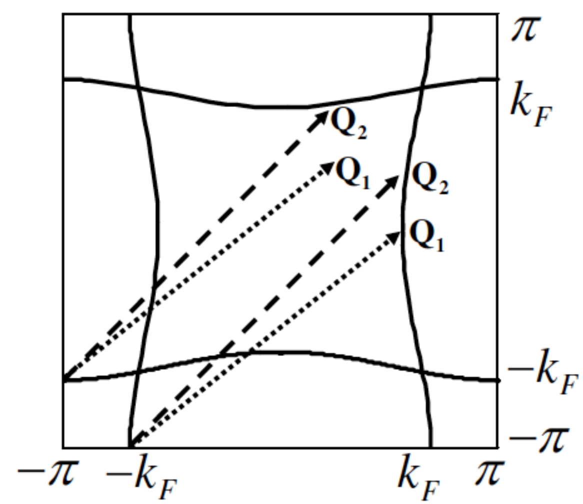
$\chi(\vec{Q}, T = 0)$





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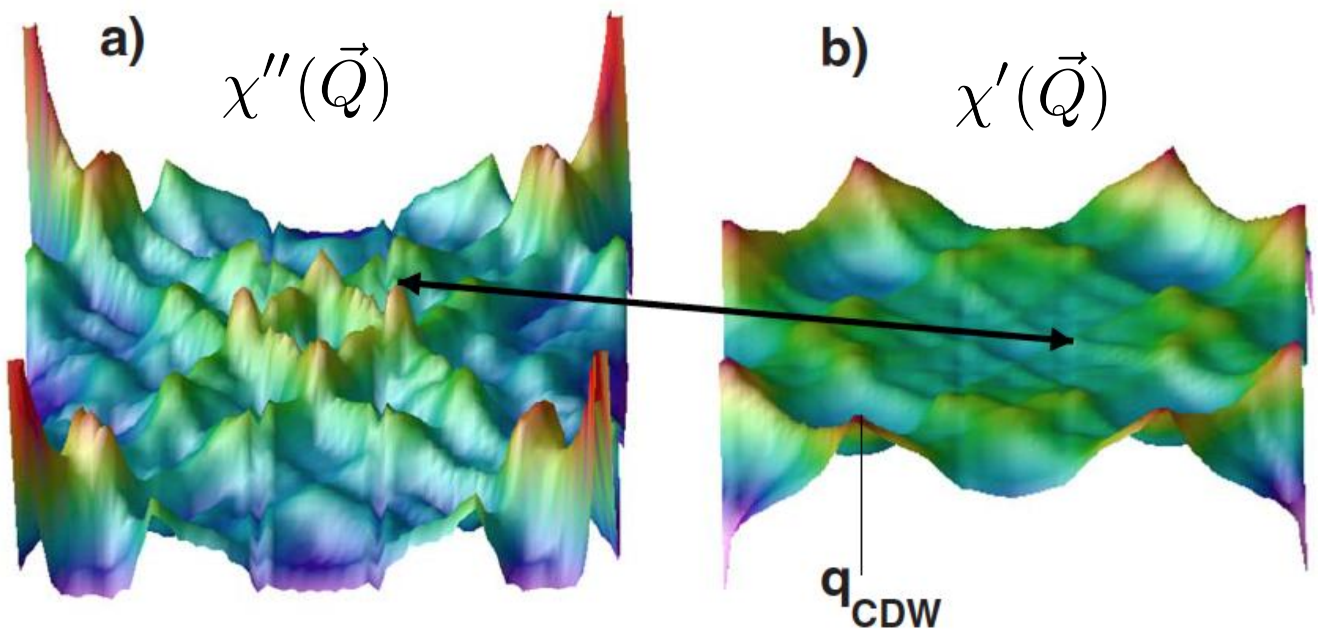

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- *Wave vector dependent electron-phonon coupling drives charge-density-wave formation in $TbTe_3$*, M. Maschek, S. Rosenkranz, R. Heid, A. H. Said, P. Giraldo-Gallo, I.R. Fisher, and F. Weber, unpublished.
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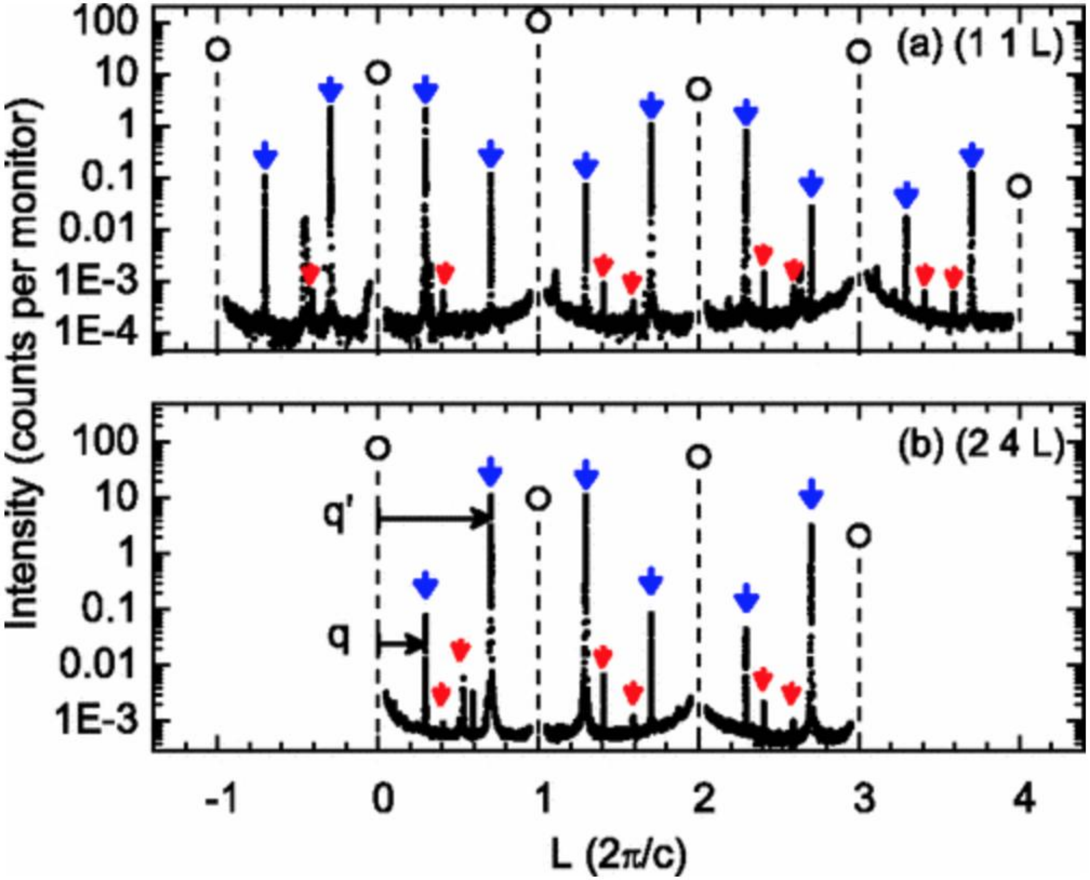
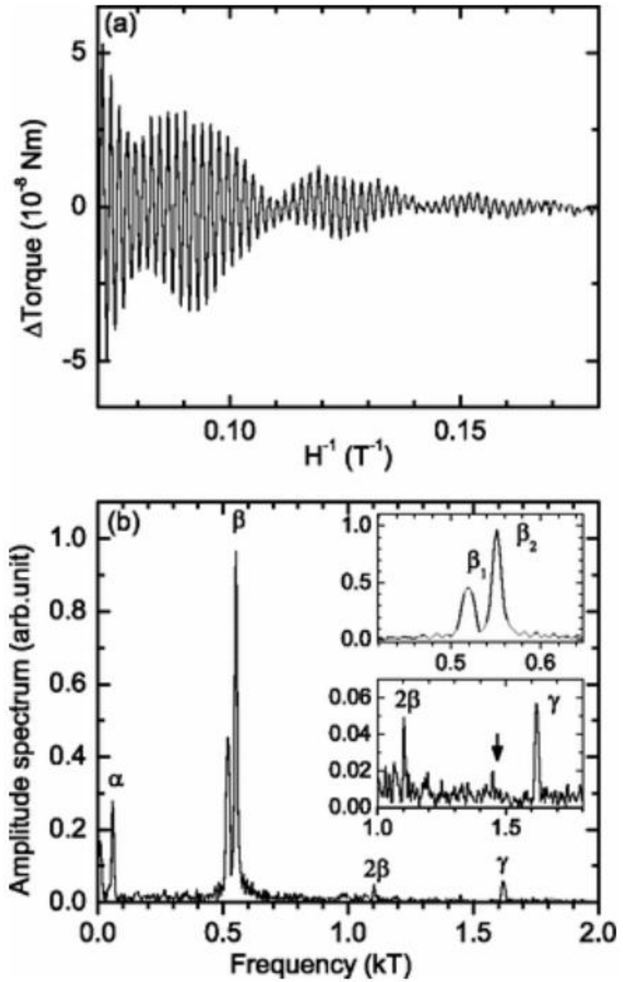
CDW in RTe_3





Effect of chemical pressure on the charge density wave transition in rare-earth tritellurides RTe_3,
N. Ru, C. L. Condron, G. Y. Margulis, K. Y. Shin, J. Laverock, S. B. Dugdale, M. F. Toney, and I. R. Fisher,
Phys. Rev. B **77**, 035114 2008;

de Haas–van Alphen oscillations in the charge density wave compound lanthanum tritellurideLaTe_3,
N. Ru, R. A. Borzi, A. Rost, A. P. Mackenzie, J. Laverock, S. B. Dugdale, and I. R. Fisher, Phys. Rev. B **78**, 2008

Some Comments About the Cuprates

The CDW tendencies in the cuprates appear to be universal:

"Bidirectional" short-range correlated (finite ξ) CDW order with ordering vectors (Q,0) and (0,Q) have been seen in:

LBCO and other 214 materials (very recently LSCO)

YBCO, Bi2201 and Bi2212, Hg1201

(In Ortho II YBCO – it is largely unidirectional but with similar Q)

and most recently in NCCO

Concerning the short-range CDW correlations observed in the cuprates

Contrary to what has been widely assumed in the cuprates, the recently discovered CDW order:

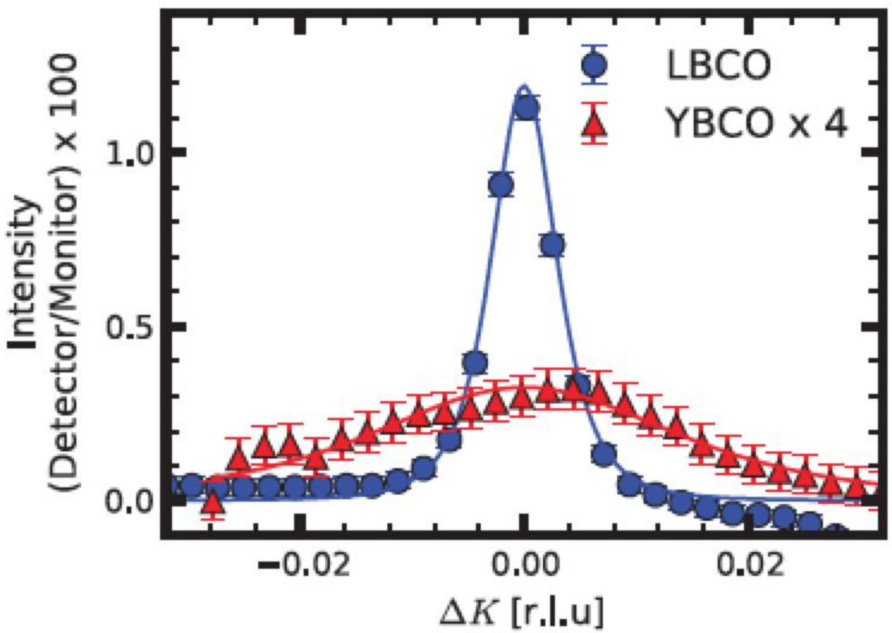
Is not related to Fermi surface nesting

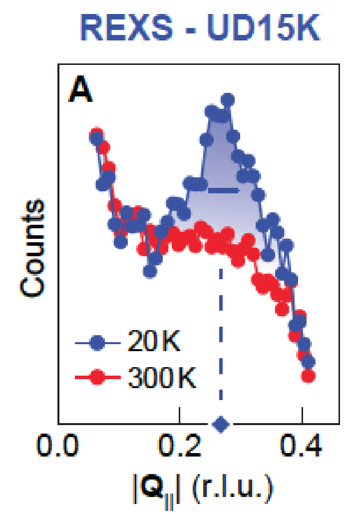
Does not much affect the quasi-particle spectrum

Is probably a parasitic order

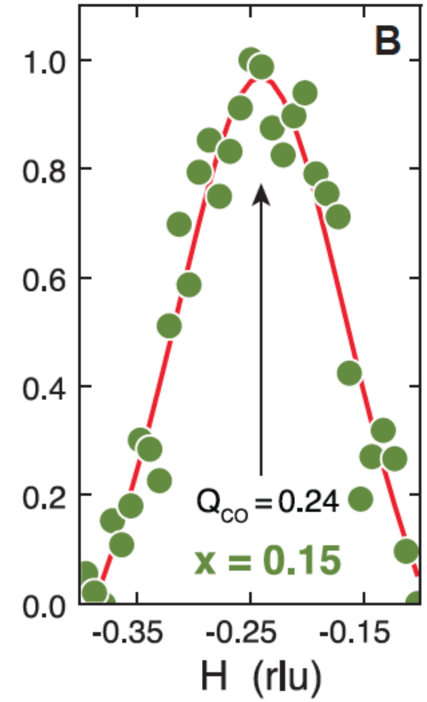
Short-range CDW order is now widely observed in the cuprates

LBCO vs YBCO with x = 1/8





BSCCO
Damascelli



NCCO
Damascelli

RXS studies by J. P. Hill and collaborators, PRB (2013)

Before discussing whether the Fermi surface structure causes the CDW, let us study the effect of the CDW on the low energy quasi-particle spectrum.

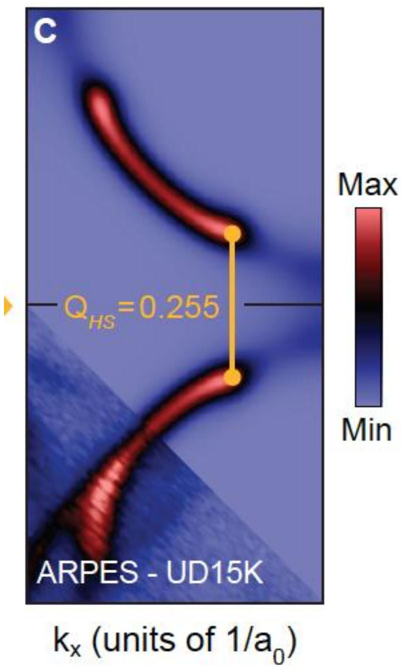
$$H_{int} = \sum_{\vec{k}} \left[\alpha(\vec{k})\ \Phi\ \psi^{\dagger}_{\vec{k}+\vec{Q}} \psi_{\vec{k}} + \text{C.C.} \right]$$

$$\text{Nesting point} : \vec{k}'_F = \vec{k}_F - \vec{Q}$$

$$E(\vec{k}_F) = E(\vec{k}'_F) = \pm |\alpha(\vec{k}_F)\Phi|$$

$$E(\vec{k}) = \pm\sqrt{|\alpha\Phi|^2 + |\vec{v}_F \cdot (\vec{k} - \vec{k}_F)|^2}$$

Concerning the short-range CDW correlations observed in the cuprates



Bi-2201
Damascelli

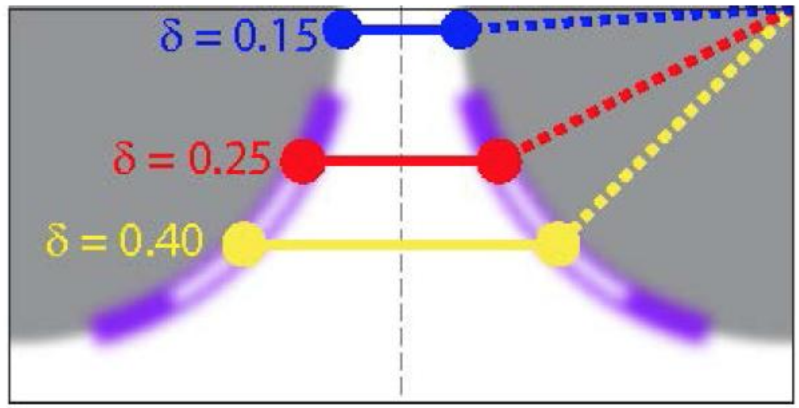
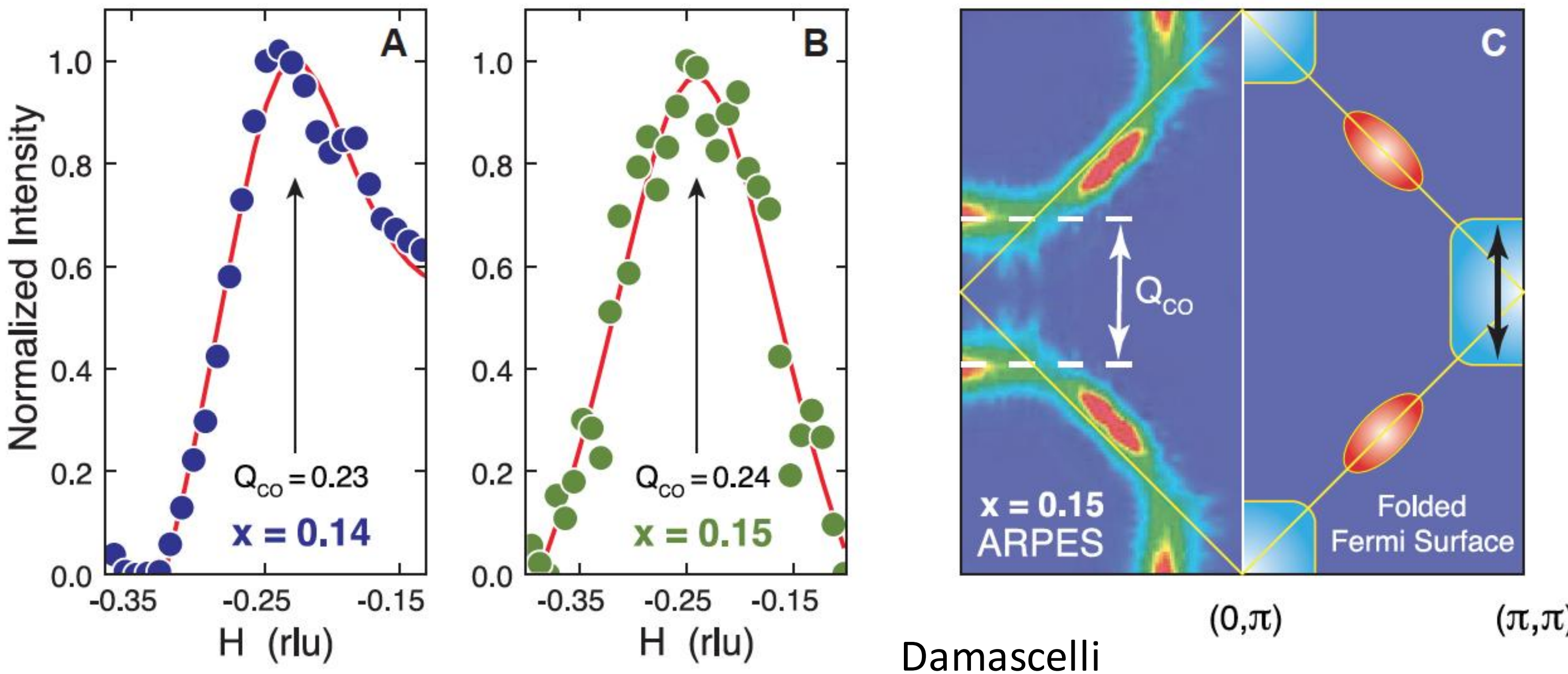


Fig. S9
Schematic of the Fermi surface of Bi-2212 for a UD75 sample showing the value of $\delta = 0.15$ for anti-nodal scattering (blue line). The red line represents the value of $\delta = 0.25$ associated to the CO in this sample. The hole barrels (dark gray) are modeled as circles, with their radii adjusted to match the location of the nodes as determined by ARPES measurements on similar samples (*29*).

Bi-2212 - Yazdani

In (certain) hole-doped cuprates, nesting occurs near "ends of nodal arcs" ---- where gap = 0

Concerning the short-range CDW correlations observed in the cuprates



Damascelli

In electron-doped cuprates, nesting condition occurs at antinodes -- where gap = 0

Before discussing whether the Fermi surface structure causes the CDW, let us study the effect of the CDW on the low energy quasi-particle spectrum.

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$$\text{Nesting point} : \vec{k}'_F = \vec{k}_F - \vec{Q}$$

$$E(\vec{k}_F) = E(\vec{k}'_F) = \pm|\alpha(\vec{k}_F)\Phi|$$

Expected gap if electrons at F.S. drive condensation :

$$\Delta \geq 2T_{CDW} \sim 40\text{meV}$$

Experimental bound roughly $\Delta \leq 5\text{meV}$

Transport measurements show strong changes at $T \sim T_{cdw}$

Therefore probably $\alpha \sim 1$ and $\Phi =$ "small"

Before discussing whether the Fermi surface structure causes the CDW, let us study the effect of the CDW on the low energy quasi-particle spectrum.

$$\text{If } \Phi \ll 2T_{cdw} \text{ it must be a subsidiary order :}$$

$$\Phi \sim \Psi^2 \;\rightarrow\; \Delta_{cdw} \sim \rho(E_F)[\Delta_{primary}]^2 \sim 2T_{cdw}[\rho(E_F)T_{cdw}]$$

Leaves open the question – what is the primary order?

$$\text{Expected gap if Fermi if electrons at F.S. drive condensation :}$$

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CDWs in the cuprates:

- *Charge order driven by Fermi-arc instability in Bi2201, R. Comin*, A. Frano, M.M.Yee, Y. Yoshida, H. Eisaki, E. Schierle, E. Weschke, R. Sutarto, F. He, A.Soumyanarayanan, Y. He, M. Le Tacon, I.S.Elfimov, J.E. Hoffman, G.A.Sawatzky, B. Keimer, and A. Damascelli, Science **343**, 390-392 (2014)
- *Ubiquitous Interplay between Charge Ordering and High-Temperature Superconductivity in Cuprates*, E.H.daSilva Neto, P.Aynajian, A. Frano, R. Comin, E. Schierle, E. Weschke, A. Gyenis, J. Wen, J. Schneeloch, Z. Xu, S. Ono, G. Gu, M. Le Tacon, A. Yazdani, Science **343**, 393-396 (2014)
- *Charge ordering in the electron-doped superconductor* $Nd_{2-x}Ce_xCuO_4$**,** E.H. da Silva Neto, R. Comin, F.He, R.Sutarto, Y.Jiang, R.L.Greene, G.A.Sawatzky, and A. Damascelli, arXiv:1410.2253
- *Theory of Intertwined Orders in High Temperature Superconductors,* E. Fradkin, S.A.Kivelson, and J.M.Tranquada, arXiv:1407.4480.
- *Quenched disorder and vestigial nematicity in the pseudo-gap regime of the cuprates,* L. Nie, G. Tarjus, and S.A.Kivelson, PNAS **111**, 7980 (2014).

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- *Extended Phonon Collapse and the Origin of the Charge-Density-Wave in $NbSe_2$*, F. Weber, S. Rosenkranz, J.-P. Castllan, R. Osborn, R. Hott, R. Heid, K.-P. Bohnen, T. Egami, A. H. Said, and D. Reznik, Phys. Rev. Lett. 107, 107403 (2011)