Title: Phenomenology of charge order in underdoped cuprates

Date: May 27, 2014 03:00 PM

URL: http://pirsa.org/14050147

Abstract: In the past few years substantial evidence has been collected that points to coexistence of charge correlations with long range superconductivity in underdoped cuprate superconductors. In this talk I will review some of this evidence, then show that a charge density wave with precisely the same signatures is a natural instability of an antiferromagnetic metal, and finally derive some phenomenological consequences, with special focus on quantum oscillation experiments.

Phenomenology of charge order in underdoped cuprates

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Harvard University

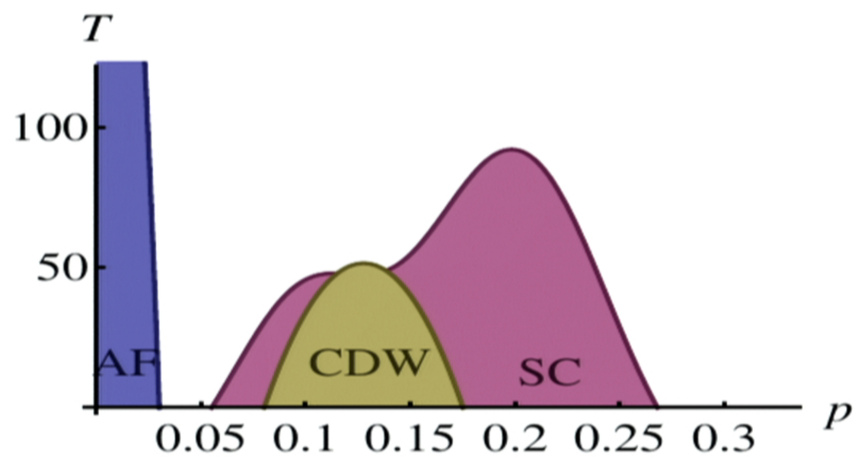
1402.4807, 1402.6311 AA, J. Bauer and S. Sachdev

1405.???? AA, D. Chowdhury and S. Sachdev

Outline

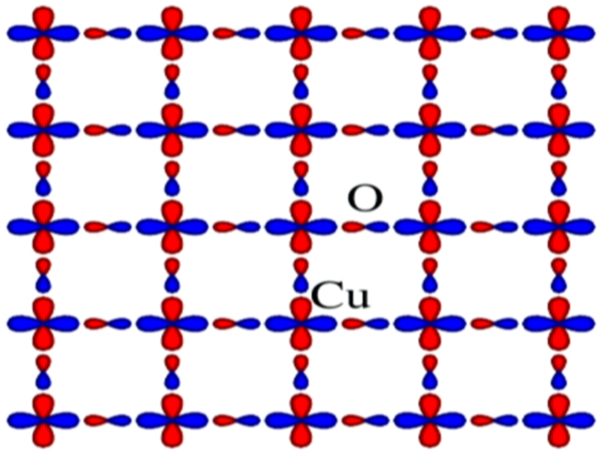
Charge order correlations ubiquitous in underdoped cuprates

- Review of experimental evidence
- Derive as natural consequence of simple model
- Some model phenomenology, especially quantum oscillations



Cuprates

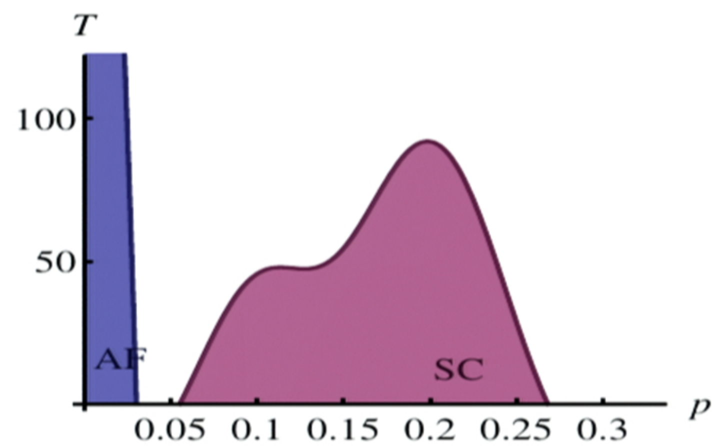
- Layered, quasi 2d materials
- Intrinsic material: 1 electron per unit cell, but insulating (Mott insulator)
- Long range antiferromagnetic (AF) order



Cuprates

When doped with holes:

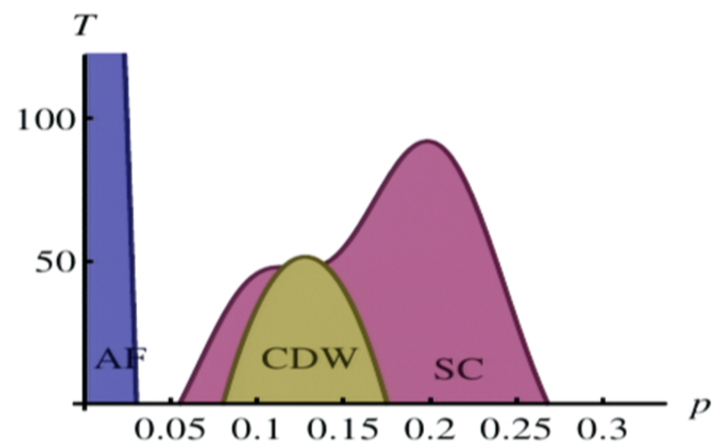
- AF order destroyed
- Bad conductor
- Superconducting at (not so) low temperature



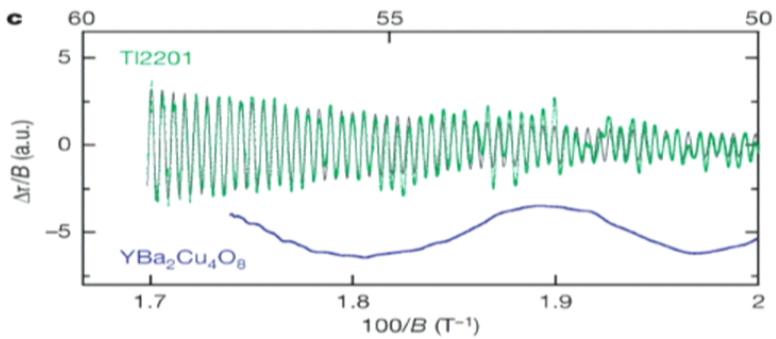
Charge density wave

Now also charge density wave

- Indications from quantum oscillations, transport, STM, Resonant and hard X ray scattering
- Short range at $\boldsymbol{B} = 0$. Stabilized, possibly long range at large $\boldsymbol{B}$.
- Competes with SC

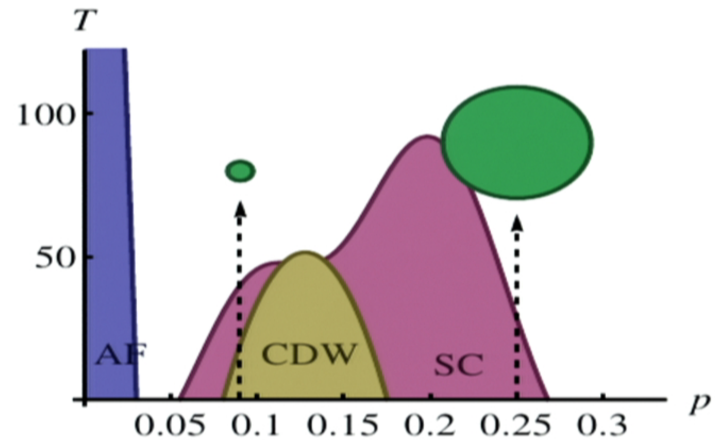


Quantum oscillations



Vignolle *et al.* Nature 2008

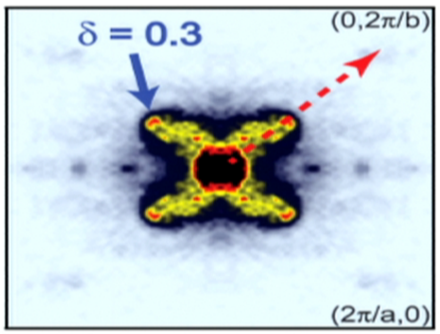
Fermi surface reconstruction.



STM and REXS

Charge density wave

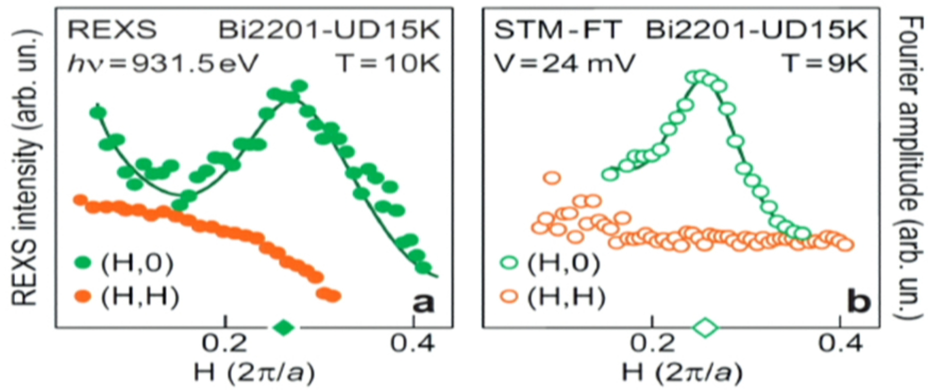
$$\rho(\boldsymbol{x}) \sim \cos \boldsymbol{Q} \cdot \boldsymbol{x} \qquad \boldsymbol{Q} \parallel \text{CuO bonds}$$



Neto *et al.* Sci. **343**, 393

Bi-2212, STM Fourier space

$T \sim T_c = 45K$

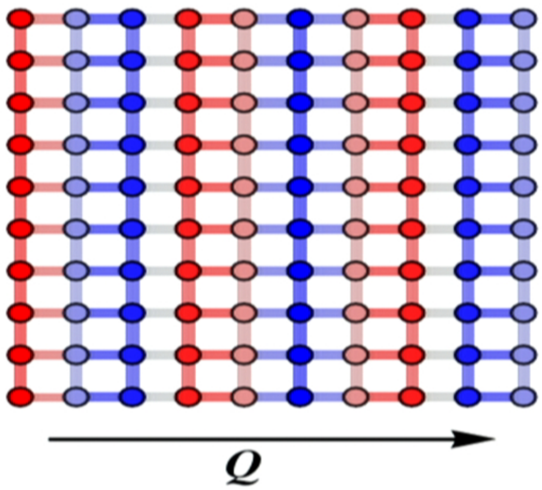


Comin *et al.* 1402.5415

Nontrivial form factor

$$\left\langle c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}} \right\rangle = -T_{\boldsymbol{a}} + \phi_{\boldsymbol{a}} \cos \boldsymbol{Q} \cdot (\boldsymbol{x} + \boldsymbol{a}/2)$$

- Disks represent $\langle c^\dagger_{\boldsymbol{r}} c_{\boldsymbol{r}} \rangle$
- Bonds represent $\langle c^\dagger_{\boldsymbol{r}} c_{\boldsymbol{r}+\boldsymbol{a}} \rangle$
- Blue is above average, red is below average
- s-wave form factor



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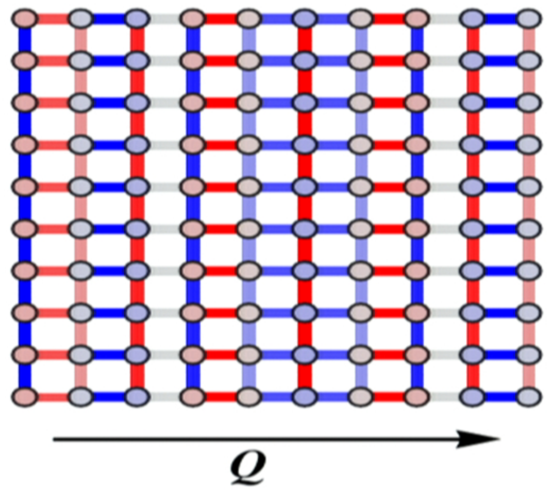
- Blue is above average, red is below average
- d-wave form factor



Nontrivial form factor

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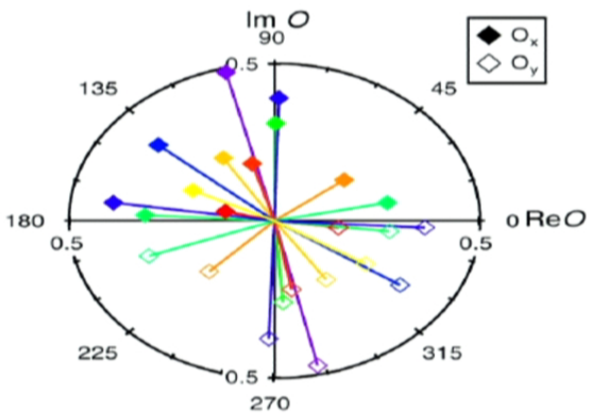
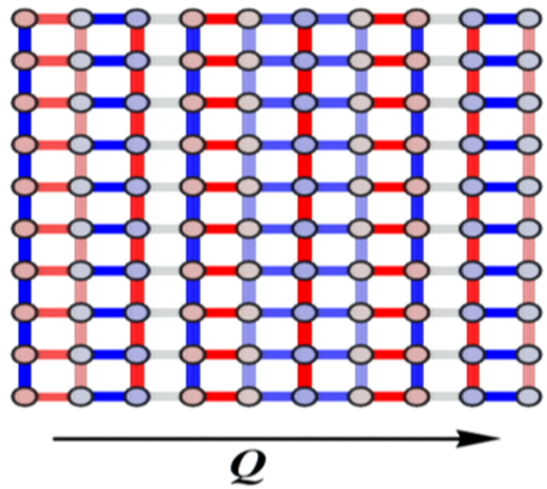
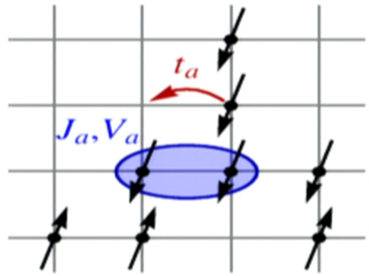


Fujita *et al.* 1404.0362



From a model

t-J-V model



$$H_{tJV} = \sum_{\boldsymbol{x},\boldsymbol{a}} \left[-t_{\boldsymbol{a}} c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}} + \frac{1}{2} J_{\boldsymbol{a}} \, \boldsymbol{S}_{\boldsymbol{x}+\boldsymbol{a}} \cdot \boldsymbol{S}_{\boldsymbol{x}} + \frac{1}{2} V_{\boldsymbol{a}} \, n_{\boldsymbol{x}+\boldsymbol{a}} n_{\boldsymbol{x}} \right]$$

$$n_{\boldsymbol{x}}(n_{\boldsymbol{x}} - 1)\,|\mathrm{phys}\rangle = 0 \quad \text{(no double occupancy)}$$

Look for order

$$\left\langle c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}} \right\rangle = -\bar{T}_{\boldsymbol{a}} + \bar{\phi}_{\boldsymbol{a}} \cos \boldsymbol{Q} \cdot (\boldsymbol{x} + \boldsymbol{a}/2)$$

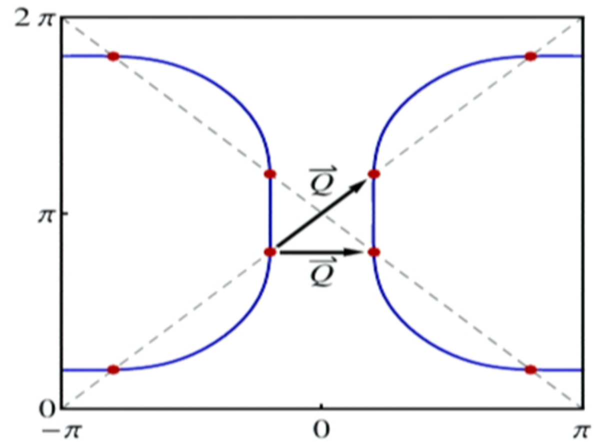
Hot spots

Without constraint (antiferromagnetic metal):

- d-wave CDW
- Wavevector $\boldsymbol{Q}$ connecting hot spots
- Diagonal $\boldsymbol{Q}$ always preferred

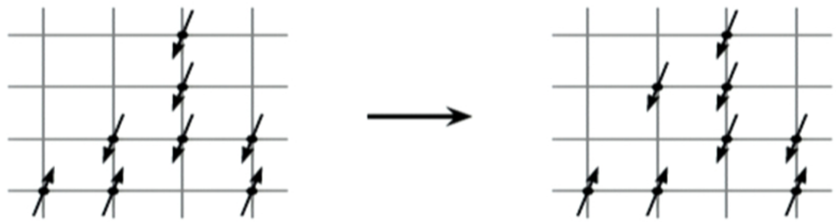
Sachdev *et al.* PRL **111** 027202

Metlitsky *et al.* PRB **82**, 075128

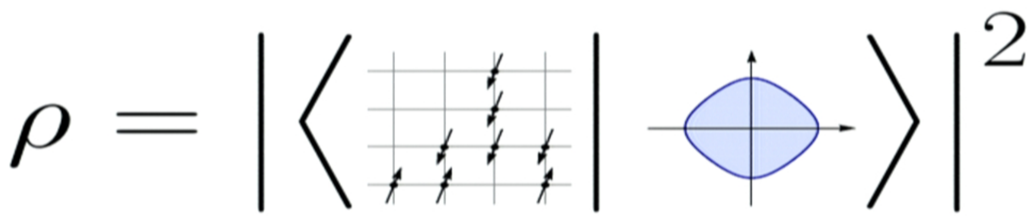


Variational Monte Carlo

Monte Carlo sample configurations



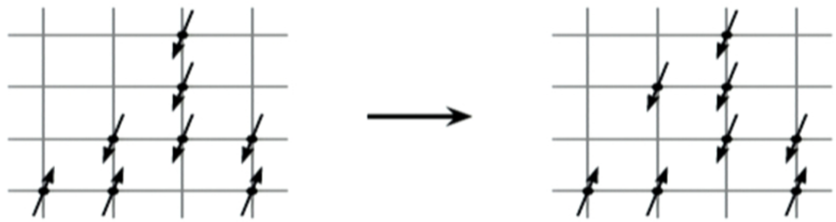
according to weight



excluding doubly occupied states.

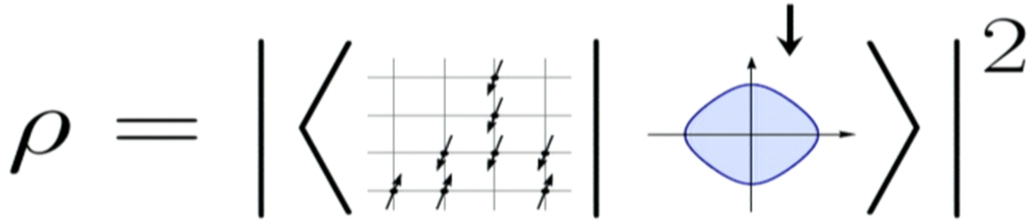
Variational Monte Carlo

Monte Carlo sample configurations



according to weight

Ground state of free fermion hamiltonian H_{var}



excluding doubly occupied states.

Variational hamiltonian

$$H_{\rm var} = \sum_{\boldsymbol{x},\boldsymbol{a}} \left[-T_{\boldsymbol{a}} + \phi_{\boldsymbol{a}} \cos \boldsymbol{Q} \cdot (\boldsymbol{x} + \boldsymbol{a}/2)\right] c^{\dagger}_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}}$$

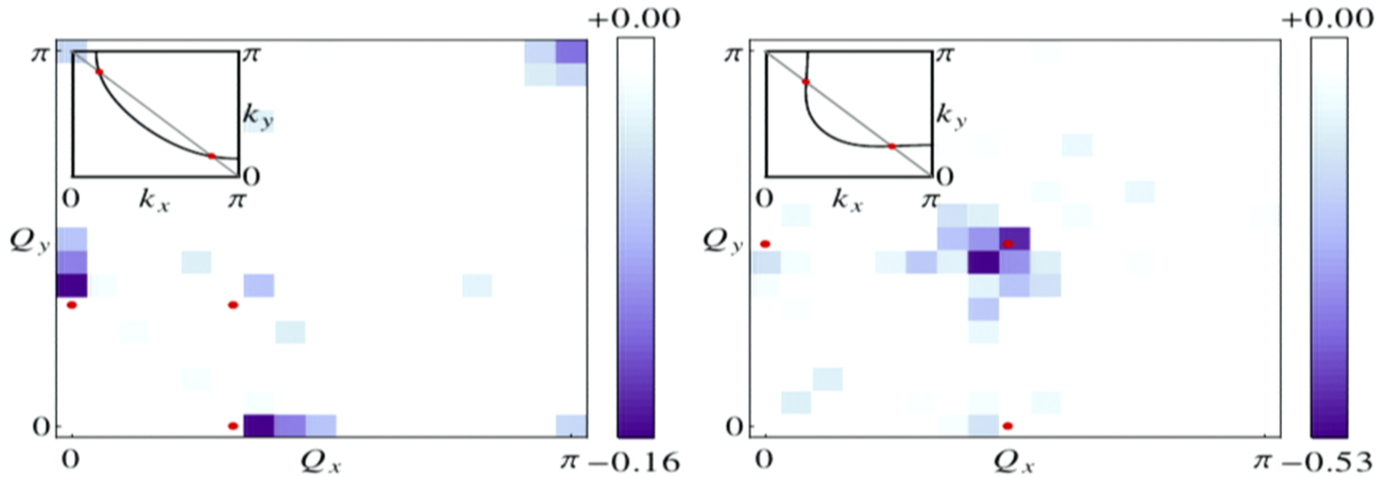
Minimize

$$E_{\rm var} = \langle H_{tJV} \rangle_{\rm var} \ ,$$

with $T_{\boldsymbol{a}}$, $\phi_{\boldsymbol{a}}$, $\boldsymbol{Q}$ variational parameters. If optimal $\phi_{\boldsymbol{a}} \neq 0$, then order is induced

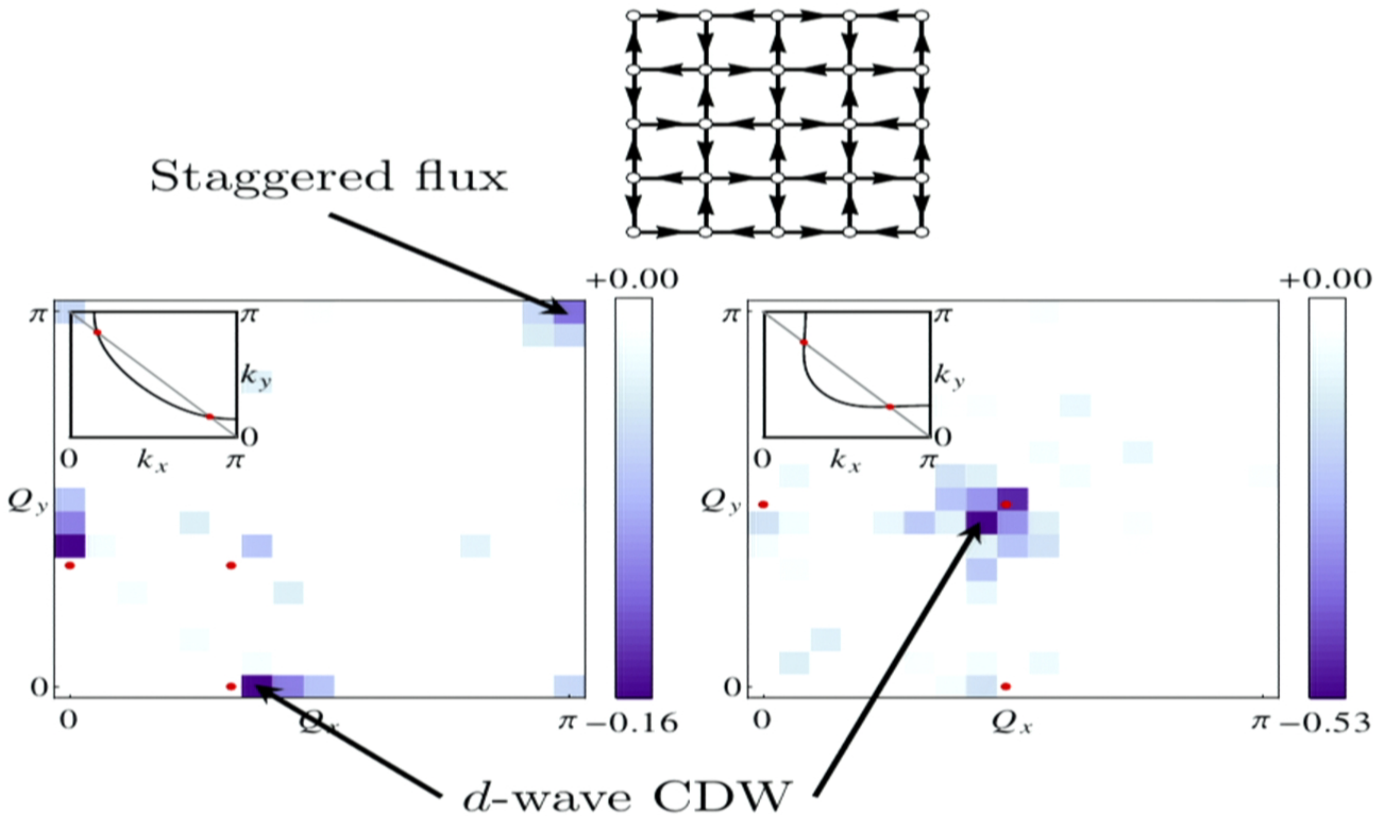
$$\left\langle c^{\dagger}_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}} \right\rangle = -\bar{T}_{\boldsymbol{a}} + \bar{\phi}_{\boldsymbol{a}} \cos \boldsymbol{Q} \cdot (\boldsymbol{x} + \boldsymbol{a}/2)$$

Variational analysis

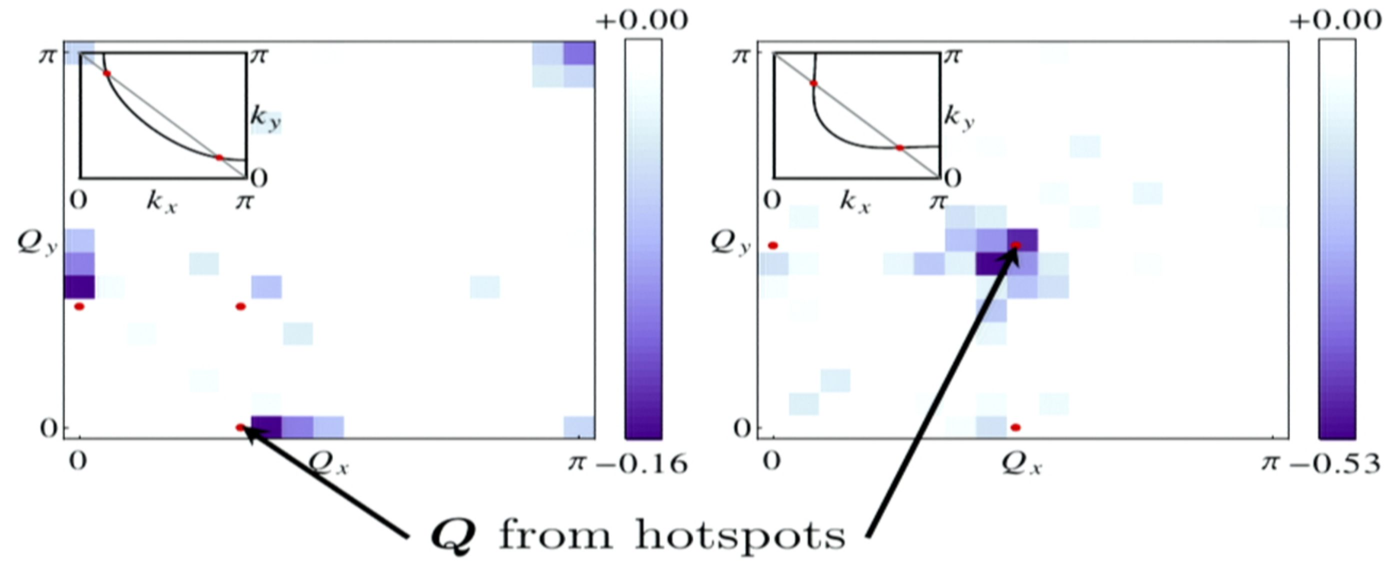


Allais *et al.* 1402.4807

Variational analysis

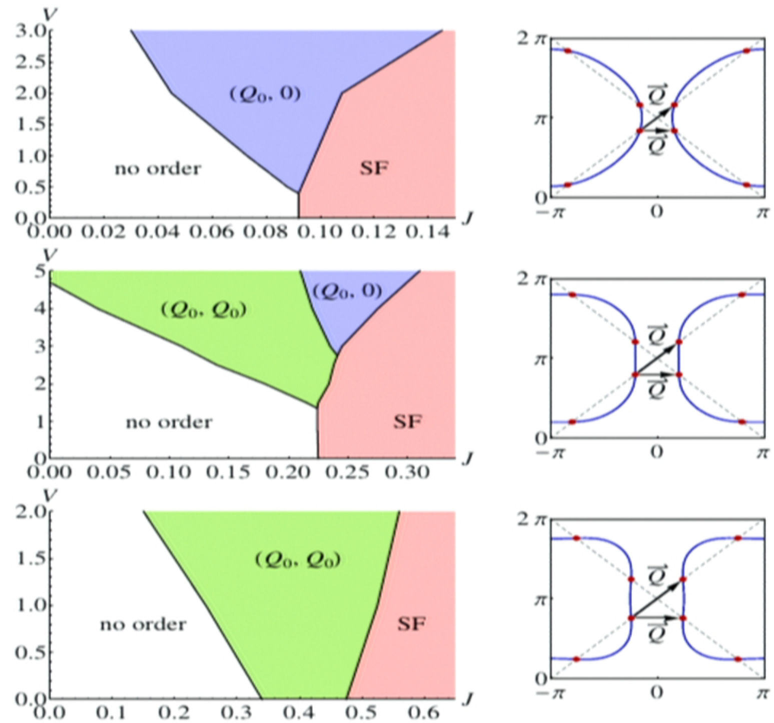


Variational analysis



Variational analysis

- CDW with diagonal wavevector
- CDW with wavevector || CuO bond
- Staggered flux state
- Correlations and V necessary



Quantum oscillations phenomenology

Landau quantization

$$H = -\sum_{\boldsymbol{r},\boldsymbol{a}} t_a \exp\left[\mathrm{i}\int_{\boldsymbol{r}}^{\boldsymbol{r}+\boldsymbol{a}} \boldsymbol{A}(\boldsymbol{\ell}) \cdot \mathrm{d}\boldsymbol{\ell}\right] |\boldsymbol{r}+\boldsymbol{a}\rangle \langle \boldsymbol{r}|$$

Make wavepacket

$$|\Psi(t)\rangle = \sum_{\boldsymbol{r}'} e^{\mathrm{i}\boldsymbol{k}(t)\cdot\boldsymbol{r}' - \frac{[\boldsymbol{r}'-\boldsymbol{r}(t)]^2}{2L^2}} |\boldsymbol{r}'\rangle$$

Get dynamics of $\boldsymbol{k}(t)$, $\boldsymbol{r}(t)$ from

$$S = \int \mathrm{d}t \, \langle \Psi(t)| \left(\mathrm{i}\partial_t - H\right) |\Psi(t)\rangle$$

Landau quantization

$$S = \int \mathrm{d}t \left[\boldsymbol{k} \cdot \dot{\boldsymbol{r}} - \varepsilon(\boldsymbol{k} - \boldsymbol{A}(\boldsymbol{r}))\right] , \quad \varepsilon(\boldsymbol{k}) = -\sum_{\boldsymbol{a}} t_a e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}}$$

Call $\boldsymbol{p} = \boldsymbol{k} - \boldsymbol{A}(\boldsymbol{r})$. For $\boldsymbol{B} = B\hat{\boldsymbol{z}}$

- ε is conserved (it's the Hamiltonian).
- p_z is conserved
- p_x and p_y are canonically conjugate.
- A complementary pair (X, P) exists (gauge dependent).

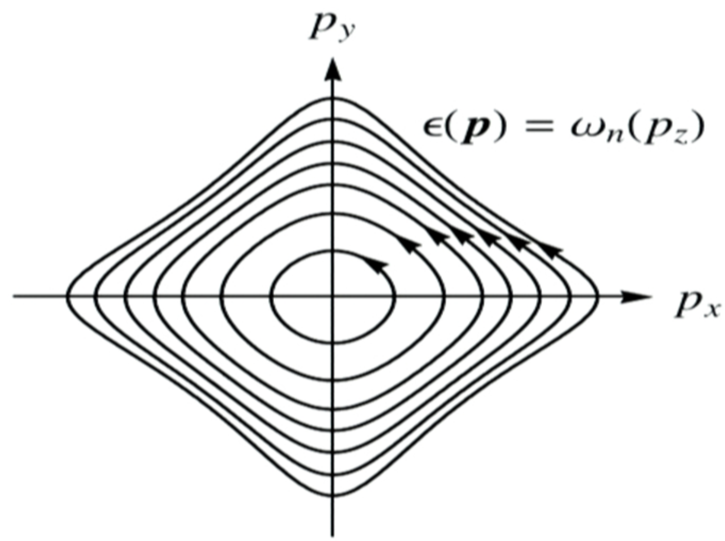
Landau quantization

$$S = \int \mathrm{d}t \left[p_x \dot{p}_y + p_z \dot{z} + P\dot{X} - \varepsilon(\boldsymbol{p}) \right]$$

- p_x, p_y describe constant-ε orbits.
- Bohr Sommerfeld quantization

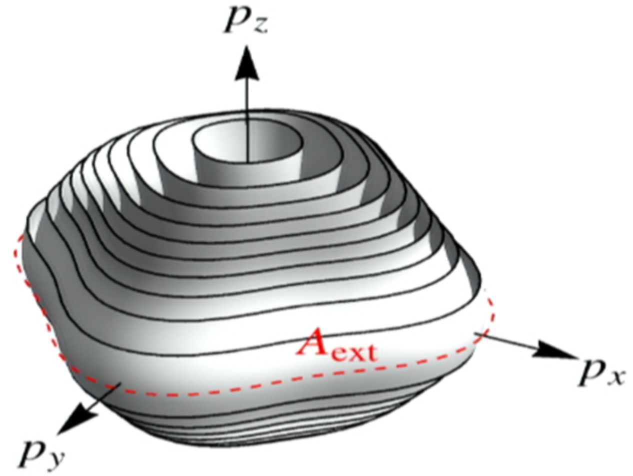
$$\frac{1}{B} \oint_{\varepsilon(\boldsymbol{p})=\omega} p_x \, \mathrm{d}p_y = 2\pi n$$

- Landau energy level $\omega_n(p_z)$: energy of contour with area $2\pi n B$.



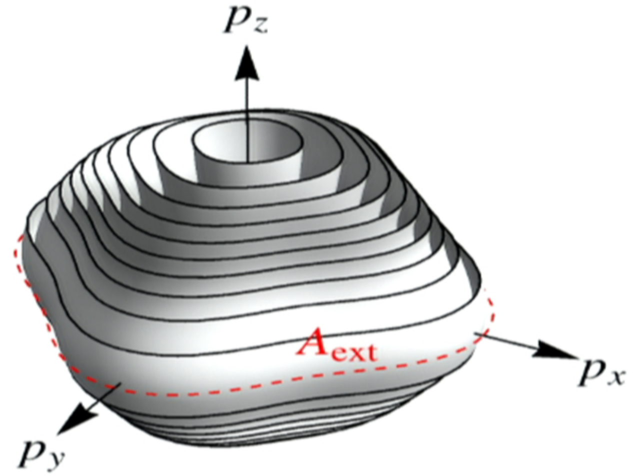
Oscillation of the density of states

- Cross sections have constant energy and quantized area
- Envelope is the Fermi surface
- Edges add up to give the density of states at the Fermi level.



Oscillation of the density of states

- Increasing B pushes shells out
- Peak in the density of states as outer shell crosses A_{ext} and disappears



Oscillation of the density of states

$$D(\omega) = \sqrt{\frac{B}{A''_{\text{ext}}(\omega)}}m(\omega)\sum_{n=1}^{\infty}\frac{1}{\sqrt{n}}\cos\left(n\frac{A_{\text{ext}}(\omega)}{B} - \phi_n\right)$$

- Thermodynamic quantities oscillate periodically in $1/B$
- Magnetization (de Haas-van Alphen)
- Resistivity (Shubnikov-de Haas)
- Hall resistance

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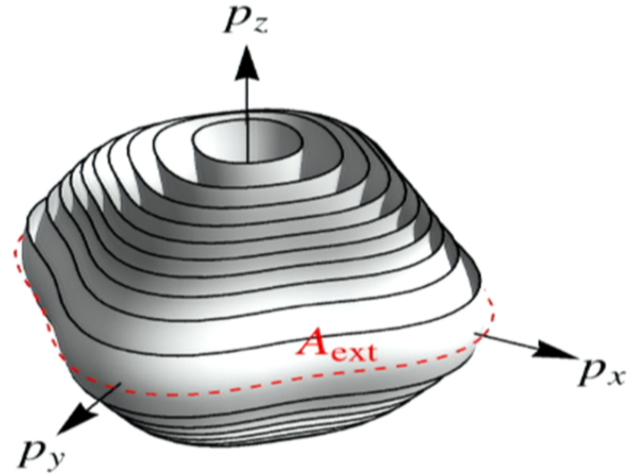

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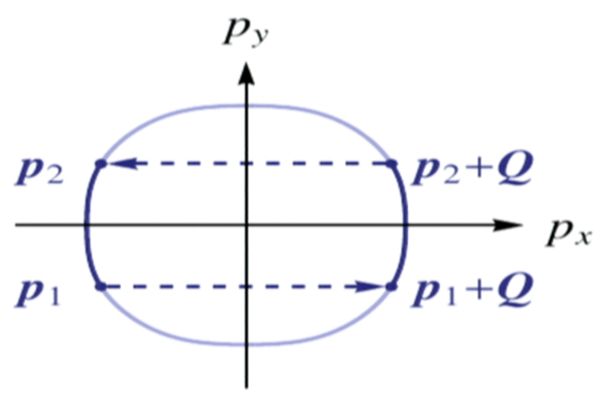
Fermi surface reconstruction

Add a periodic charge modulation

$$H = -\sum_{\boldsymbol{r},\boldsymbol{a}} t_a e^{\mathrm{i}\int_{\boldsymbol{r}}^{\boldsymbol{r}+\boldsymbol{a}} \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{\ell}} \left|\boldsymbol{r}+\boldsymbol{a}\right\rangle \left\langle \boldsymbol{r}\right| + \sum_{\boldsymbol{r}} P \cos \boldsymbol{Q}\cdot\boldsymbol{r} \left|\boldsymbol{r}\right\rangle \left\langle \boldsymbol{r}\right|$$

- Potential P causes scattering across Fermi surface
- Intuitively, different closed orbits are possible



Fermi surface reconstruction

More general wavepacket

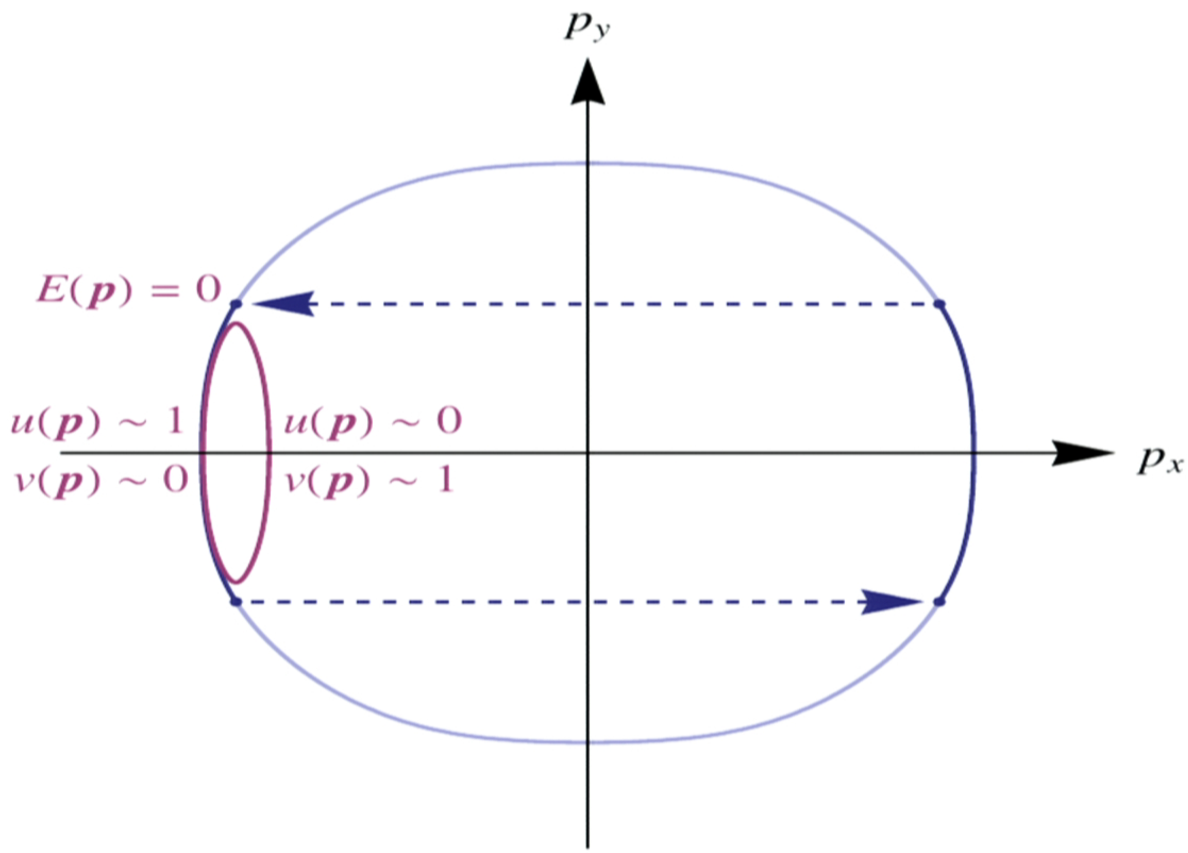
$$|\Psi(t)\rangle = \sum_{\boldsymbol{r}'} \left[u(t) + v(t) e^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}'} \right] e^{\mathrm{i}\boldsymbol{k}(t)\cdot\boldsymbol{r}' - \frac{[\boldsymbol{r}' - \boldsymbol{r}(t)]^2}{2L^2}} \left|\boldsymbol{r}'\right\rangle$$

Take $u(t) = u_{\boldsymbol{p}(t)}$, $v(t) = v_{\boldsymbol{p}(t)}$

$$\begin{pmatrix} \epsilon_{\boldsymbol{p}} & P \\ P & \epsilon_{\boldsymbol{p}+\boldsymbol{Q}} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{p}} \\ v_{\boldsymbol{p}} \end{pmatrix} = E(\boldsymbol{p}) \begin{pmatrix} u_{\boldsymbol{p}} \\ v_{\boldsymbol{p}} \end{pmatrix}$$

$$S = \int \mathrm{d}t \left[p_x \dot{p}_y + p_z \dot{z} + P\dot{X} - E(\boldsymbol{p}) \right]$$

Fermi surface reconstruction



Limitations of semiclassical treatment

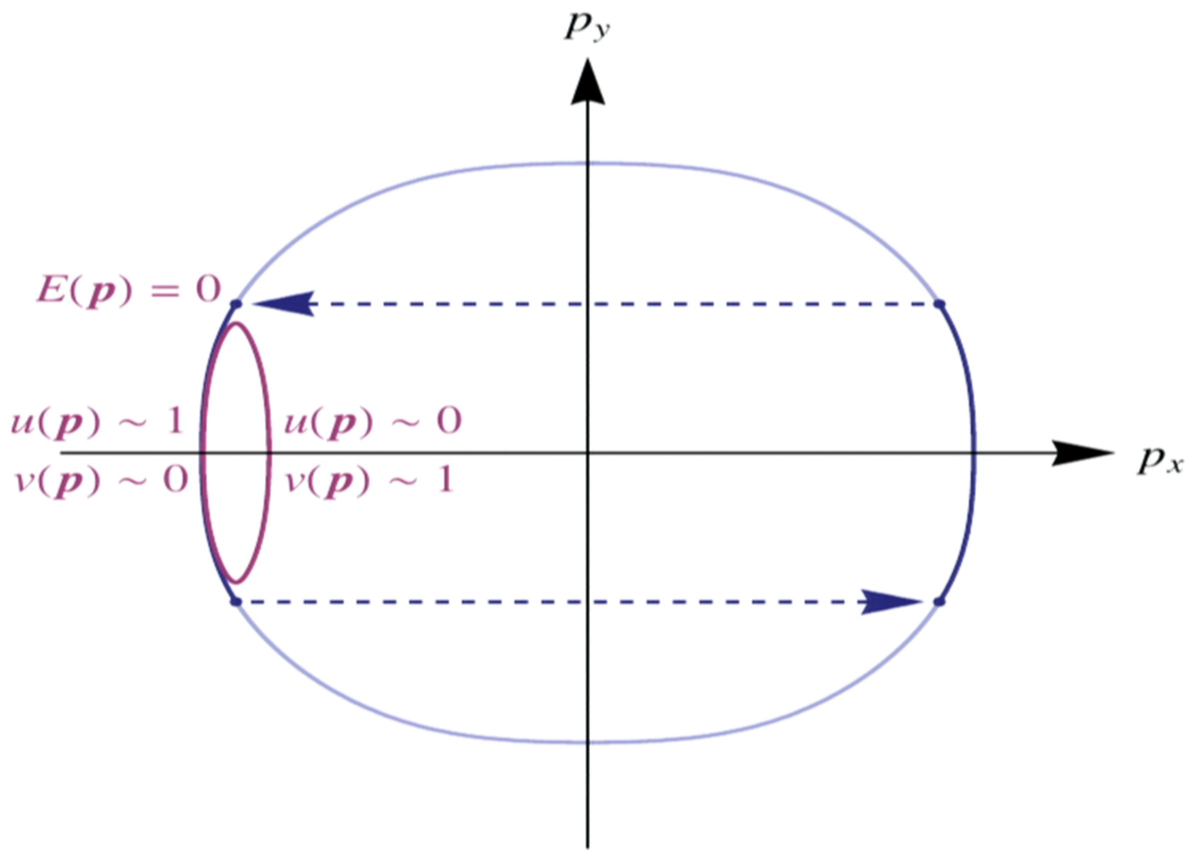
Semiclassical treatment

- Neglects higher order processes of scattering $\boldsymbol{k} \to \boldsymbol{k} + n\boldsymbol{Q}$
- Cannot handle magnetic breakdown

Solve exactly:

$$D(\omega) = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr} \frac{1}{\omega - H + \mathrm{i}\eta}$$

Fermi surface reconstruction



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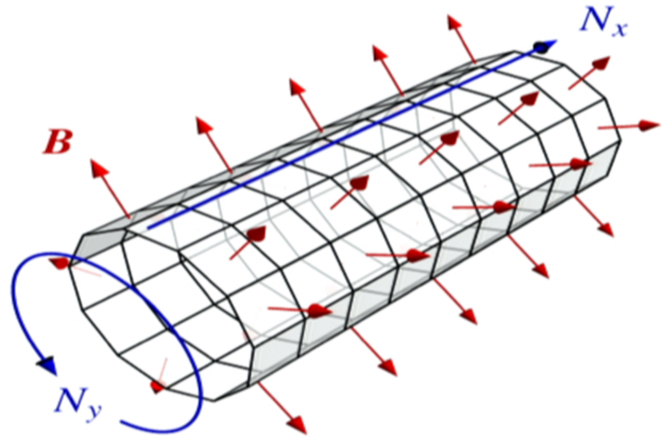
Exact treatment

$$D(\omega) = -\frac{1}{\pi} \mathrm{Im}\,\mathrm{Tr} \frac{1}{\omega - H + \mathrm{i}\eta}$$

- Put the system on an open cylinder (B not quantized)

$$H = \begin{pmatrix} h_{11} & t_{12} & 0 & \dots \\ t_{21} & h_{22} & t_{23} & \dots \\ 0 & t_{32} & h_{33} & \dots \\ \vdots & \vdots & \vdots & \end{pmatrix} .$$

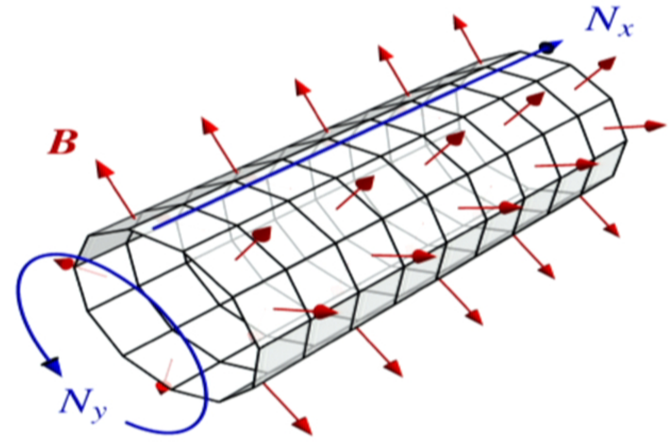
- Complexity $\sim N_x N_y^3$



Exact treatment

$$D(\omega) = -\frac{1}{\pi} \mathrm{Im}\,\mathrm{Tr} \frac{1}{\omega - H + \mathrm{i}\eta}$$

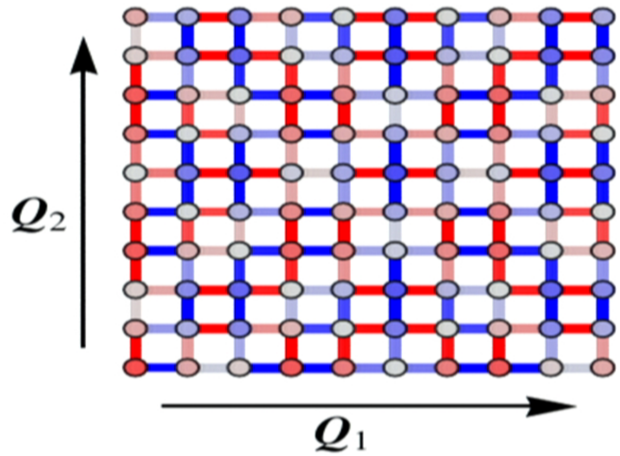
- Exact solution of the model
- Very large system size 1000×50 (continuous d.o.s., small finite-size effects)
- Commensurate as well as incommensurate CDW.



Model hamiltonian

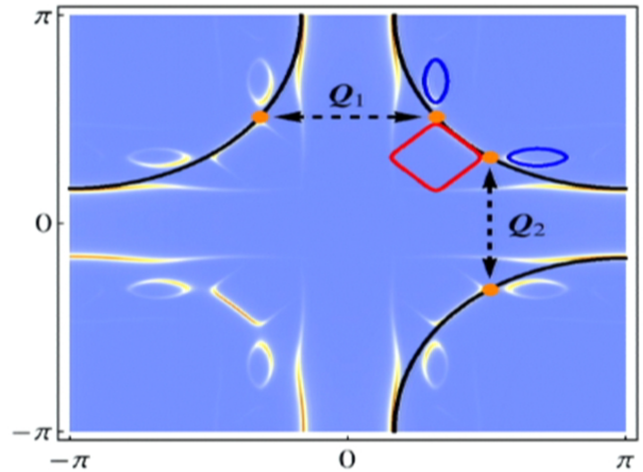
$$H = \sum_{\boldsymbol{r},\boldsymbol{a}} \left[-t_a + P_{\boldsymbol{a}} \cos \boldsymbol{Q} \cdot (\boldsymbol{r} + \boldsymbol{a}/2)\right] |\boldsymbol{r} + \boldsymbol{a}\rangle \langle \boldsymbol{r}|$$

- d-wave charge density wave
- Checkerboard
- $\boldsymbol{Q}_1 \sim (0.3, 0)2\pi$,
  $\boldsymbol{Q}_2 \sim (0, 0.3)2\pi$

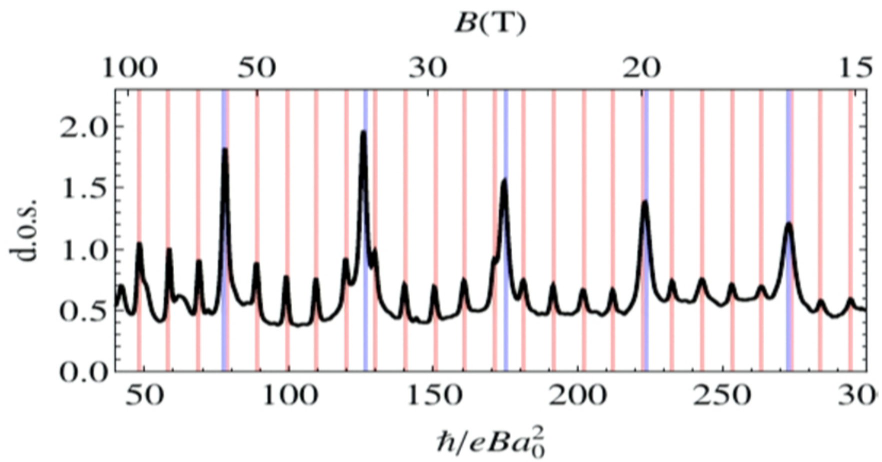


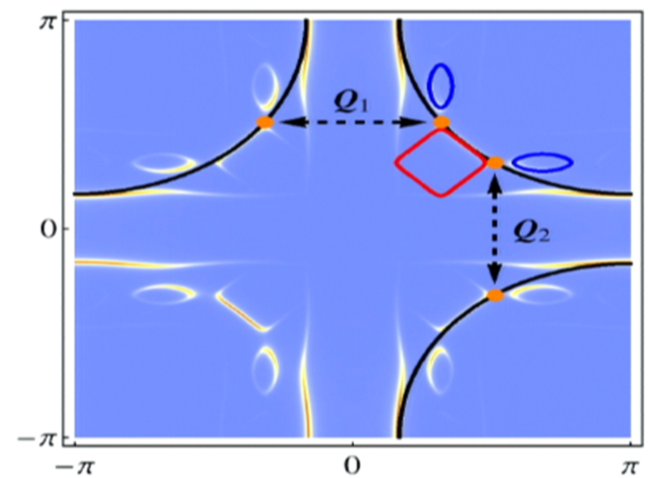
Fermi surface reconstruction

- Fermi surface appropriate for YBCO
- CDW opens up gaps at nested points
- Small *electron* pocket
- Harrison *et al.* PRL 2011

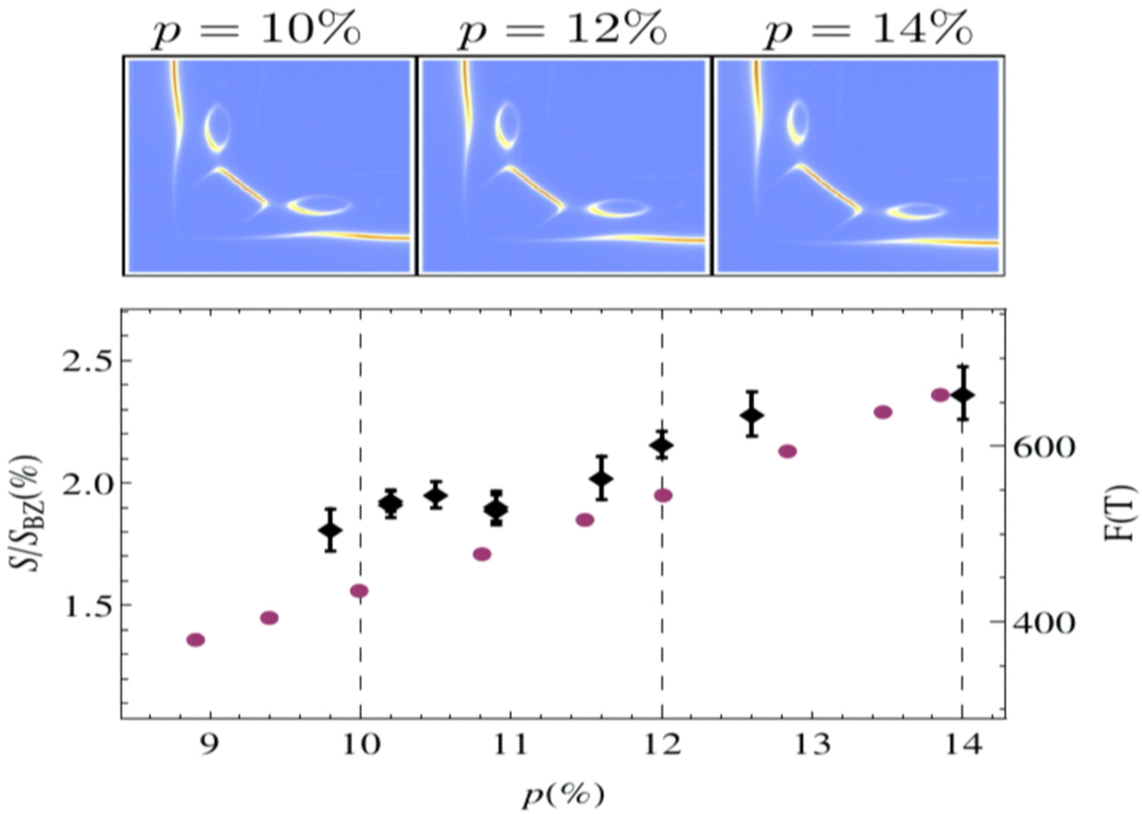


Fermi surface reconstruction





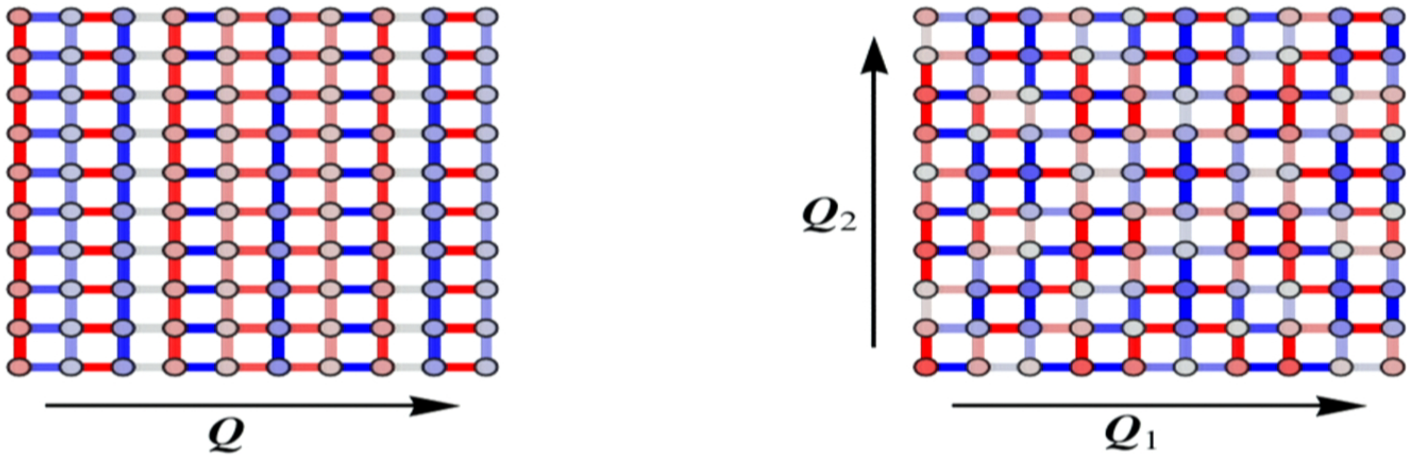
Doping dependence



Experimental data from Vignolle *et al.* C. R. Physique 2013

Stripe to checkerboard

What happens in going from stripe to checkerboard order?



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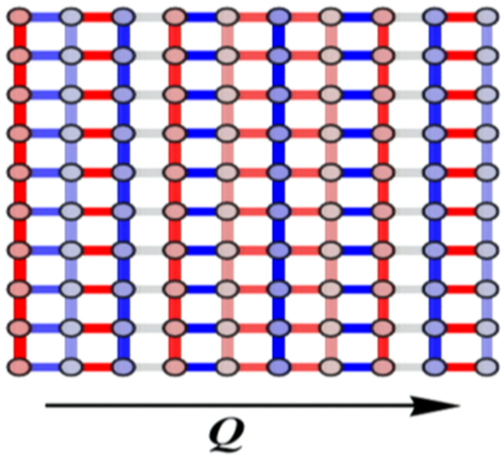

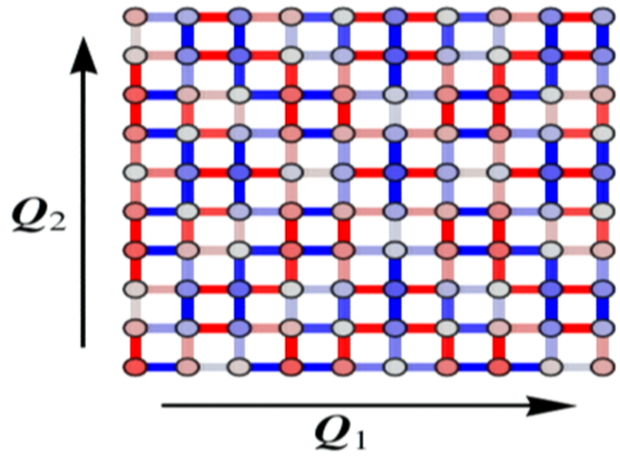

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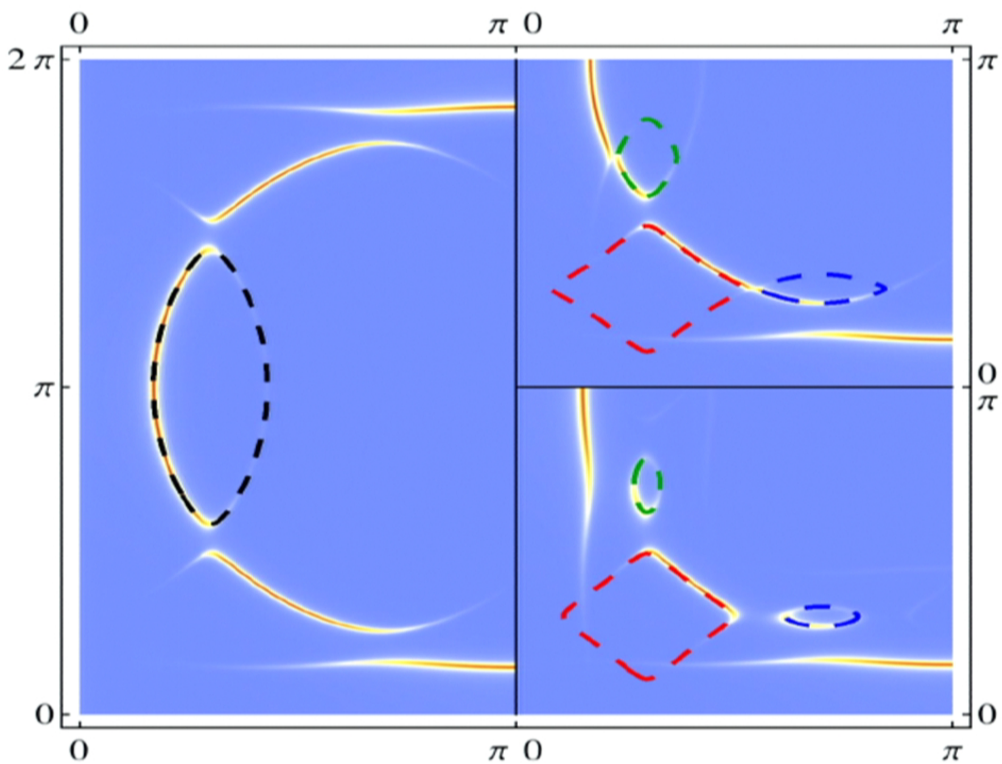

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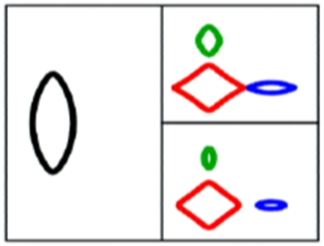
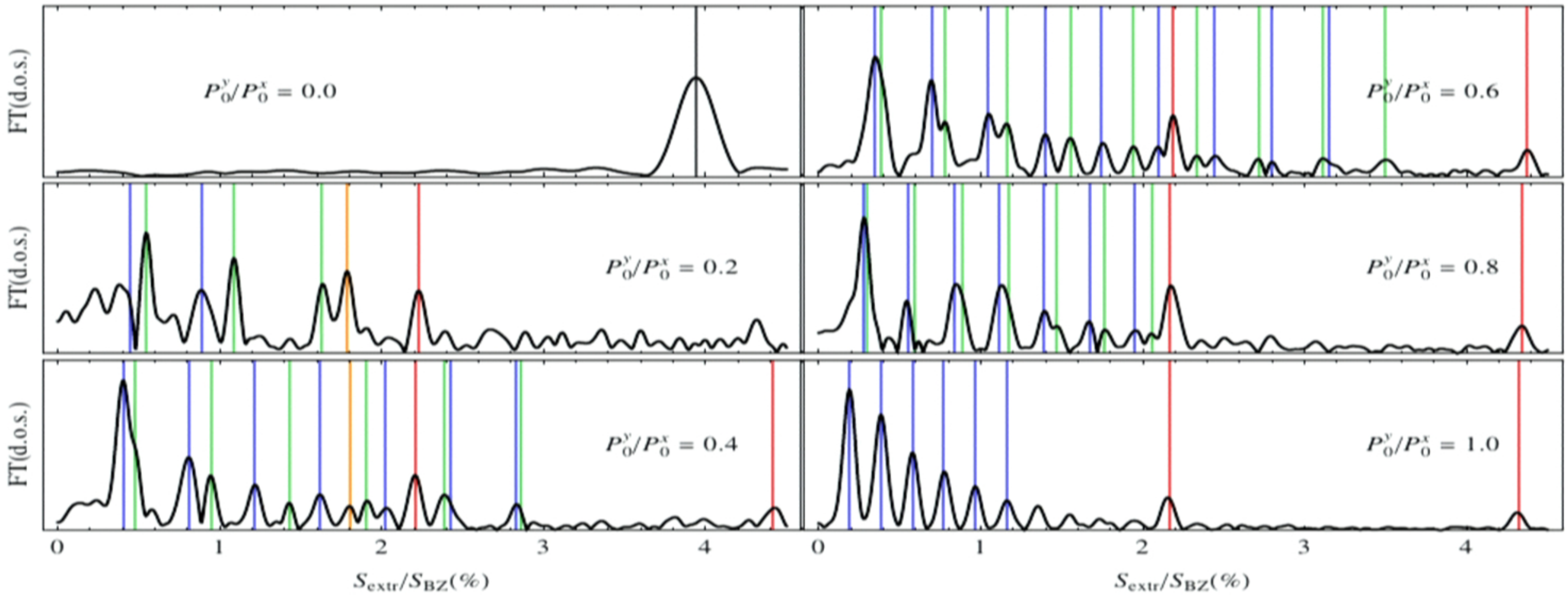
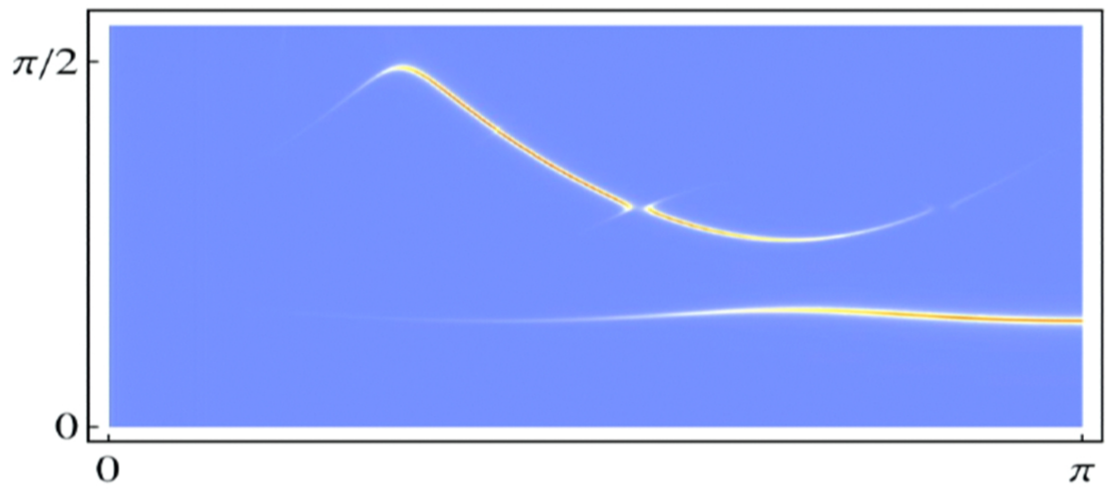
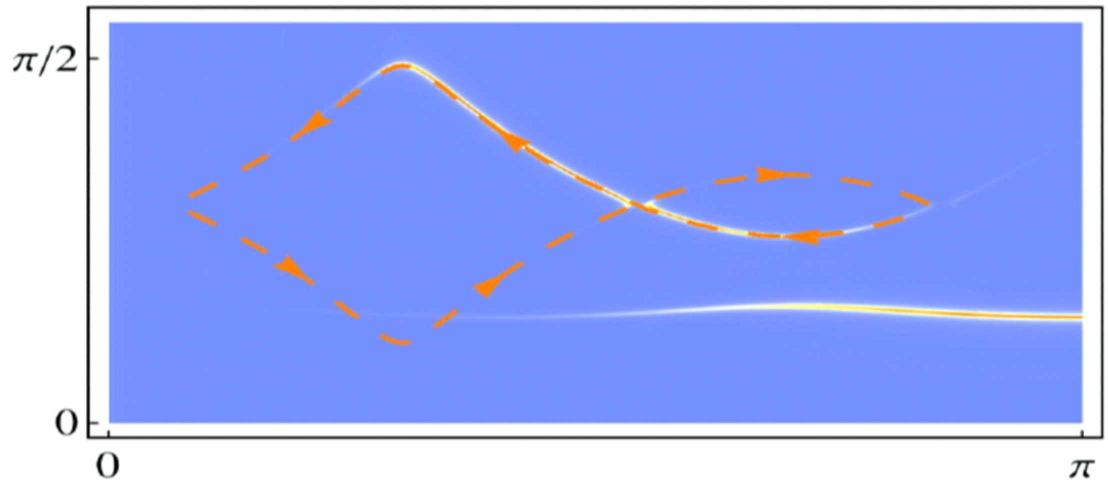




Higher order processes



Higher order processes



Summary

- Charge density wave arises naturally from a simple model
- It fits many experimental signatures
- Analysis of quantum oscillations beyond semiclassical theory
  - Doping dependence of oscillation frequency
  - Transition from stripe to checkerboard
  - Robustness of electron pocket to stripy order