Electron-Phonon Interaction and Charge Instabilities in Strongly Correlated Electron Systems

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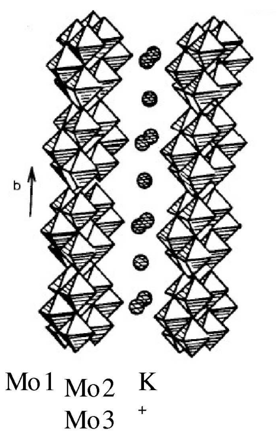
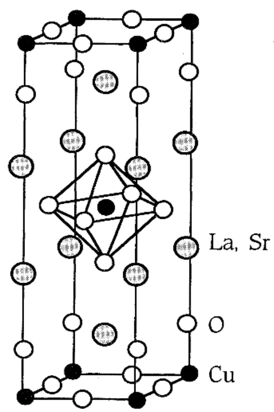
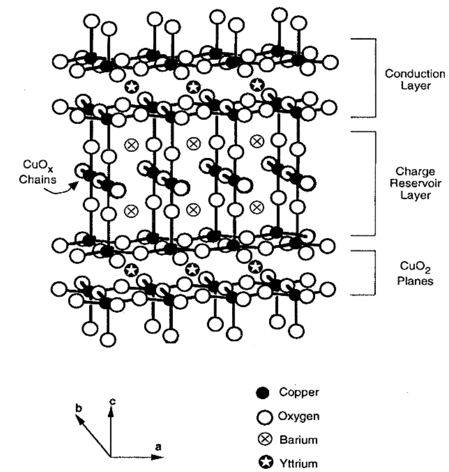
Charge Density Wave (CDW) Materials



$K_{0.30}MoO_3$



$La_{2-x}Sr_xCuO_4$



$YBa_2Cu_3O_{7-x}$

- **CLASSICAL CDW's**

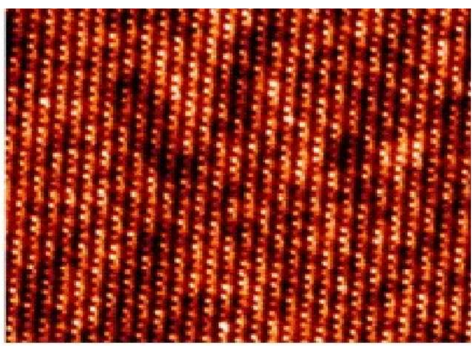
  1D-blue bronzes ($A_{0.30}MoO_3$ with $A = K, Rb$);

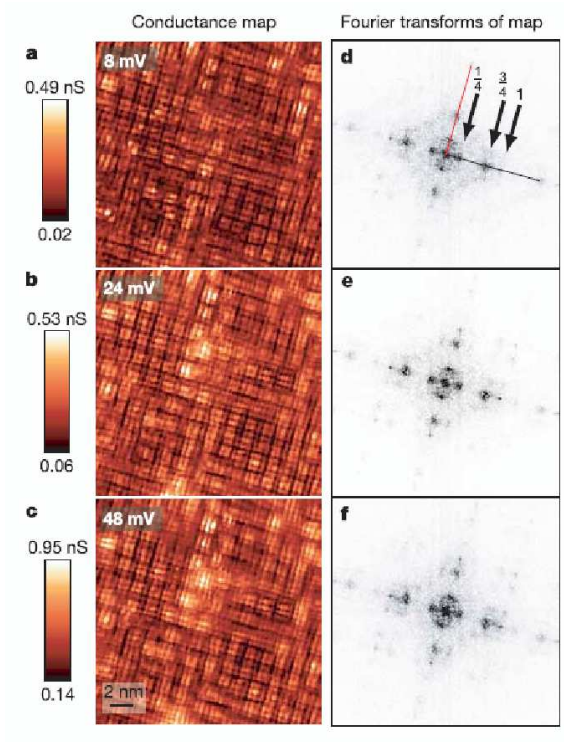
  2D-dichalcogenides (MC_2 with M=Ta,Ti,Nb,Mo and C=S,Se) ...

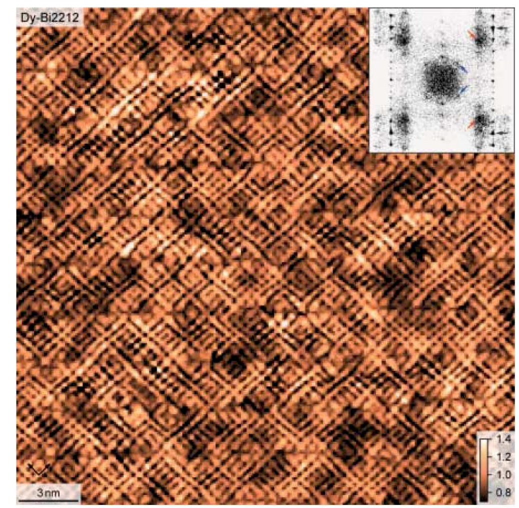
- **STRONGLY CORRELATED CDW's**

  cuprates, manganites, nickelates, cobaltites ...

Charge Density Wave (CDW) Materials



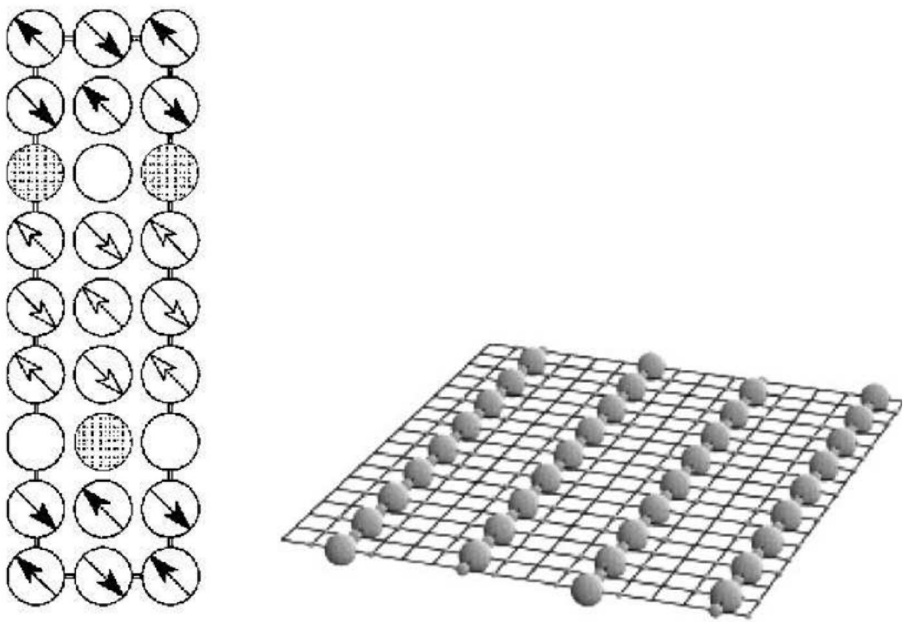


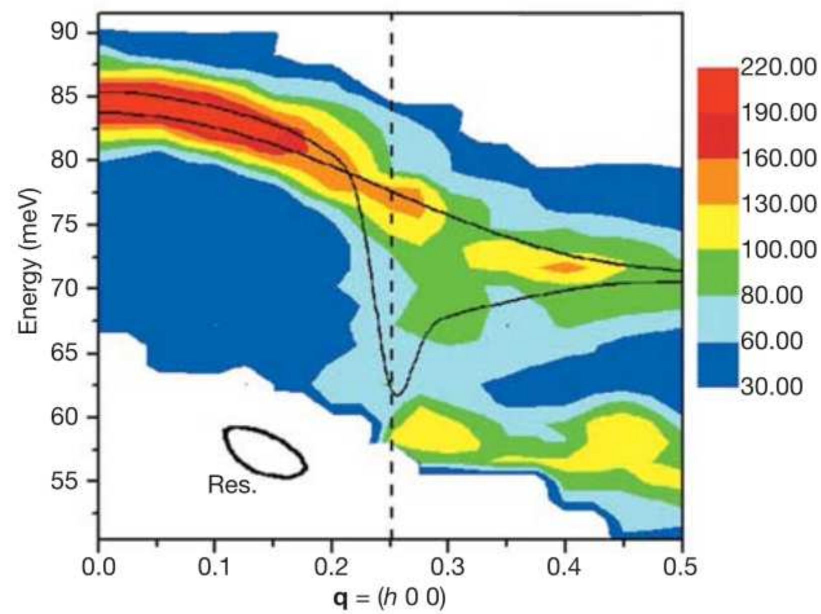


$Rb_{0.3}MoO_3$[Brun05] $Ca_{2-x}Na_xCuO_2Cl_2$[Hanaguri04] Dy-BSCCO[Kohsaka07]

CDW's in STM (Scansion Tunnelling Microscope) experiments

Anomalous Phonon Softening in the Cuprates





Stripe Phase[Tranquada96,Bosch01] *Bond-Stretching Phonon Branch in LBCO[Reznik06]*

OUR IDEA: STRIPES $\Rightarrow$ Nearly 1D-metallic structures

$\Longrightarrow [Kohn\ Anomaly]$ ANOMALOUS SOFTENING OF THE BOND-STRETCHING PHONON BRANCH

Hubbard-Holstein Model + Gutzwiller-RPA Method

- $\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$ $\Longrightarrow$ ELECTRONIC KINETIC TERM

  $\sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ $\Longrightarrow$ E-E INTERACTIONS

  $\sum_i \beta x_i (\hat{n}_i - n)$ $\Longrightarrow$ E-PH COUPLING

  $\sum_i \left(\frac{1}{2M} P_i^2 + \frac{1}{2} K x_i^2 \right)$ $\Longrightarrow$ PHONONIC TERM

- **ADIABATIC LIMIT** $(M \rightarrow \infty) \Rightarrow \kappa_{\mathbf{q}}^{eph} = \dfrac{\kappa_{\mathbf{q}}}{1 - \lambda \kappa_{\mathbf{q}} / \chi_0^0}$ **exact relation**

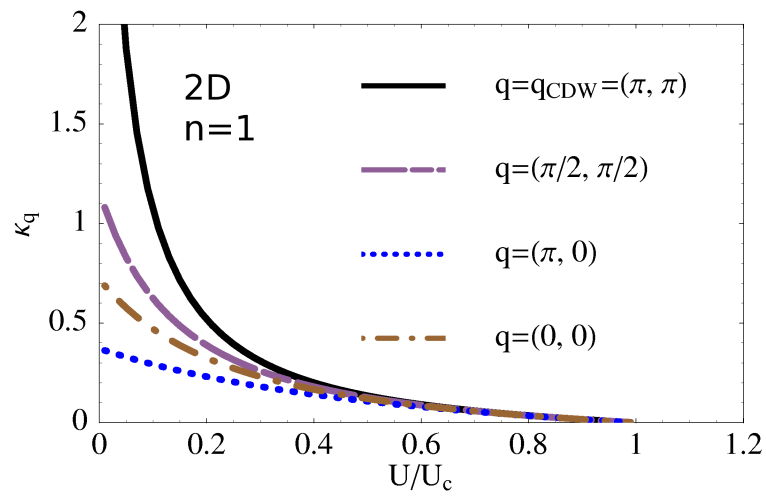
  $\lambda = \chi_0^0 \beta^2 / K \rightarrow e$-$ph$ coupling

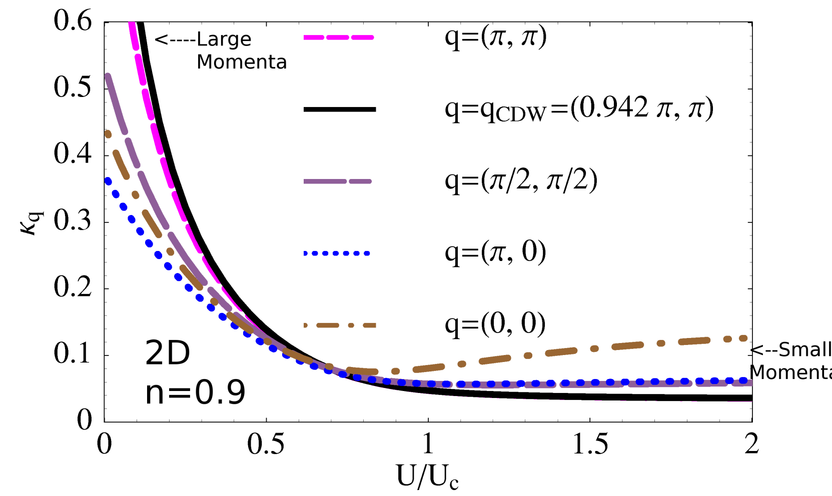
  $\chi_0^0 \rightarrow$ density of states of the non-interacting system

- **GUTZWILLER APPROXIMATION (GA)** $\Longrightarrow$ electronic GROUND STATE + low-energy excitations (quasiparticles)

  RANDOM PHASE APPROXIMATION (RPA) $\Longrightarrow$ FLUCTUATIONS $\Rightarrow$ dressed ELECTRONIC SUSCEPTIBILITY:
  $\kappa_{\mathbf{q}}$ (without e-ph coupling) $\Rightarrow$ $\kappa_{\mathbf{q}}^{eph}$ (with e-ph coupling)

Homogeneous Metal $\Longrightarrow$ Charge Inhomogeneities





n=1, U=U_c $\rightarrow$ Metal-Insulator Transition

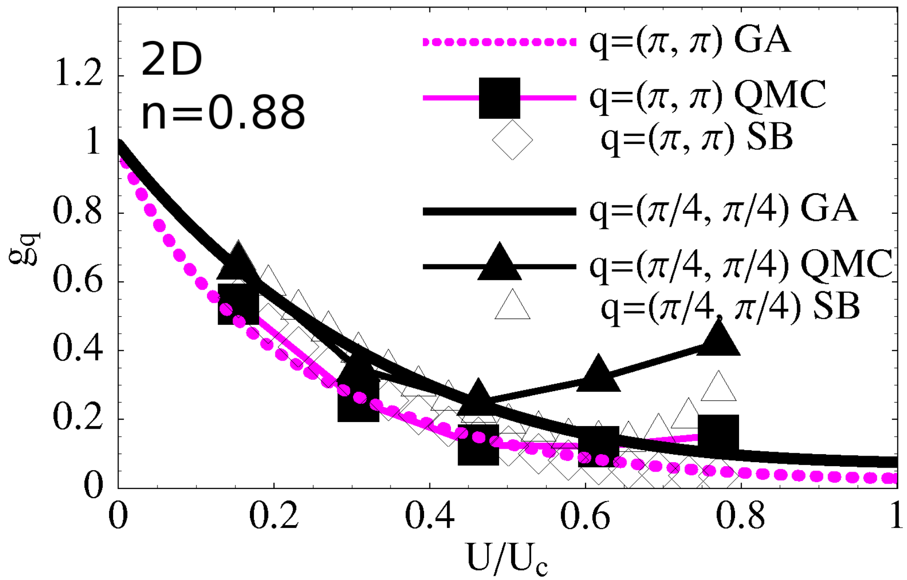
$$\kappa_{\mathbf{q}}^{eph} = \frac{\kappa_{\mathbf{q}}}{1-\lambda\kappa_{\mathbf{q}}/\chi_0^0}$$

U=0 $\Longrightarrow$ $\kappa_{\mathbf{q=2k_F}}$ maximum $\Longrightarrow$ strong phonon anomaly (KOHN ANOMALY)

SMALL U $\Longrightarrow$ PEIERLS CDW

LARGE U $\Longrightarrow$ PHASE SEPARATION (PS)

Homogeneous Metal $\Longrightarrow$ Charge Inhomogeneities



GA is accurate

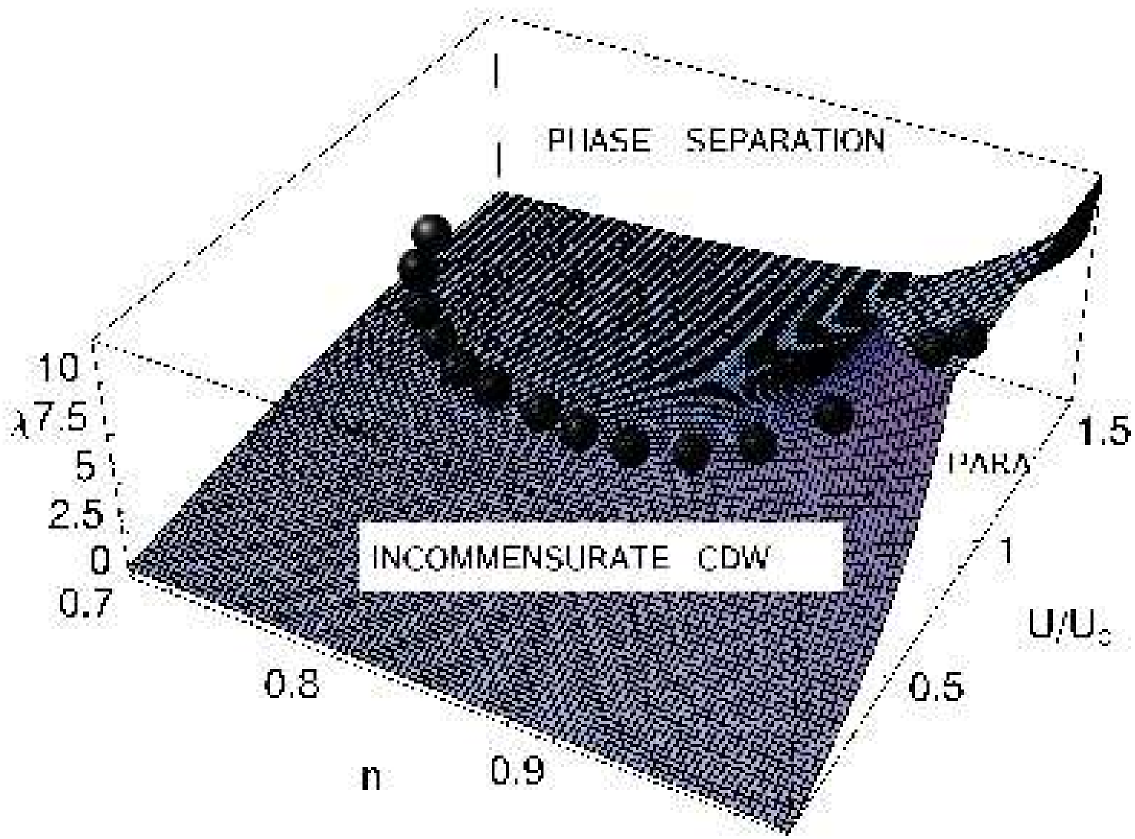
U WEAKENS THE EFFECTIVE E-PH COUPLING

$$g_{\mathbf{q}} = z_0^2 \frac{\kappa_{\mathbf{q}}}{\kappa_{\mathbf{q}}^0}$$

$z_0 \Rightarrow$ GA renormalized hopping

$t \longrightarrow t z_0^2$

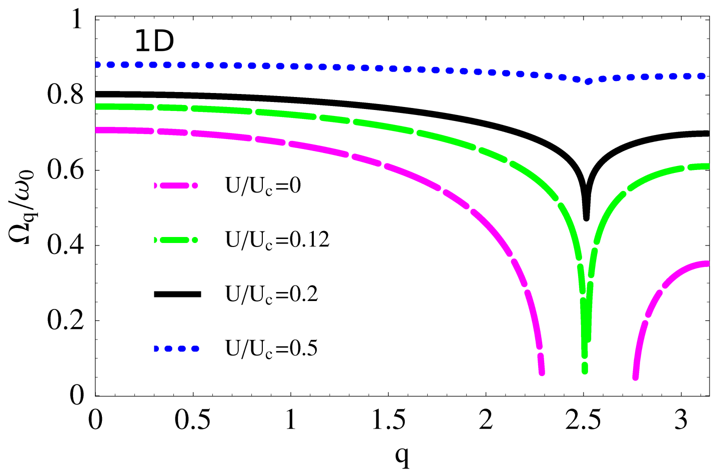
Homogeneous Metal ⟹ Charge Inhomogeneities

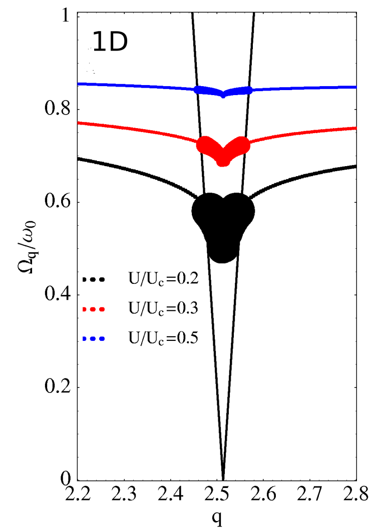


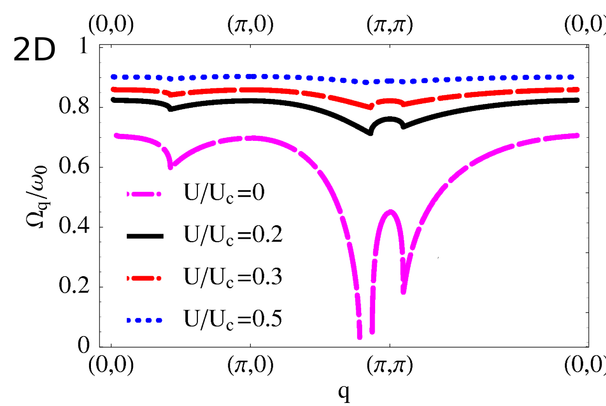
2D - PHASE DIAGRAM OF THE PARAMAGNETIC METAL

Kohn Anomaly in 1D and 2D

$\omega_0 \rightarrow$ bare phonon frequency

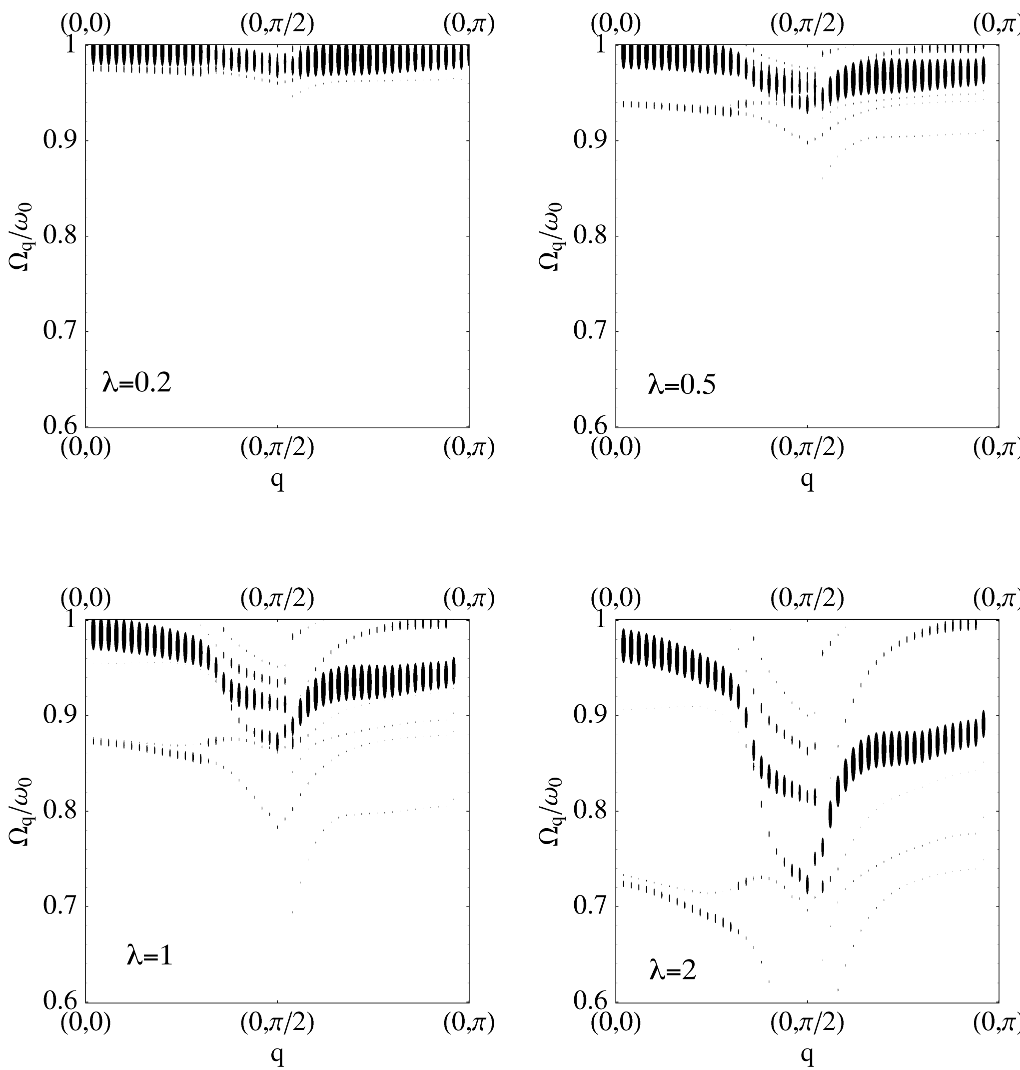






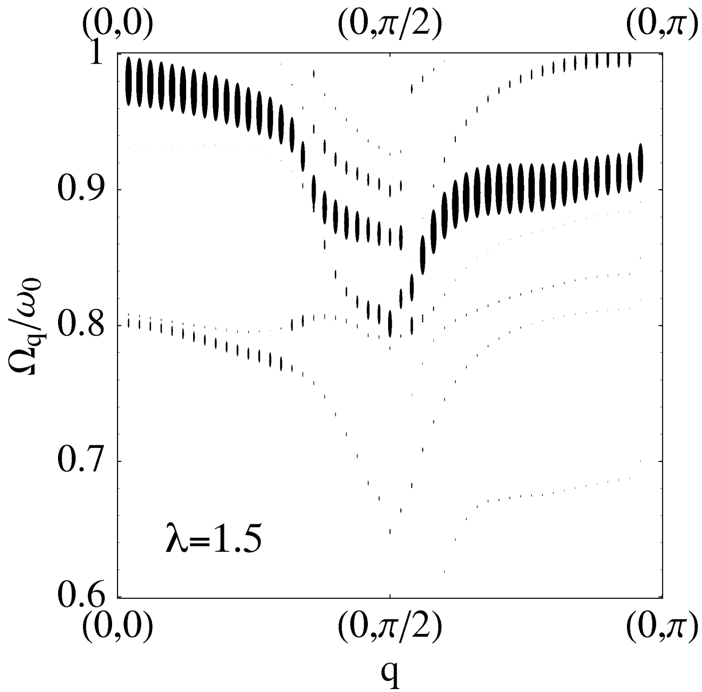
Results for $n = 0.8$ and $\lambda = 0.5$. **U SUPPRESSES THE KOHN ANOMALY**.

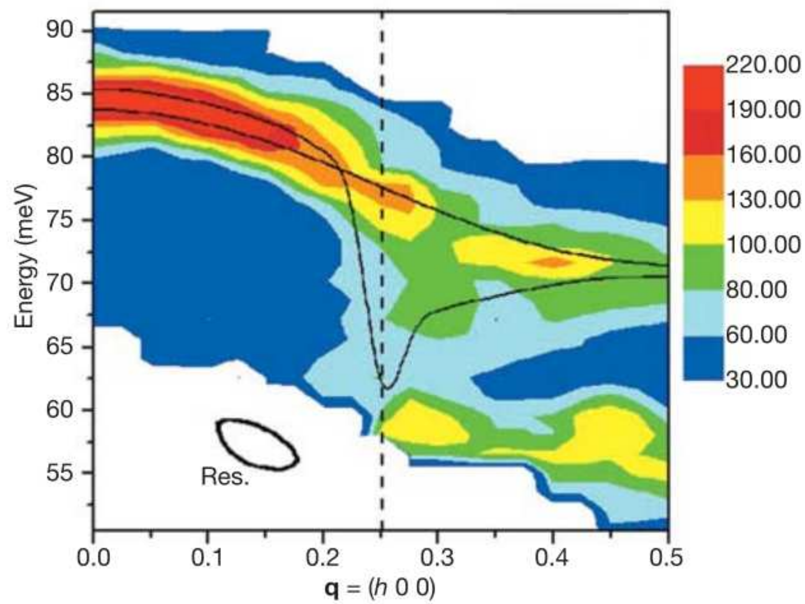
Stripes $\Longrightarrow$ Anomalous Phonon Softening



REALISTIC PARAMETERS$\Longrightarrow$ $n = 0.875$, $U/t = 8$, next-nearest hopping $t'/t = -0.2$

Stripes $\Longrightarrow$ Anomalous Phonon Softening





OUR OPTICAL PHONON BRANCHES VS EXPERIMENTAL BRANCHES

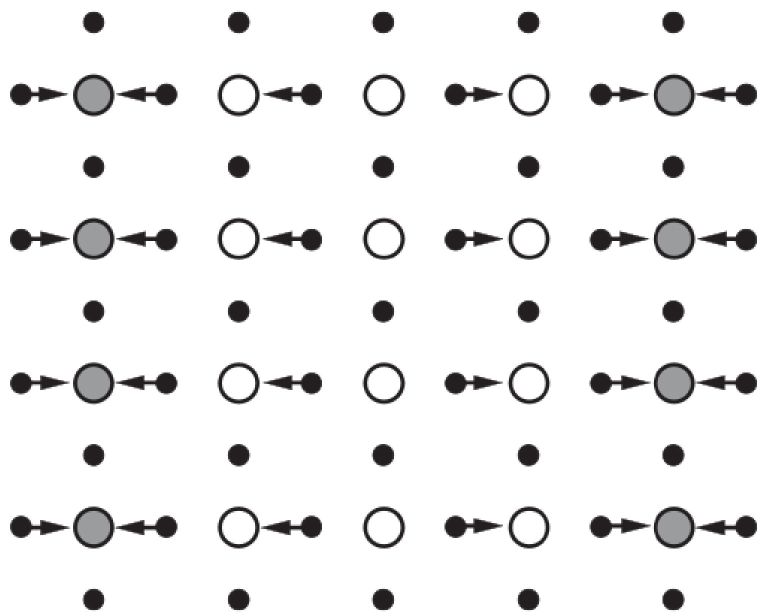
STRONG ASYMMETRY WELL REPRODUCED

NOT TRIVIAL RESULT

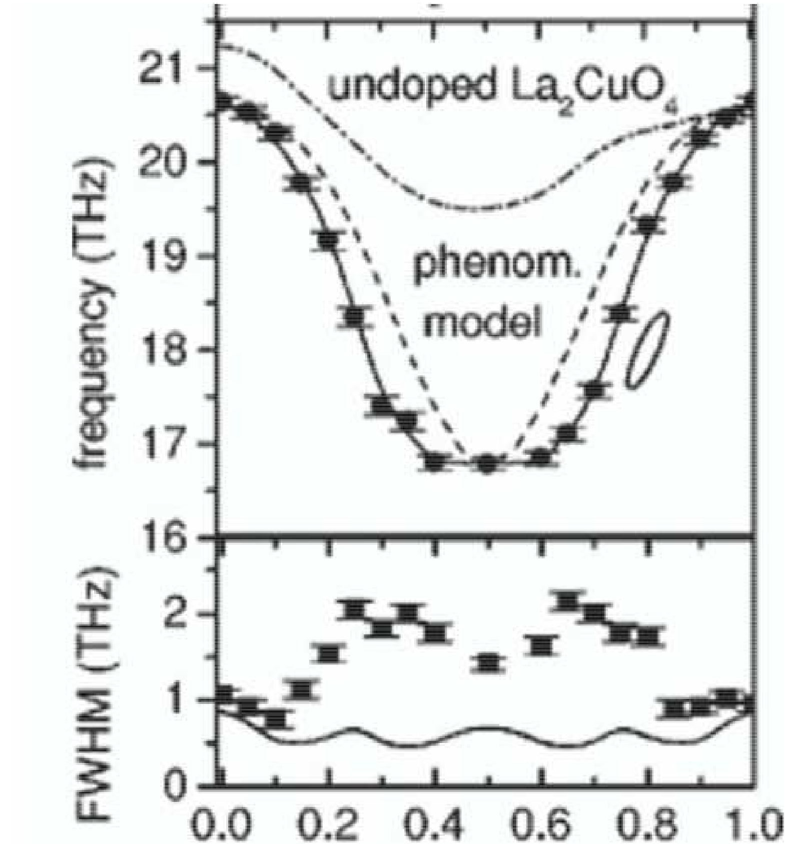
Conclusions

- e-ph coupling suppressed by e-e interaction
- Homogeneous Metal $\Rightarrow \lambda \Rightarrow$ Charge Inhomogeneities
- Peierls CDW $\Longrightarrow U \Longrightarrow$ PS
- Optical Phonons + Stripes $\Rightarrow U \Rightarrow$ Anomalous Phonon Softening

Anomalous Phonon Softening in the Cuprates



Half-Breathing Phonon Mode



Longitudinal Optical Branch[Pintschovius99]

Hubbard-Holstein Model + Gutzwiller-RPA Method

The susceptibility $\kappa_{\mathbf{q}}$ has all the information on how e-e interaction renormalizes e-ph interaction:

$$\kappa_{\mathbf{q}}^{eph} = \frac{\kappa_{\mathbf{q}}}{1 - \lambda \kappa_{\mathbf{q}} / \chi_0^0} = \frac{\kappa_{\mathbf{q}}}{1 - \tilde{\lambda}_{\mathbf{q}}} \quad , \qquad \tilde{\lambda}_{\mathbf{q}} = \lambda \frac{\kappa_{\mathbf{q}}}{\chi_0^0}$$

- In the absence of other (first-order) instabilities, for $\lambda = \lambda_c = \chi_0^0 / \kappa_{\mathbf{q_c}}$ the system undergoes a transition to a CDW state with a typical $\mathbf{q_c}$.
- Increasing $U \Rightarrow \kappa_{\mathbf{q}}$ reduced with respect to $\kappa_{\mathbf{q}}^0 \Rightarrow$ $\tilde{\lambda}_{\mathbf{q}}$ reduced $\Longrightarrow$ U WEAKENS the e-ph coupling.
- The problem is then reduced to the study of the electronic susceptibility for $\lambda = 0$.

Hubbard-Holstein Model + Gutzwiller-RPA Method

The Hubbard model: $H_e = \sum_{ij\sigma} t_{ij}(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \sum_i U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$

- GZW TRIAL STATE: $|\psi_G\rangle = \hat{P}_g |Sd\rangle \Longrightarrow$

  $|Sd\rangle \rightarrow$ SLATER DETERMINANT

  $\hat{P}_g = \prod_i [1 - (1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}] = \prod_i [1 - (1-g)\hat{D}_i]$

  For $g < 1$, $\hat{P}_g$ suppresses double occupancies D_i.

  For $g = 0$, all the configurations with $D_i \neq 0$ are ruled out.

- $E_e[\rho, D] = \langle \psi_G | H_e | \psi_G \rangle \simeq \sum_{ij\sigma} t_{ij} z_{i\sigma} z_{j\sigma} \rho_{ji\sigma} + \sum_i U D_i$

- $z_{i\sigma}[\rho_{ii\sigma}, \rho_{ii,-\sigma}, D_i] \rightarrow$ GZW-renormalized hopping factors

- $\rho_{ji\sigma} = \langle Sd | c^\dagger_{i\sigma} c_{j\sigma} | Sd \rangle \rightarrow$ uncorrelated single fermion

  DENSITY MATRIX

Hubbard-Holstein Model + Gutzwiller-RPA Method

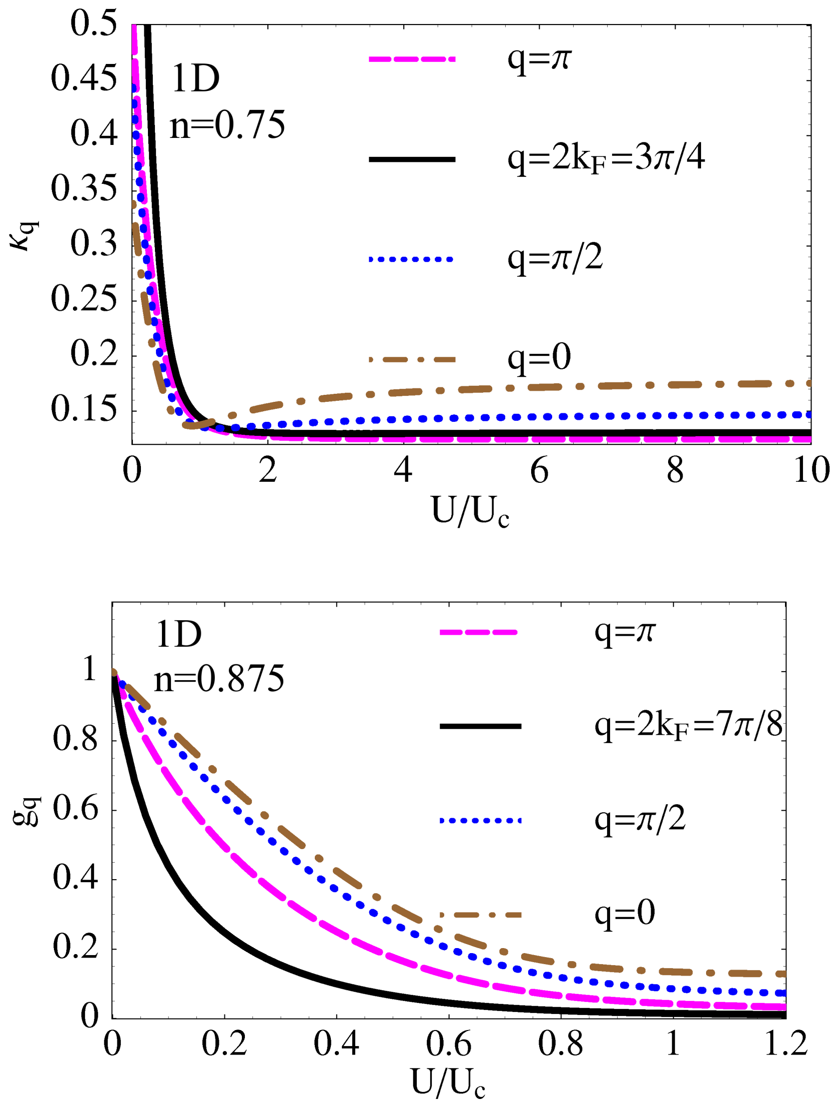
- Computations with the GA+RPA method [Seibold-Lorenzana0103], generalization of the HF+RPA technique [Ring80, Blaizot86]

- An external field induces small amplitude deviations δD and $\delta\rho$ around the GA saddle point $\Longrightarrow$
  $E_e[\rho, D] = E_{e0} + Tr[h_0\delta\rho] + \frac{1}{2}\delta\rho^\dagger L_0\delta\rho + \delta D S_0\delta\rho + \frac{1}{2}\delta D^t K_0\delta D$
  with $h = \delta E_e/\delta\rho$.

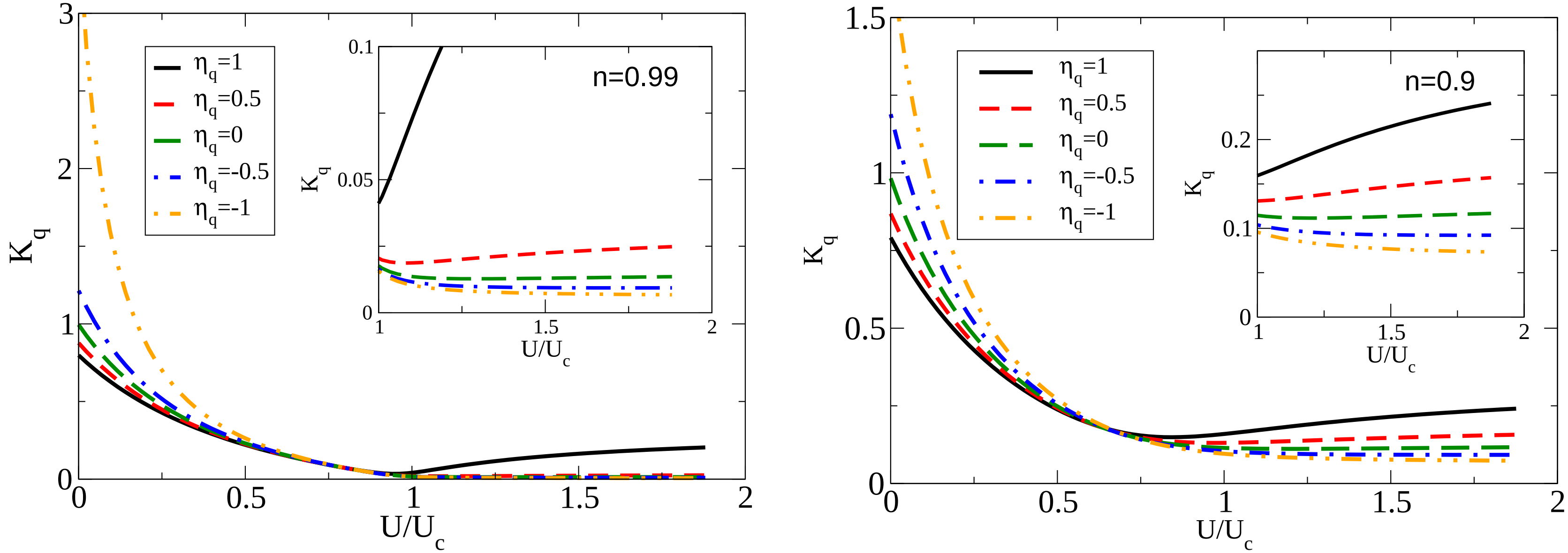
- $\dfrac{\partial E}{\partial\delta D} = 0$ eliminates the δD deviations $\Longrightarrow$
  2nd order energy deviation: $\delta E_e = \frac{1}{2}\delta\rho^\dagger W\delta\rho$

- The interaction kernel W mediates local and intersite charge deviations.

Homogeneous Metal $\Longrightarrow$ Charge Inhomogeneities



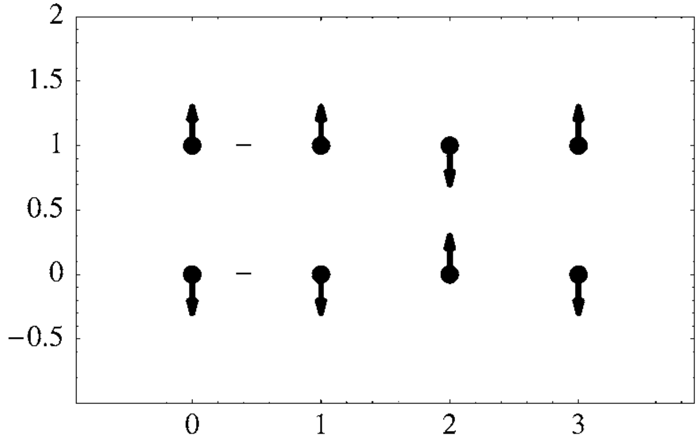
Homogeneous Metal $\Longrightarrow$ Charge Inhomogeneities

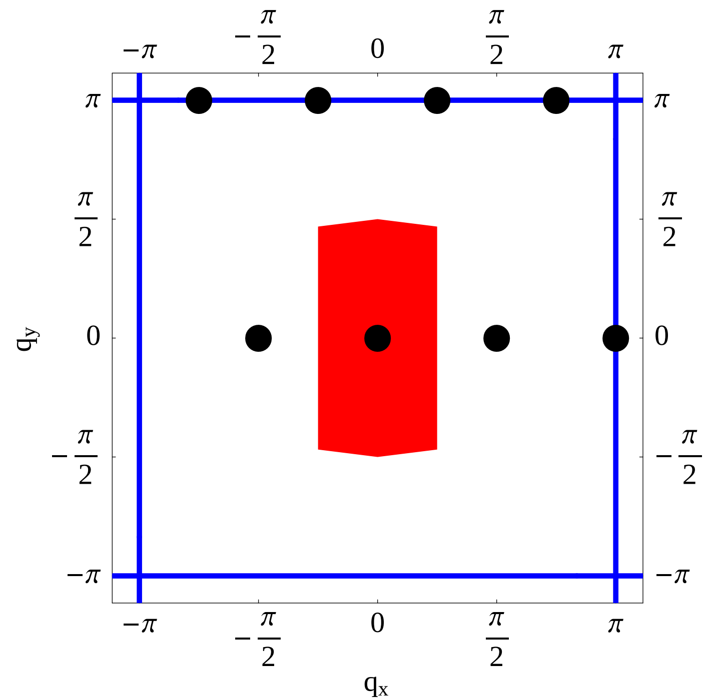


$$D = \infty$$

$$\eta_{\mathbf{q}} = \frac{1}{d} \sum_{\nu=1}^{d} \cos q_\nu$$

Stripes $\Longrightarrow$ Anomalous Phonon Softening





4×2 UNIT CELL $\Longrightarrow$ FIRST REDUCED BRILLOUIN ZONE