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

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Charge Density Wave (CDW) Materials

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**

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

$\Rightarrow$ [Kohn Anomaly] ANOMALOUS SOFTENING OF THE BOND-STRETCHING PHONON BRANCH
Hubbard-Holstein Model + Gutzwiller-RPA Method

\[ \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \implies \text{ELECTRONIC KINETIC TERM} \]
\[ \sum_{i} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \implies \text{E-E INTERACTIONS} \]
\[ \sum_{i} \beta x_{i}(\hat{n}_{i} - n) \implies \text{E-PH COUPLING} \]
\[ \sum_{i} \left( \frac{1}{2M} P_{i}^{2} + \frac{1}{2} K x_{i}^{2} \right) \implies \text{PHONONIC TERM} \]

**ADIABATIC LIMIT** \((M \to \infty) \implies \kappa_{q}^{\text{eph}} = \frac{\kappa_{q}}{1 - \lambda \kappa_{q} / \chi_{0}^{0}} \text{ exact relation} \)

\( \lambda = \chi_{0}^{0} \beta^{2} / K \to \text{e-ph coupling} \)
\( \chi_{0}^{0} \to \text{density of states of the non-interacting system} \)

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

**RANDOM PHASE APPROXIMATION (RPA) \(\implies\) FLUCTUATIONS \(\implies\)**
\( \kappa_{q} \text{ (without e-ph coupling)} \implies \kappa_{q}^{\text{eph}} \text{ (with e-ph coupling)} \)
Homogeneous Metal $\implies$ Charge Inhomogeneities

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

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

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

SMALL $U \implies$ PEIERLS CDW

LARGE $U \implies$ PHASE SEPARATION (PS)
Homogeneous Metal $\implies$ Charge Inhomogeneities

$$\overset{GA}{\Rightarrow} \text{Charge Inhomogeneities}$$

GA is accurate

**$U$ WEAKENS THE EFFECTIVE $E$-$PH$ COUPLING**

$$g_q = z_0^2 \frac{\kappa_q}{\kappa_0}$$

$z_0 \Rightarrow$ GA renormalized hopping

$$t \rightarrow t z_0^2$$
Homogeneous Metal $\rightarrow$ Charge Inhomogeneities

2D - PHASE DIAGRAM OF THE PARAMAGNETIC METAL
Kohn Anomaly in 1D and 2D

\[ \omega_0 \to \text{bare phonon frequency} \]

Results for \( n = 0.8 \) and \( \lambda = 0.5 \). **U SUPPRESSES THE KOHN ANOMALY.**
Stripes $\rightarrow$ Anomalous Phonon Softening

**REALISTIC PARAMETERS** $\rightarrow n = 0.875, \ U/t = 8, \ \text{next-nearest hopping} \ t'/t = -0.2$
Stripes $\rightarrow$ 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 $\xrightarrow{U} \text{PS}$

- Optical Phonons + Stripes $\Rightarrow U \Rightarrow$ Anomalous Phonon Softening
Anomalous Phonon Softening in the Cuprates

Half-Breathing Phonon Mode

Longitudinal Optical Branch [Pintschovius99]
The susceptibility $\kappa_q$ has all the information on how $e-e$ interaction renormalizes $e-ph$ interaction:

$$\kappa_{q}^{eph} = \frac{\kappa_q}{1 - \lambda \kappa_q/\chi_0^0} = \frac{\kappa_q}{1 - \tilde{\lambda}_q}, \quad \tilde{\lambda}_q = \lambda \frac{\kappa_q}{\chi_0^0}$$

- In the absence of other (first-order) instabilities, for $\lambda = \lambda_c = \chi_0^0/\kappa_{q_c}$, the system undergoes a transition to a CDW state with a typical $q_c$.
- Increasing $U \Rightarrow \kappa_q$ reduced with respect to $\kappa_q^0 \Rightarrow \tilde{\lambda}_q$ reduced $\Rightarrow U$ WEAKENS the $e-ph$ coupling.
- The problem is then reduced to the study of the electronic susceptibility for $\lambda = 0$. 
The Hubbard model: \( H_e = \sum_{ij\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \)

**GZW TRIAL STATE:** \( |\psi_G\rangle = \hat{P}_g |Sd\rangle \implies |Sd\rangle \rightarrow \text{SLATER DETERMINANT} \)

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

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.

\[ E_e[\rho, D] = \langle \psi_G |H_e|\psi_G\rangle \simeq \sum_{ij\sigma} t_{ij} \zeta_{i\sigma} \zeta_{j\sigma} \rho_{ji\sigma} + \sum_i UD_i \]

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

\[ \rho_{ji\sigma} = \langle Sd |c_{i\sigma}^\dagger c_{j\sigma}|Sd\rangle \rightarrow \text{uncorrelated single fermion DENSITY MATRIX} \]
Computations with the GA+RPA method [Seibold-Lorenzana0103], generalization of the HF+RPA technique [Ring80, Blaizot86]

An external field induces small amplitude deviations $\delta D$ and $\delta \rho$ around the GA saddle point $\Rightarrow$

$$E_e[\rho, D] = E_{e0} + Tr[h_0 \delta \rho] + \frac{1}{2} \delta \rho^\dagger L_0 \delta \rho + \delta DS_0 \delta \rho + \frac{1}{2} \delta D^t K_0 \delta D$$

with $h = \delta E_e / \delta \rho$.

$$\frac{\partial E}{\partial \delta D} = 0$$

eliminates the $\delta D$ deviations $\Rightarrow$

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

![Graph 1](image1.png)

1D
\( n = 0.75 \)
- \( q = \pi \)
- \( q = 2k_F = 3\pi/4 \)
- \( q = \pi/2 \)
- \( q = 0 \)

\( \kappa_q \) vs. \( U/U_c \)

![Graph 2](image2.png)

1D
\( n = 0.875 \)
- \( q = \pi \)
- \( q = 2k_F = 7\pi/8 \)
- \( q = \pi/2 \)
- \( q = 0 \)

\( \varepsilon \) vs. \( U/U_c \)
Homogeneous Metal $\implies$ Charge Inhomogeneities

\[
D = \infty
\]

\[
\eta_q = \frac{1}{d} \sum_{\nu=1}^{d} \cos q_\nu
\]
Stripes $\implies$ Anomalous Phonon Softening

$4 \times 2$ UNIT CELL $\implies$ FIRST REDUCED BRILLOUIN ZONE