



Dynamika sieci i oddziaływanie spin-fonon w nadprzewodnikach wysokotemperaturowych

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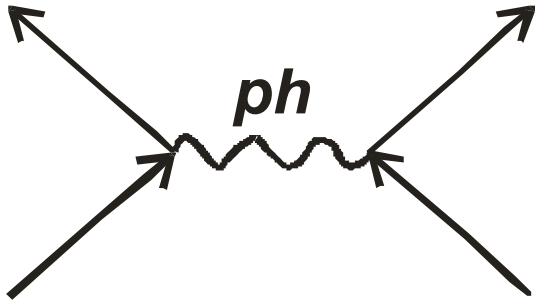
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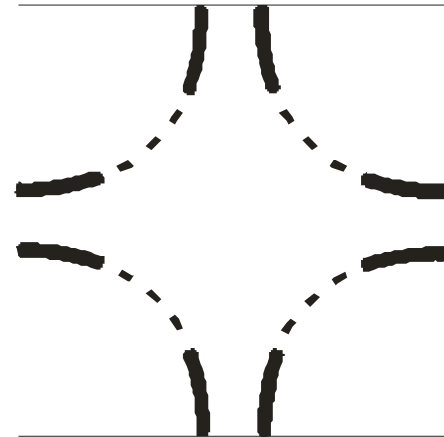
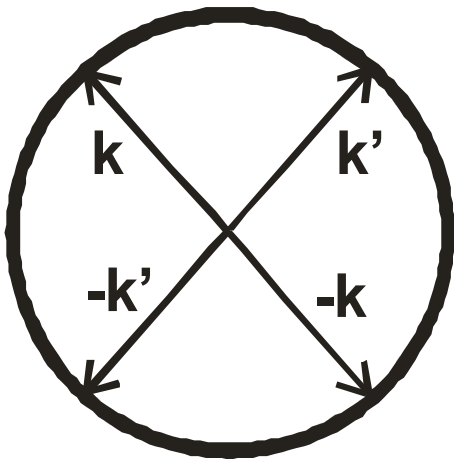
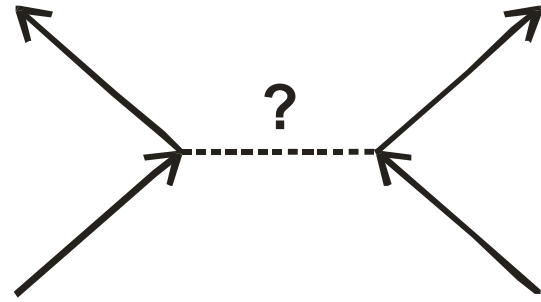
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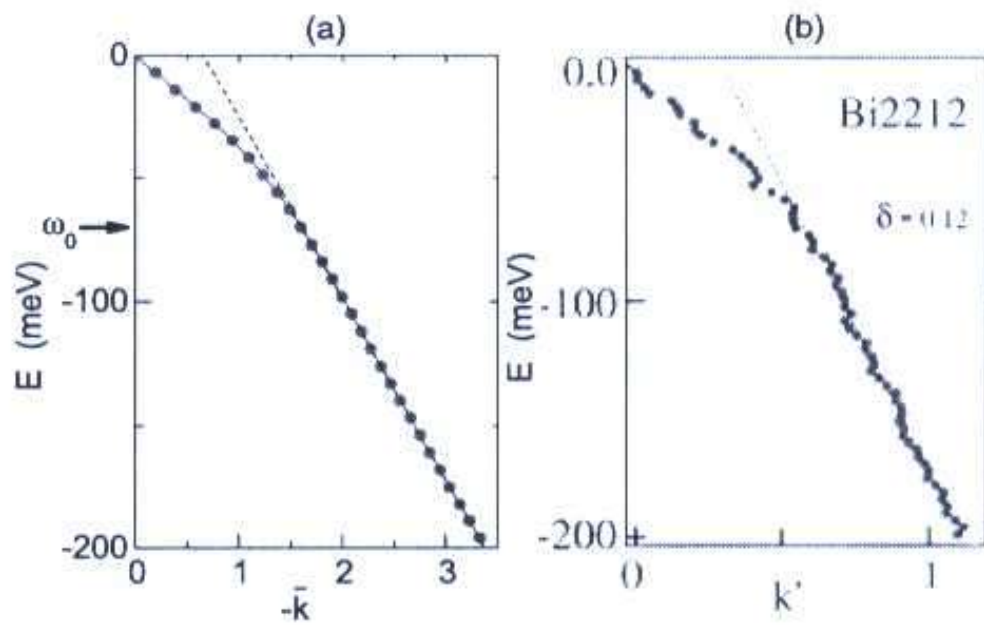
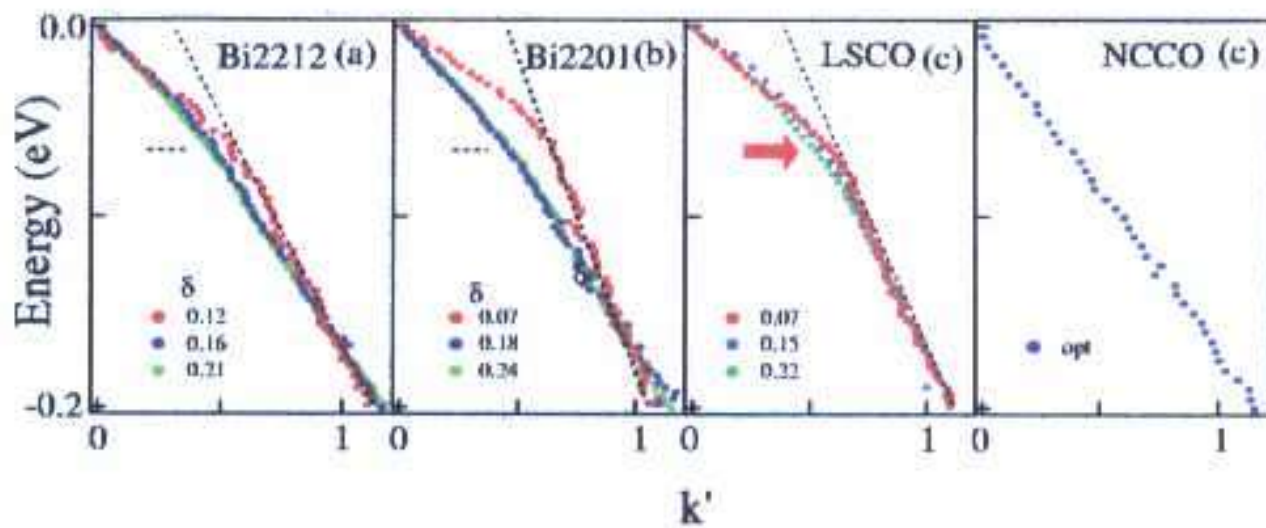
- I. Wstęp**
- II. Eksperyment neutronowy:
 $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$**
- III. Dynamika sieci – obliczenia**
 - a) model powłokowy
 - b) obliczenia *ab initio*
- VI. Model Hubbarda**
 - a) oddziaływanie *el-ph*
 - b) fluktuacje ładunkowe
 - c) dynamika spinowa

BCS

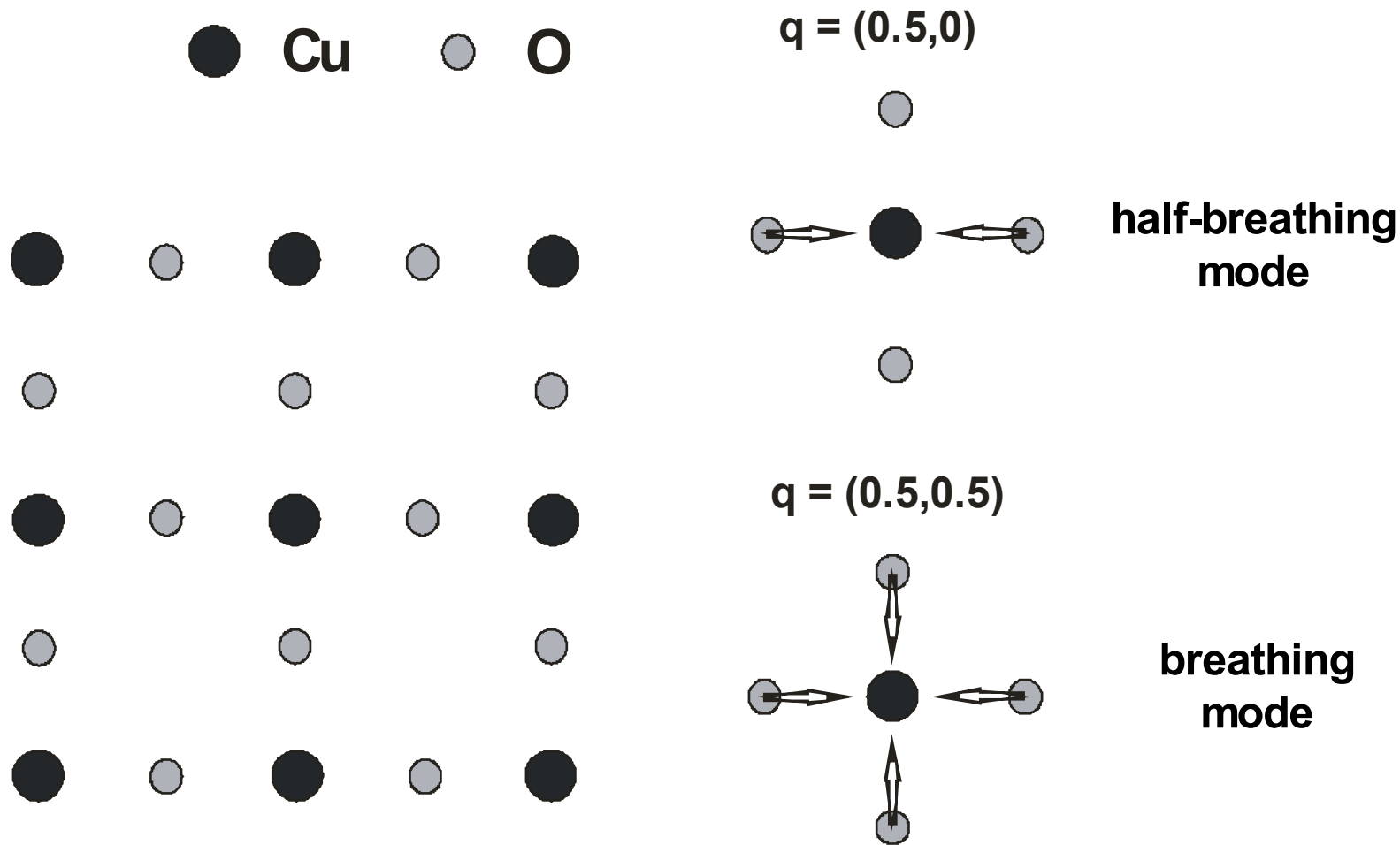


HTSC

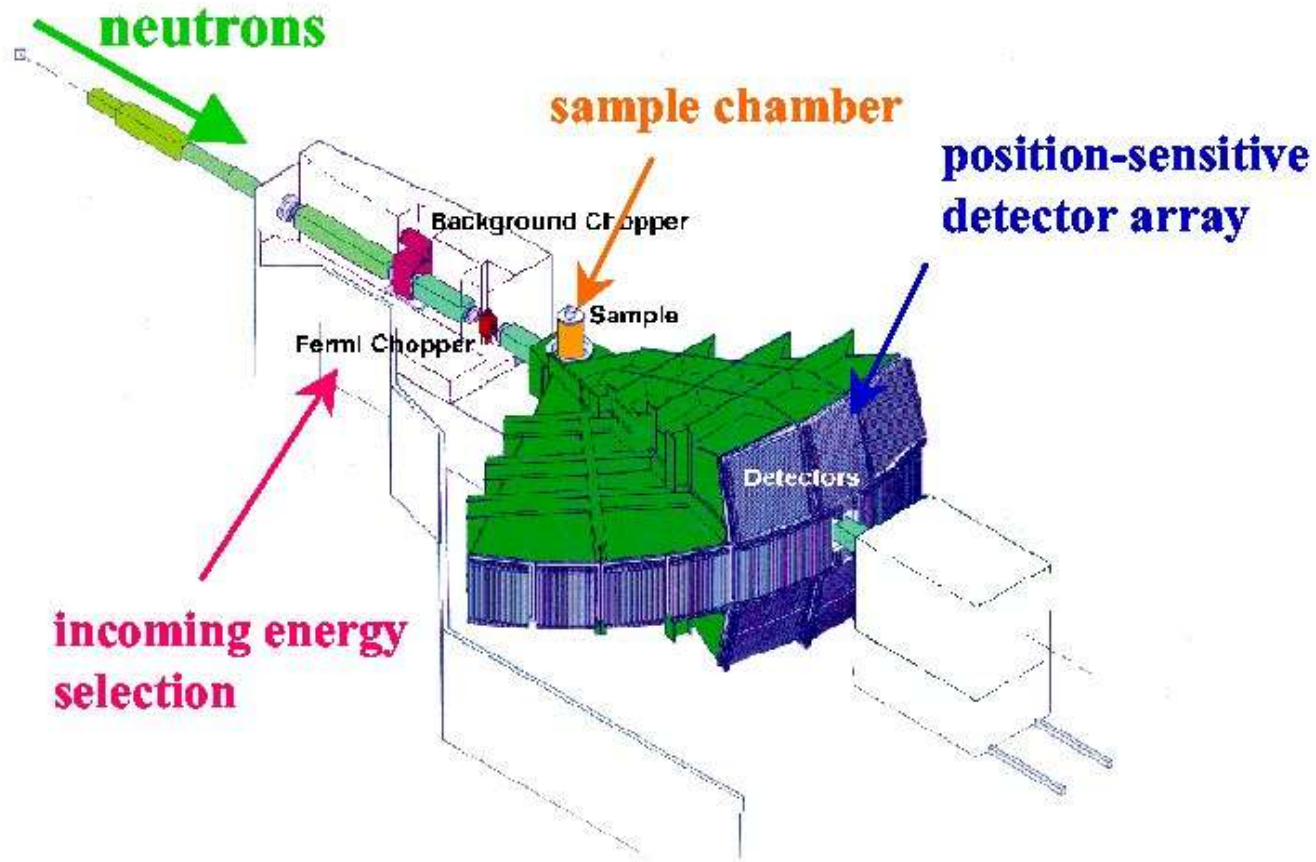




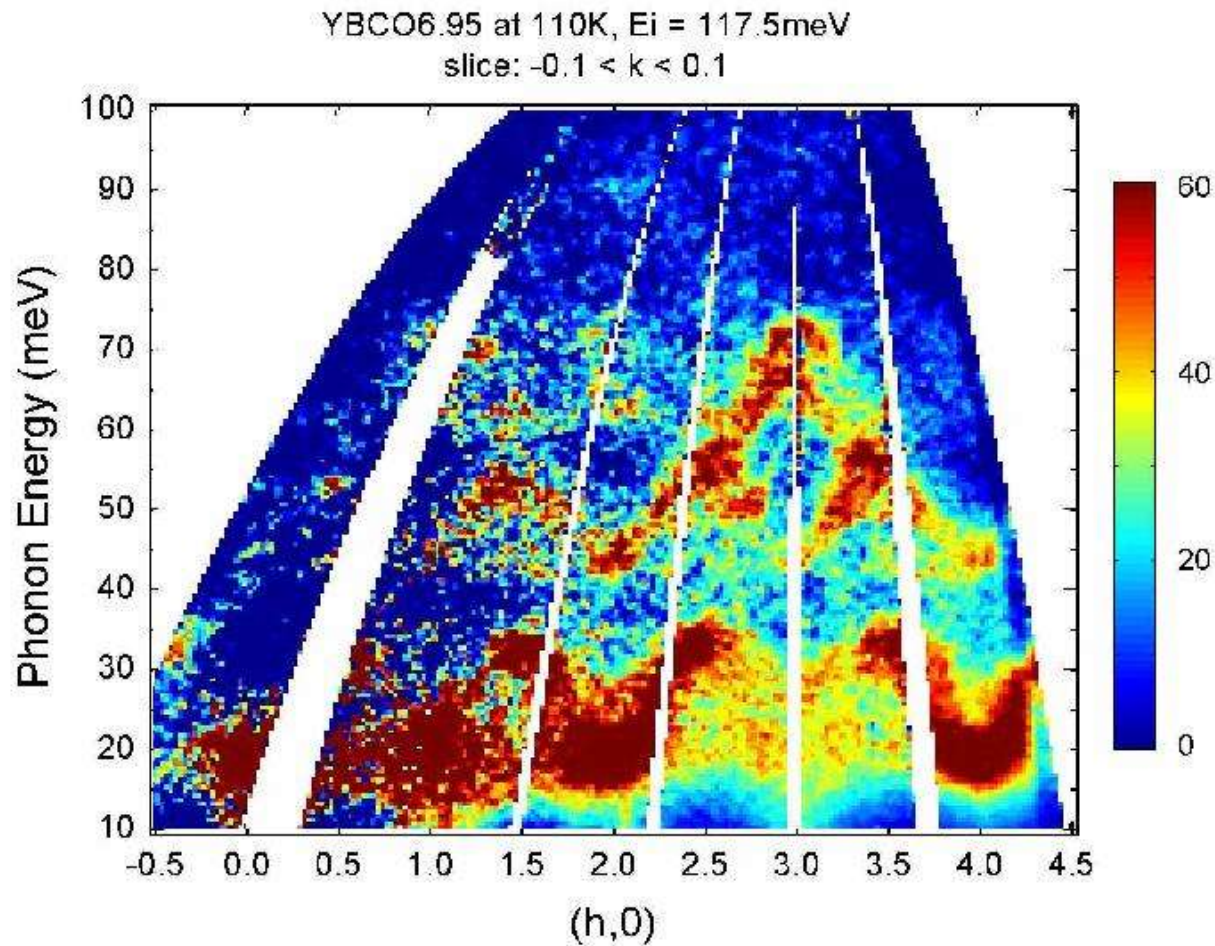
Mody fononowe w płaszczyznach CuO_2

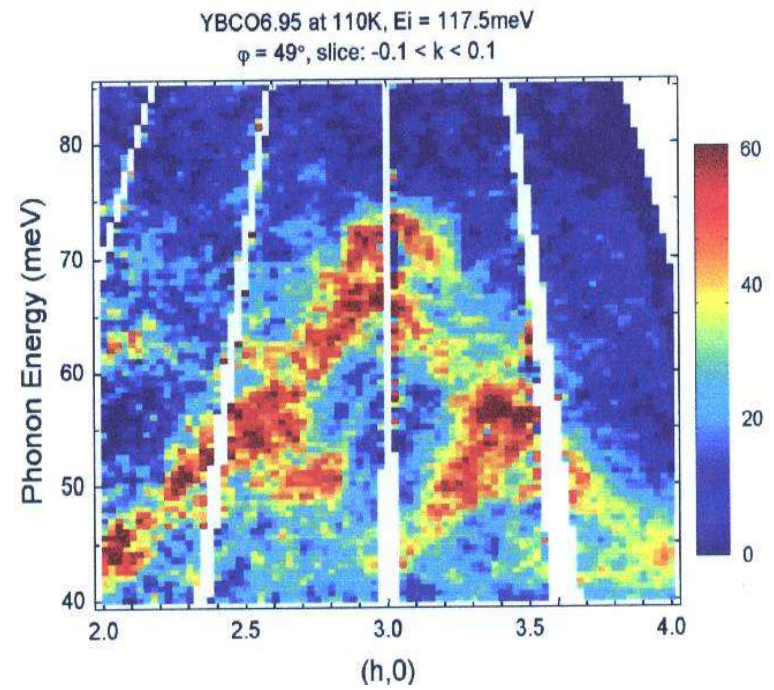
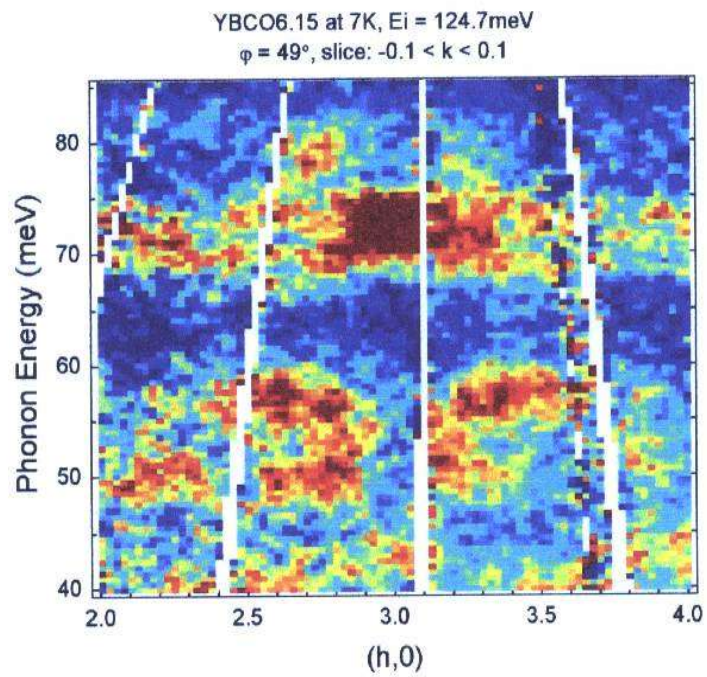


MAPS: neutronowy spektrometr czasu przelotu ISIS Rutherford Appleton Laboratory

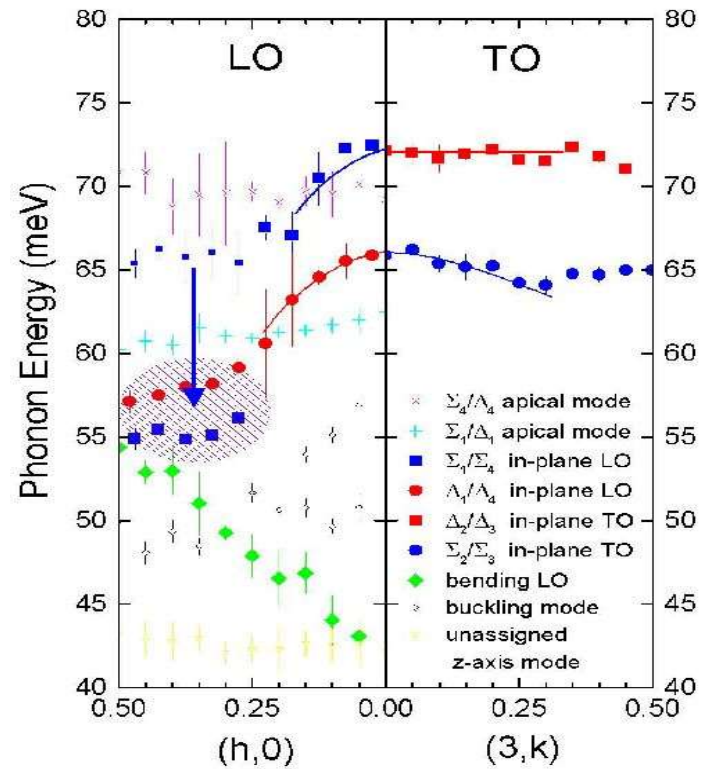
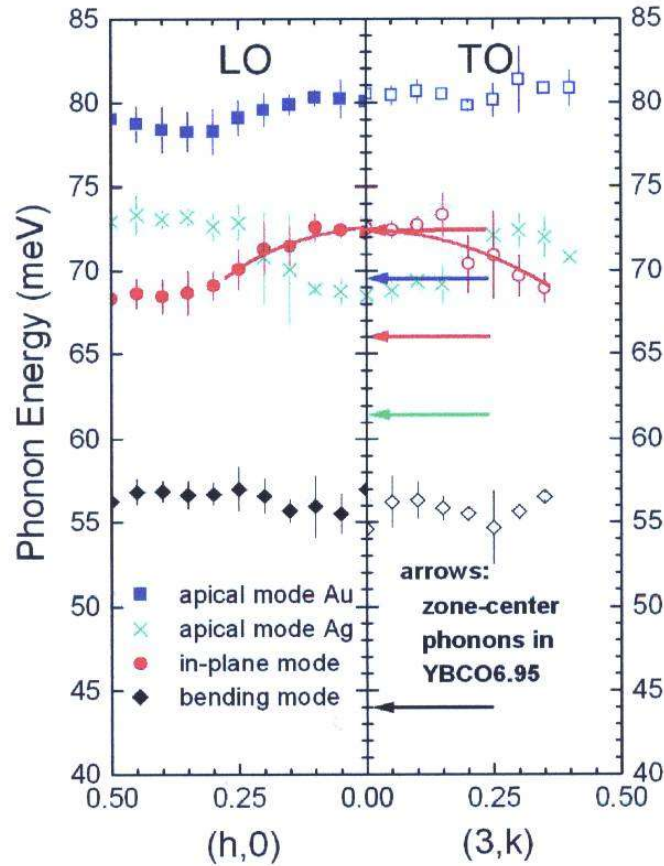


Dynamiczny czynnik strukturalny





Krzywe dyspersji



Dynamika sieci – metody obliczeniowe

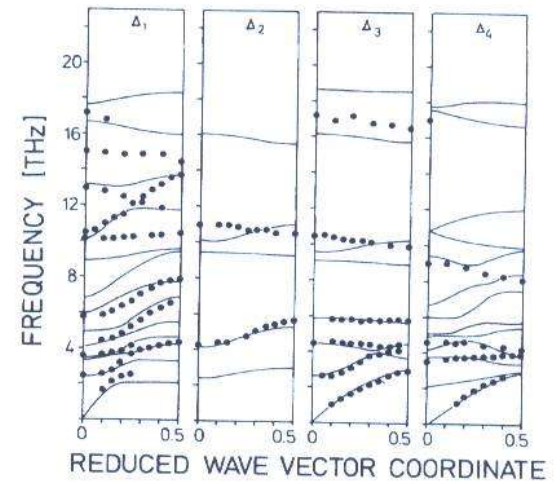
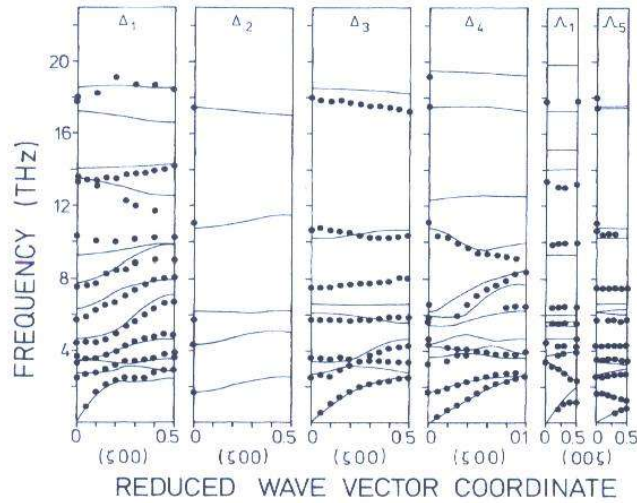
I. Obliczenia modelowe - model powłokowy



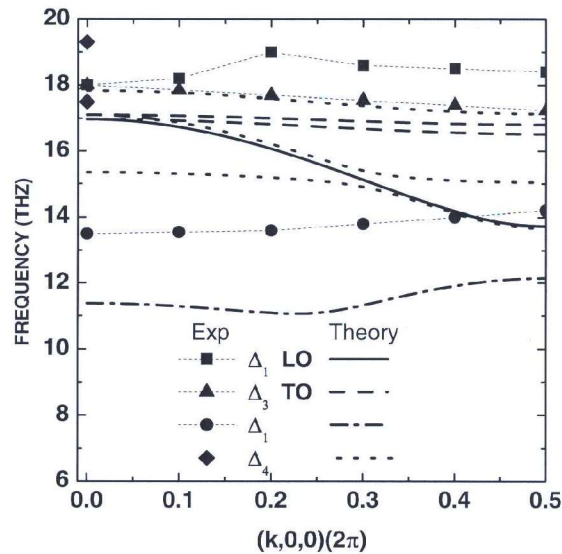
$$V(r_{ij}) = A \exp(-r_{ij}/B) - C/r_{ij}$$

II. Obliczenia *ab initio*

- metoda odpowiedzi liniowej
- metoda bezpośrednia (małych wychyleń)

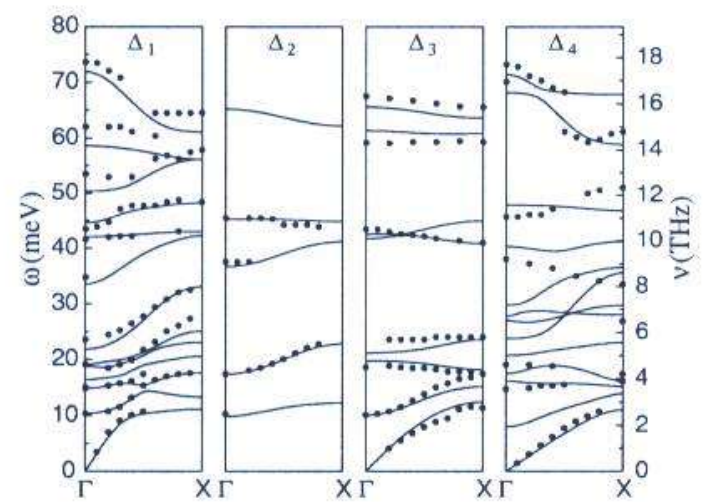


Model powłokowy



J. Łażewski

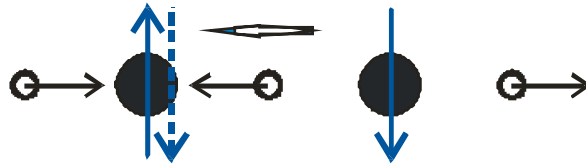
Ab initio



**K.-P. Bohnen, et al.,
Europhys. Lett. 64, 104 (2003)**

Model Hubbardda

$x = 0$

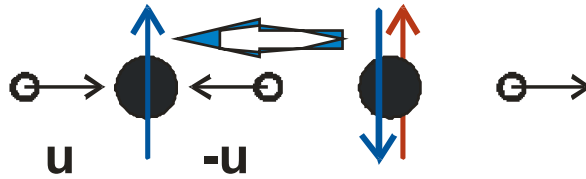


$U_d \sim 10 \text{ eV}$

$$t(u) = t_0 + u$$

$$t(u) = t_0 - u$$

$x > 0$



Electron-phonon Hamiltonian

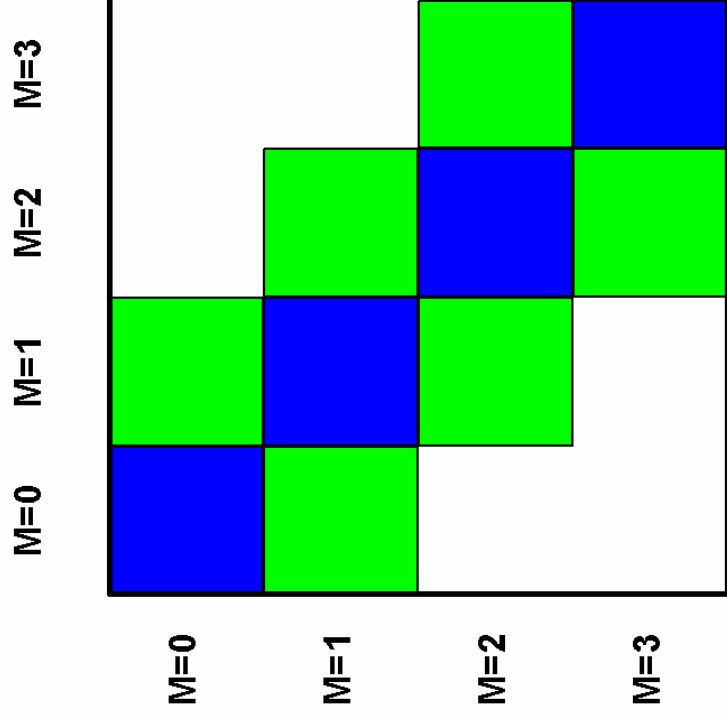
$$\begin{aligned}
 H = & \sum_{i,j,\sigma} t_{ij} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) + \sum_{i=1}^N U_i n_{i,\uparrow} n_{i,\downarrow} \\
 & + \frac{m}{2} \sum_{i=1}^N (\dot{u}_i^2 + \omega^2 u_i^2) - \lambda \sum_{i=1}^N n_i (u_i - u_{i-1})
 \end{aligned}$$

$$X_q = \frac{1}{\sqrt{N}} \sum_{i=1}^N u_i(q) = \frac{1}{\sqrt{N}} \sum_{i=1}^N u_i e^{iqr_i} = \sqrt{\frac{\hbar}{2m\omega_q}} (b_q^\dagger + b_q)$$

$$H_p + H_{e-p} = \sum_q \hbar\omega_q (b_q^\dagger b_q + \frac{1}{2}) + \sum_{i=1,q}^N g(q) n_i e^{iqr_i} (b_q^\dagger + b_{-q})$$

$$g(q) = -2i\lambda \sqrt{\frac{\hbar}{2m\omega N}} \sin\left(\frac{q}{2}\right) \qquad \hbar\omega_\alpha = \lambda \sqrt{\frac{\hbar}{2m\omega}}$$

H =



Dim = Dim_e * Dim_p Dim_p = 10-20

N=8 x = 0 Dim_e = 4900

N=8 x = 1/4 Dim_e = 3136

N=12 x = 1/6 Dim_e = 627264

Spectral properties

The energy spectrum of a given operator A can be calculated as

$$I(\omega) = \sum_n |\langle \psi_n | A | \psi_0 \rangle|^2 \delta(\omega - E_n + E_0)$$

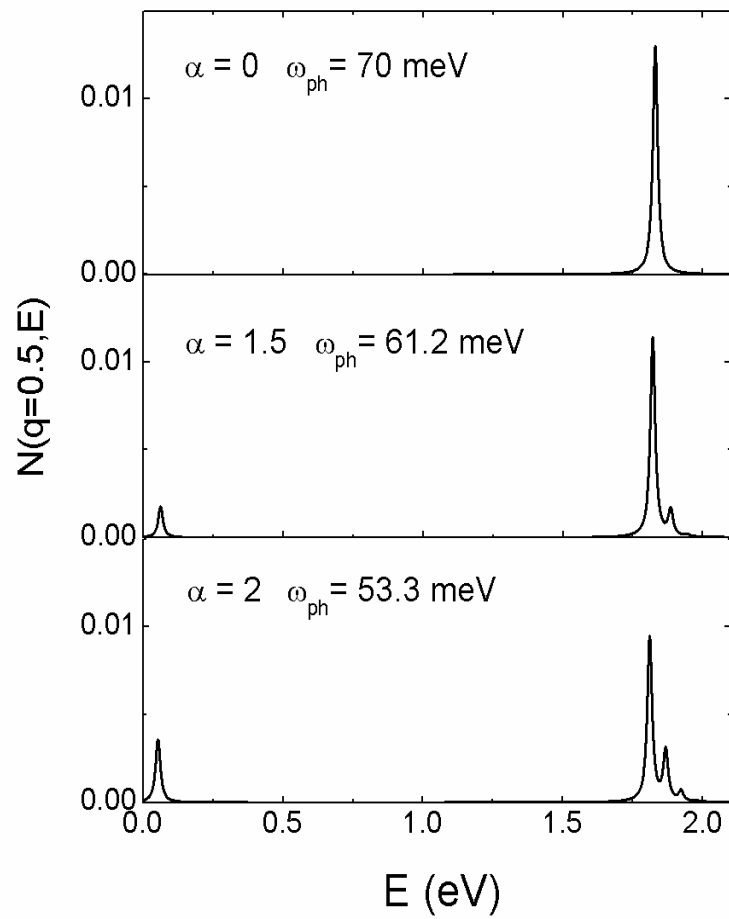
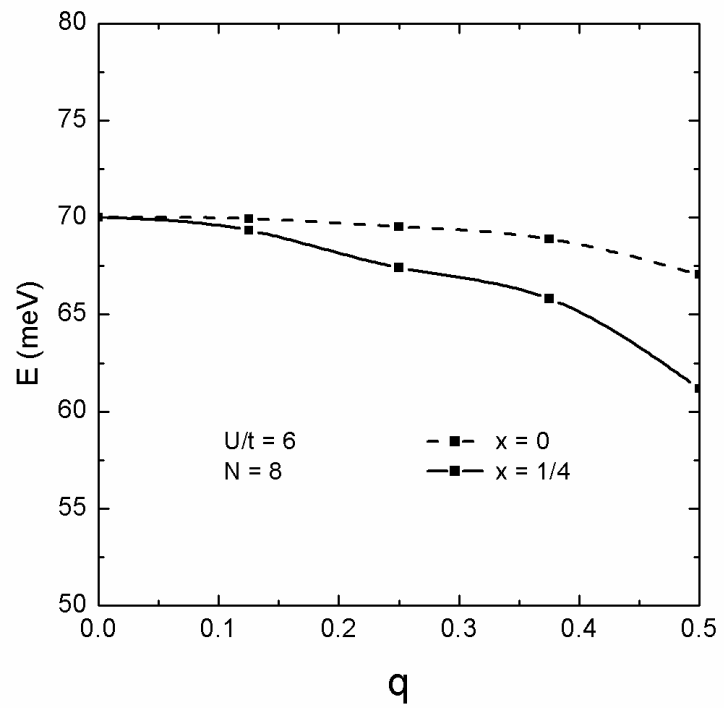
In order to evaluate $I(\omega)$ we repeat the Lanczos procedure starting with a vector

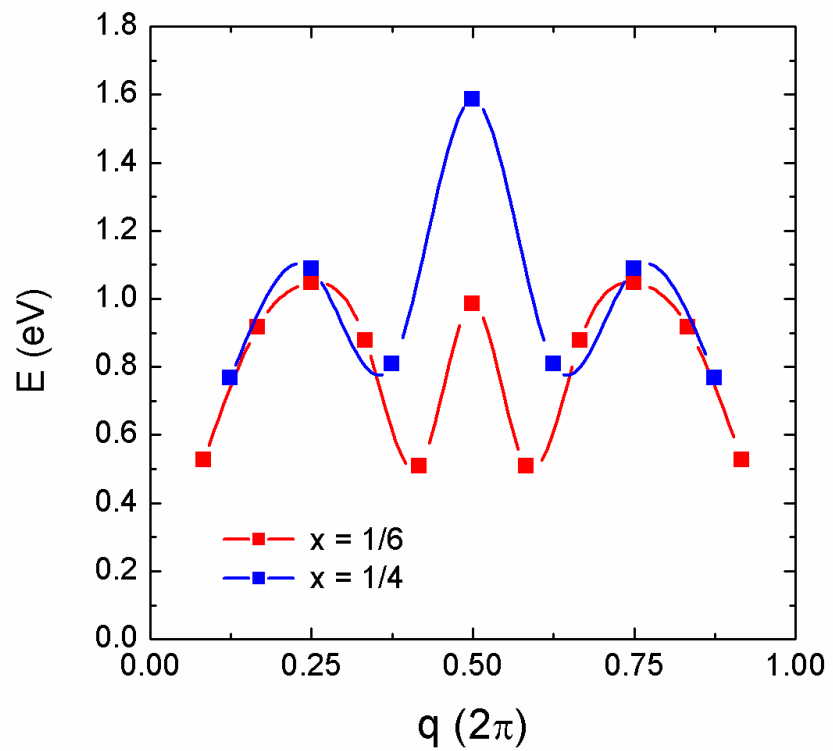
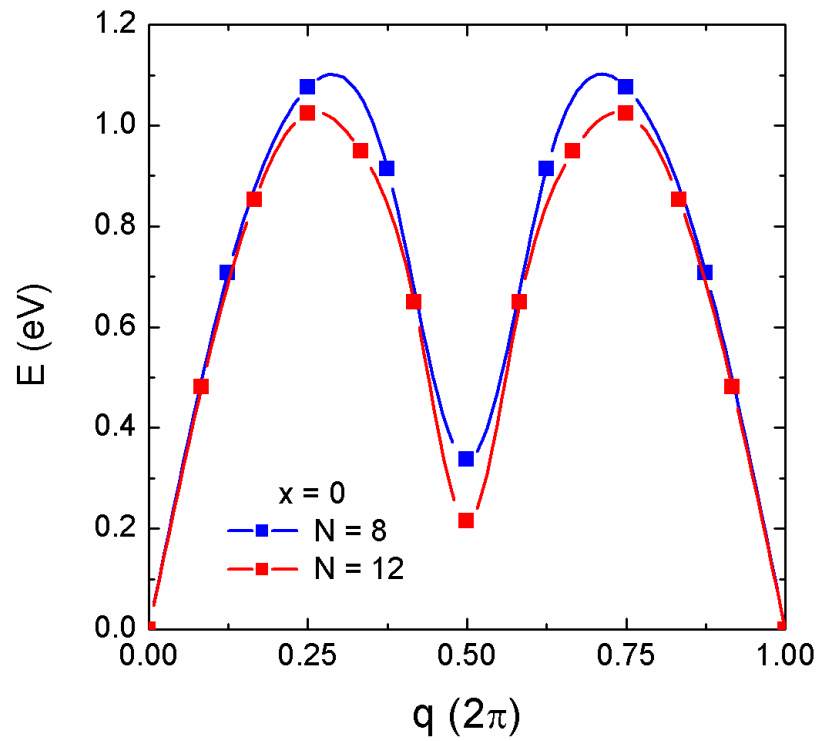
$$|\phi_0\rangle = \frac{A|\psi_0\rangle}{\sqrt{\langle \psi_0 | A^\dagger A | \psi_0 \rangle}}$$

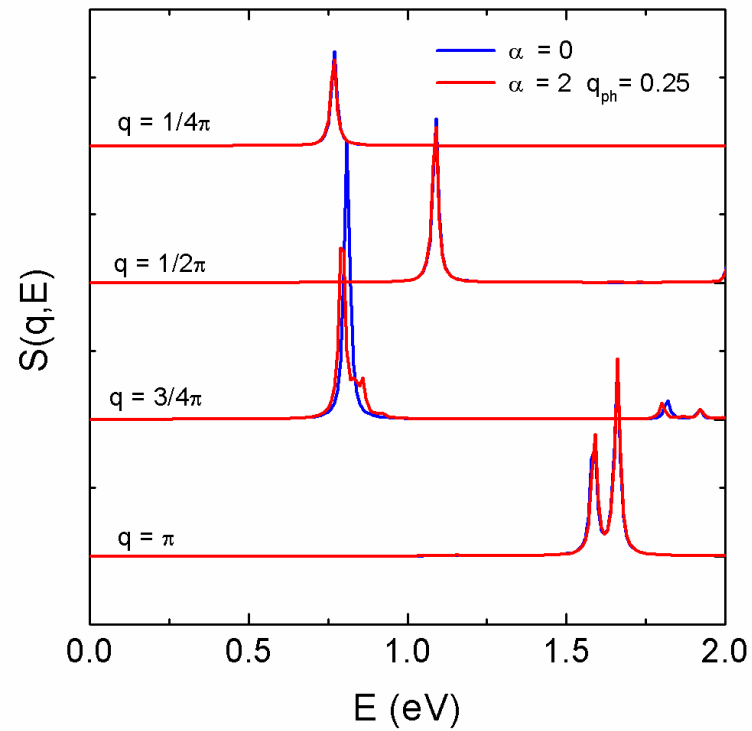
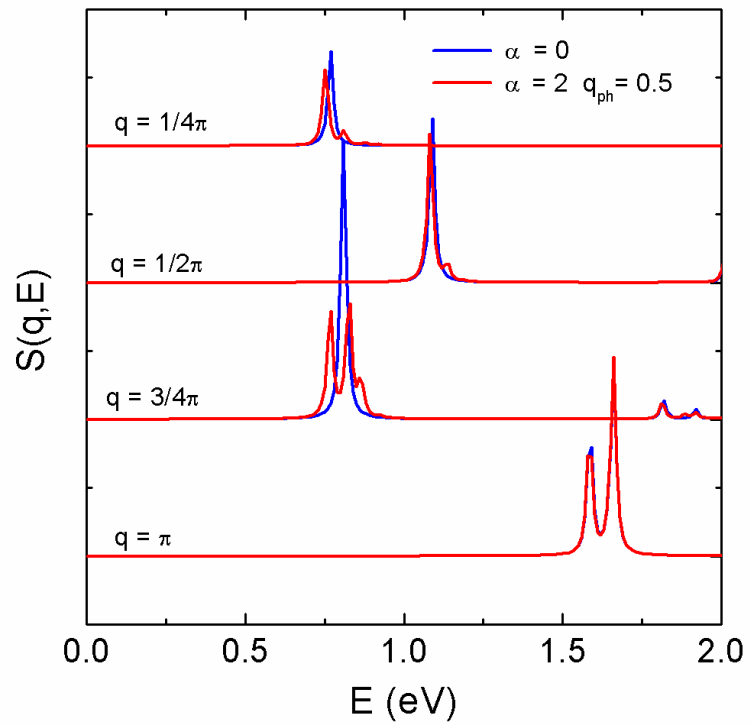
$$I(\omega) = -\frac{1}{\pi} \text{Im} \frac{\langle \psi_0 | A^\dagger A | \psi_0 \rangle}{\omega + E_0 - a_0 - \frac{b_1^2}{\omega + E_0 - a_1 - \frac{b_2^2}{\omega + E_0 - a_2 - \dots}}}$$

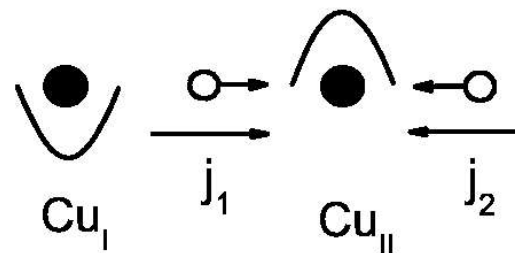
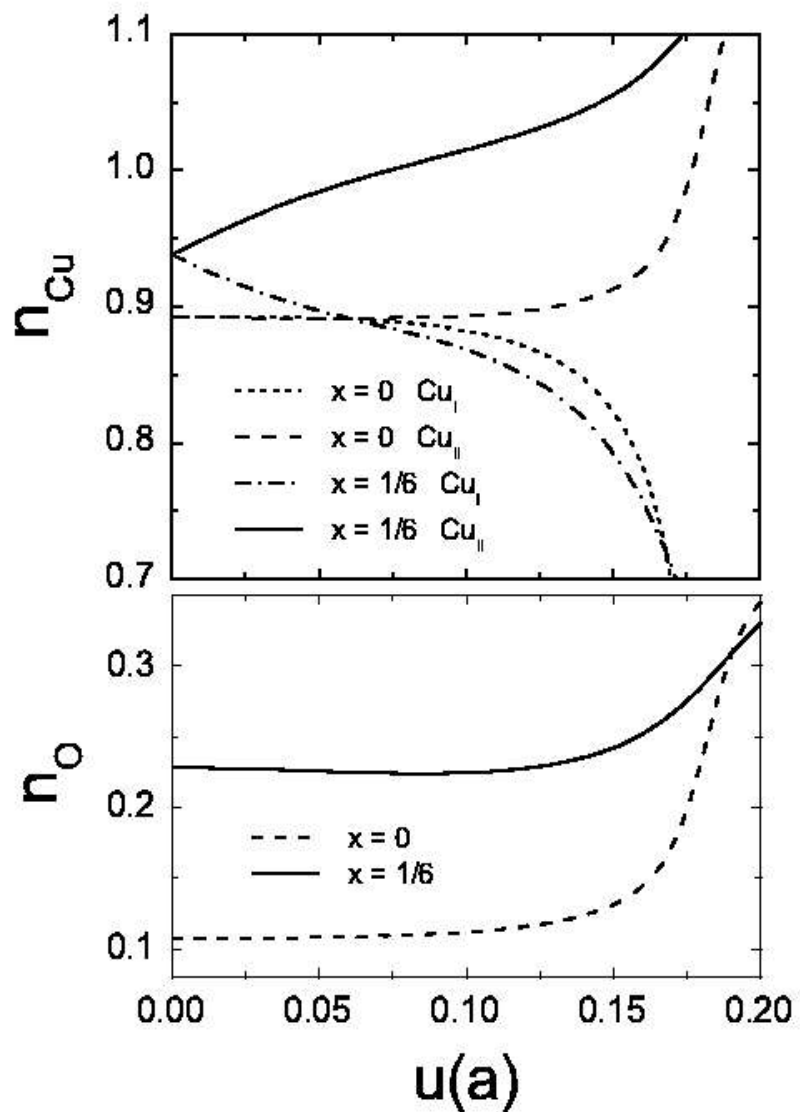
The intensity of each peak can be also written in terms of the first component of each eigenvector $|\psi_n\rangle = \sum_m c_m^n |\phi_m\rangle$

$$I(\omega) = \sum_n |c_0^n|^2 \langle \psi_0 | A^\dagger A | \psi_0 \rangle \delta(\omega - E_n + E_0)$$

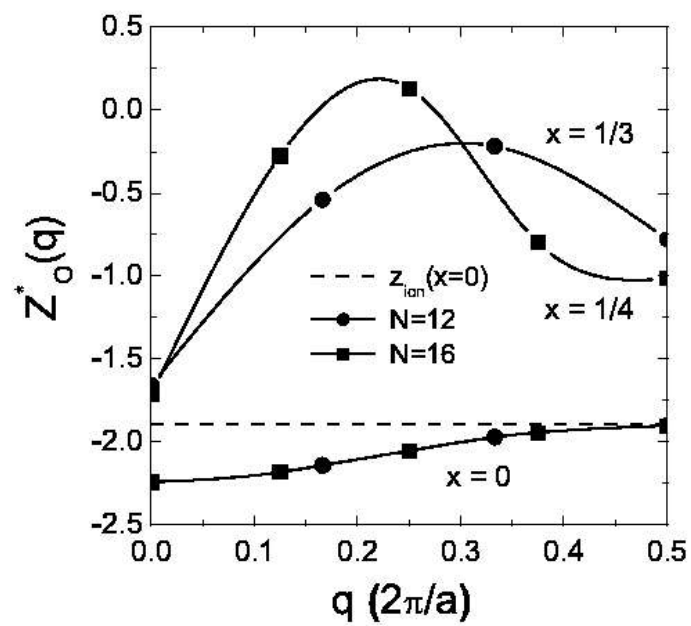




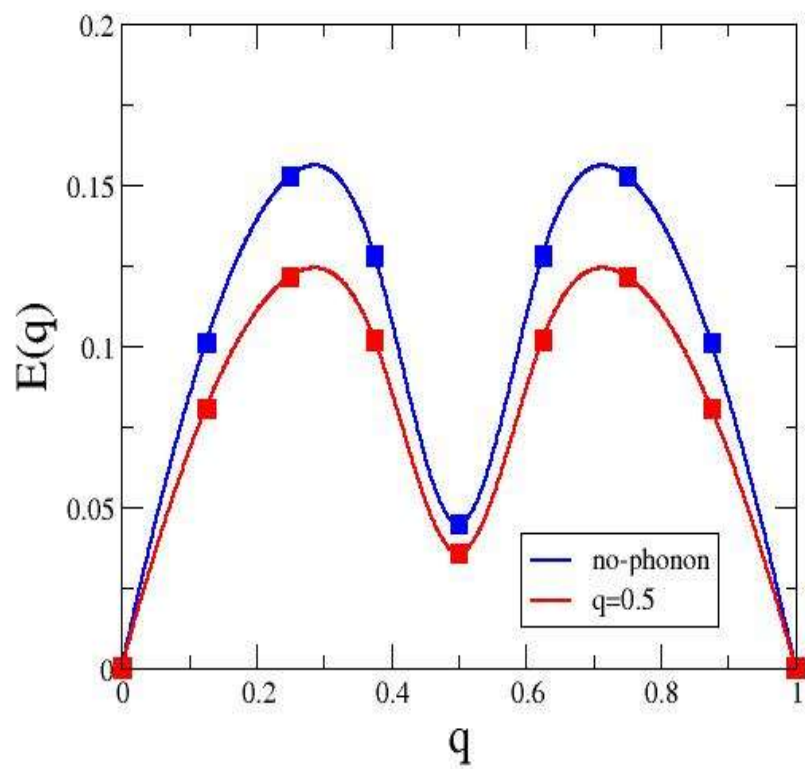




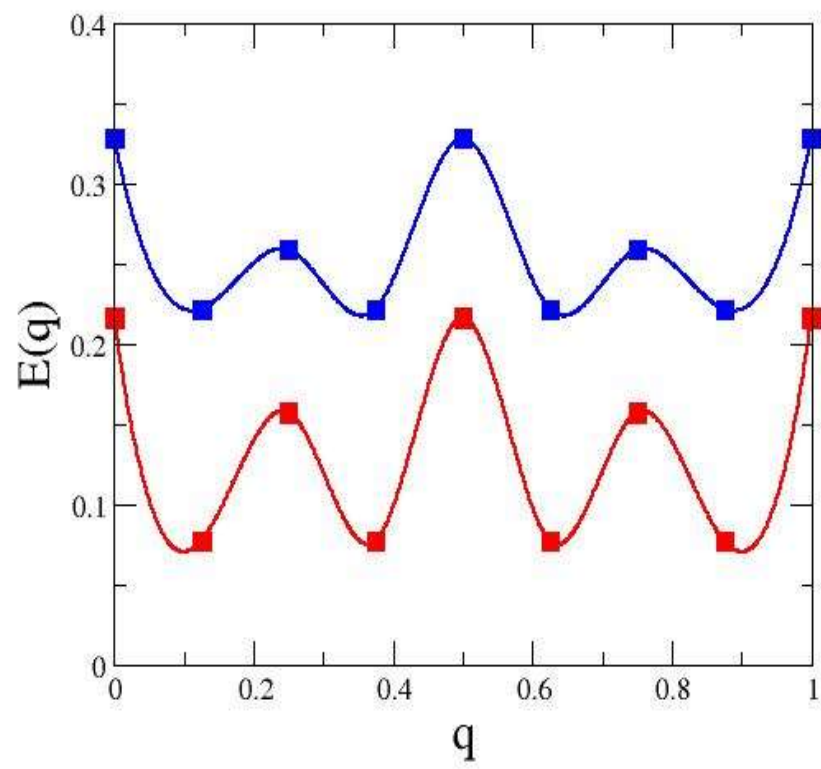
$$Z^* = Z_{\text{ion}} + DZ/u$$

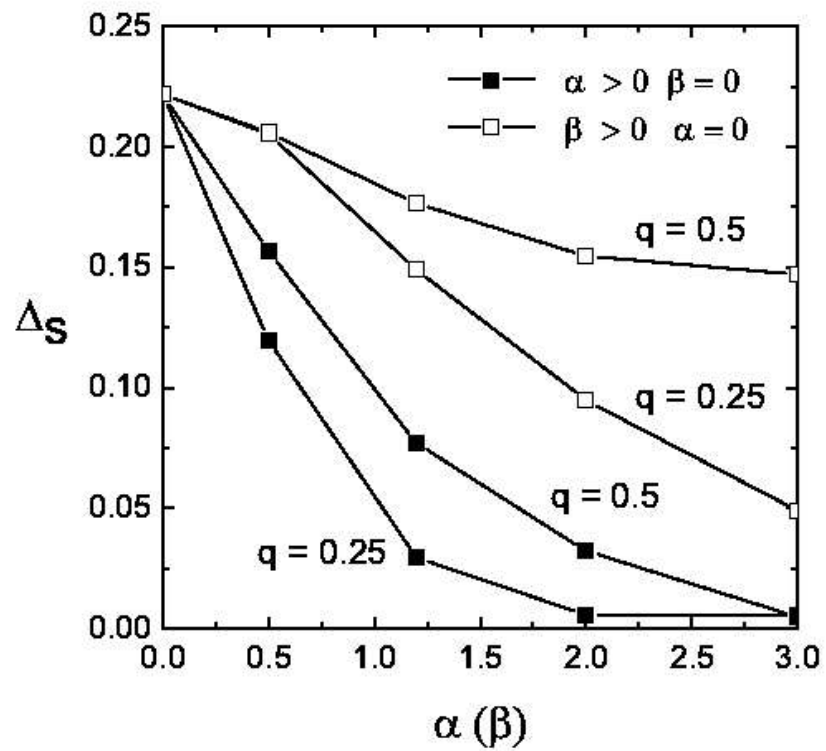
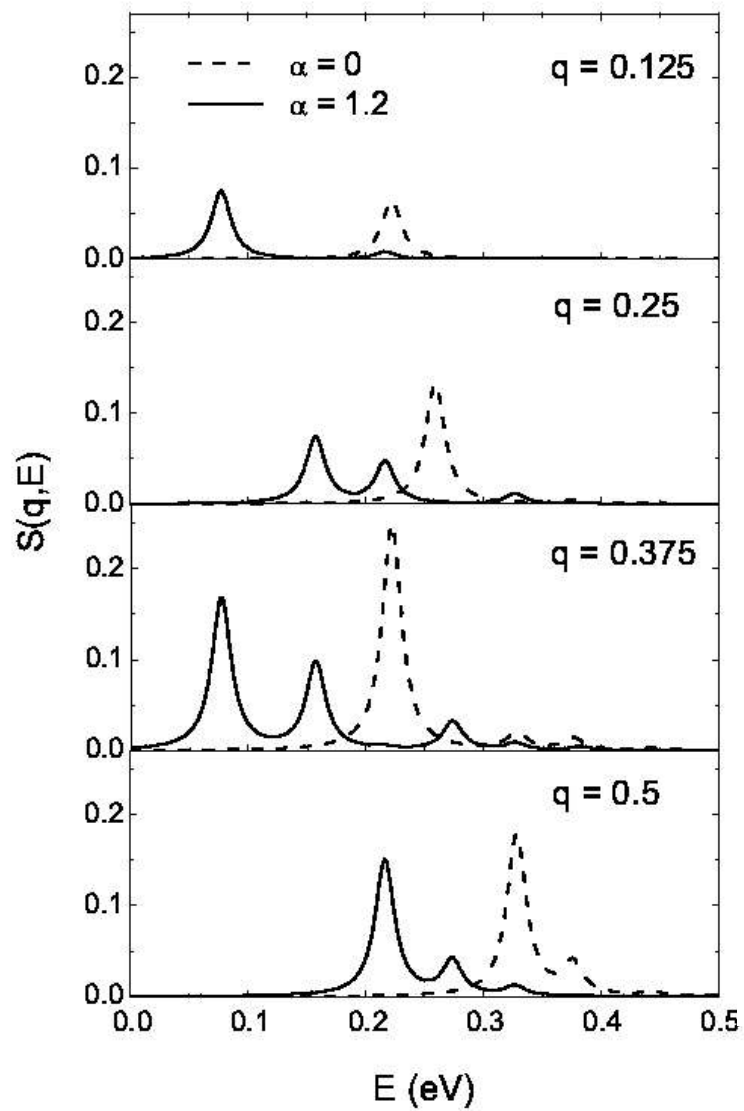


x = 0



x = 0.25

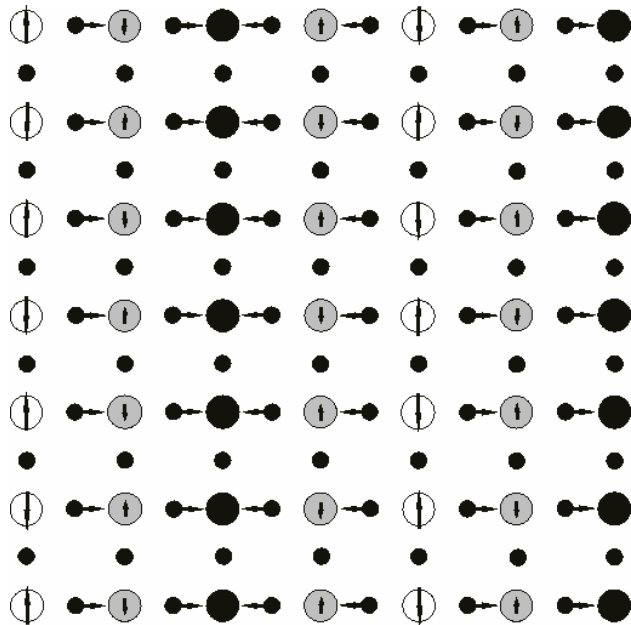




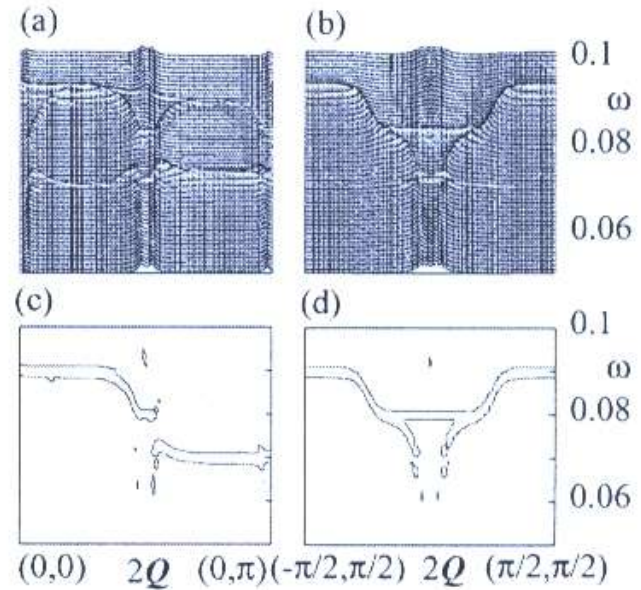
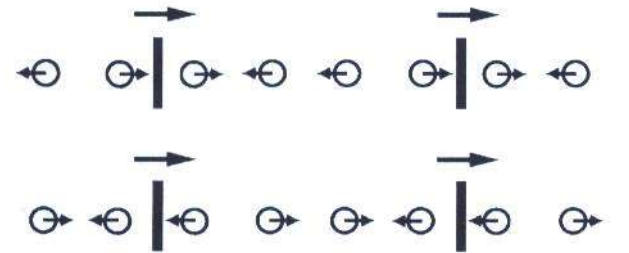
Fluktuacje ładunkowo-spinowe

J. Zaanen and O. Gunnarsson
Phys. Rev. B 40, 7391 (1989)

J.M. Tranquada *et al.*, Nature 375, 561 (1995)



A. Kaneshita *et al.*, Phys. Rev. Lett. 88, 115501 (2002)



Podsumowanie

- **Pomiary neutronowe w YBCO potwierdziły silną zmianę częstości tlenowych modów optycznych w płaszczyźnie CuO w przejściu izolator-metal**
- **Zaobserwowano anizotropie krzywych dyspersji w kierunkach a i b**
- **Porównane zostały wyniki eksperymentalne z obliczeniami modelowymi i *ab initio***
- **Obliczenia dynamiki sieci powinny uwzględniać korelacje elektronowe w stanach *d***
- **Uporządkowanie (fluktuacje) ładunkowo-spinowe mogą być odpowiedzialne za nieciągłości w krzywych dyspersji**