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

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

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

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

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

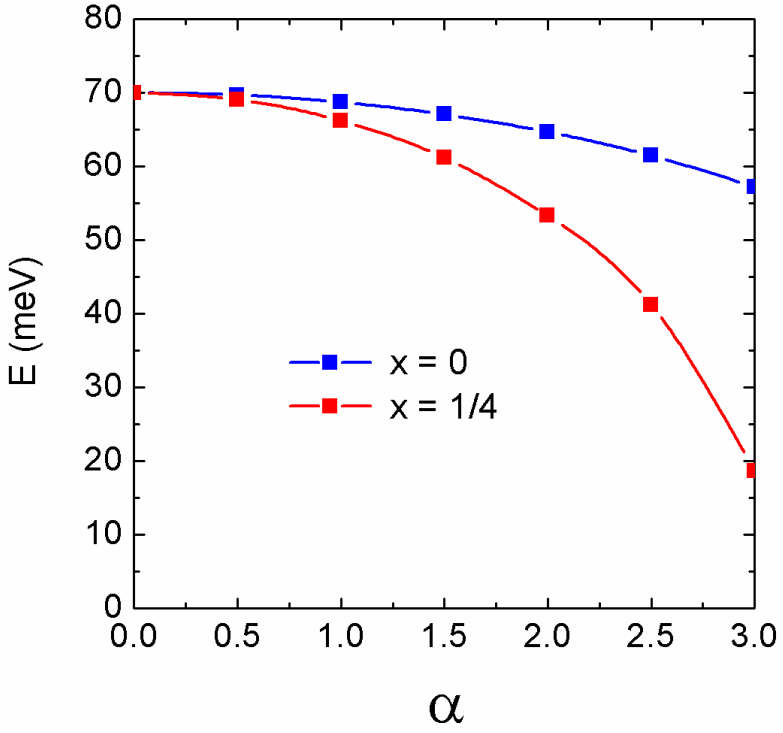
Scattering cross sections

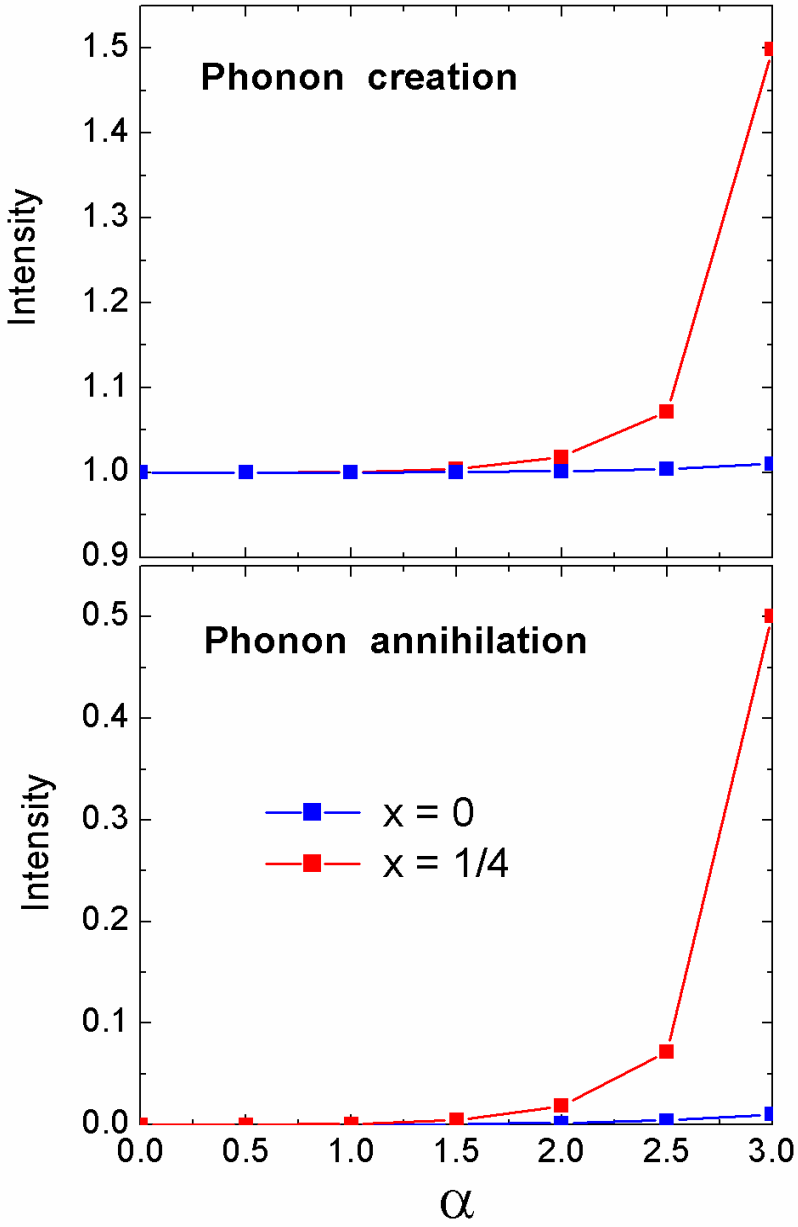
Phonon creation

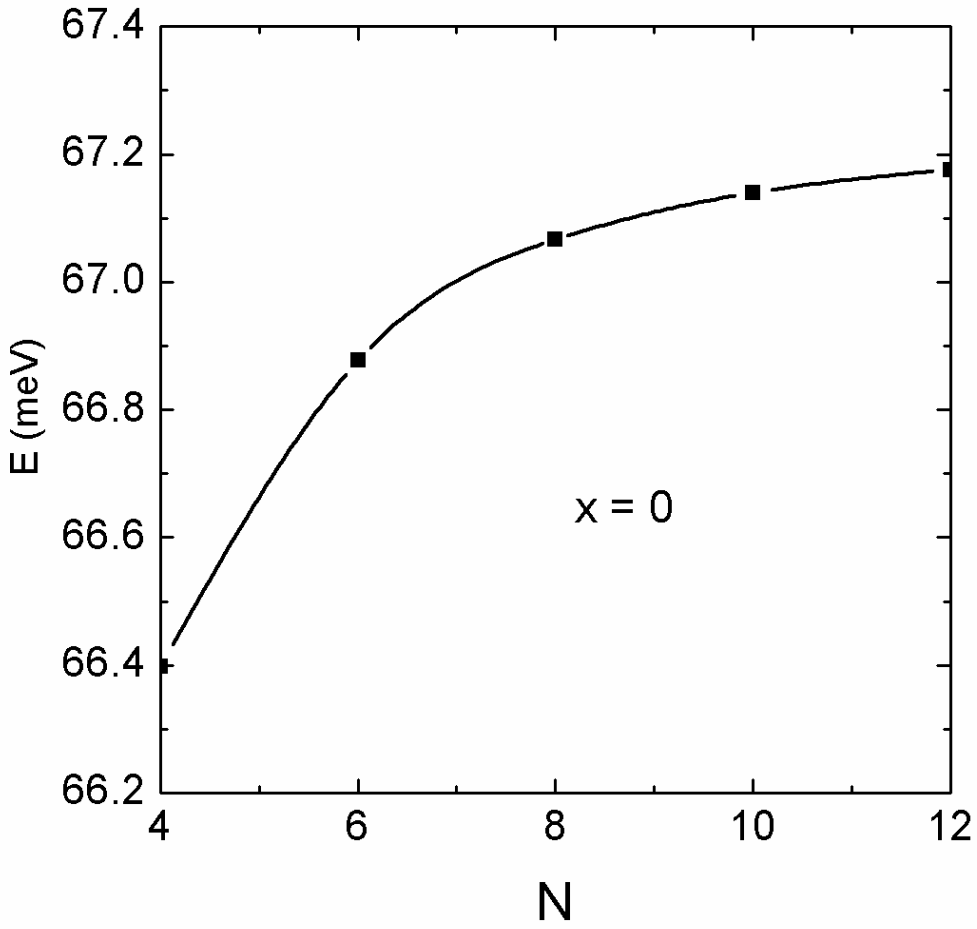
$$B_q^{>}(\omega) = \sum_n |\langle \psi_n | b_q^\dagger | \psi_0 \rangle|^2 \delta(\omega - E_n + E_0)$$

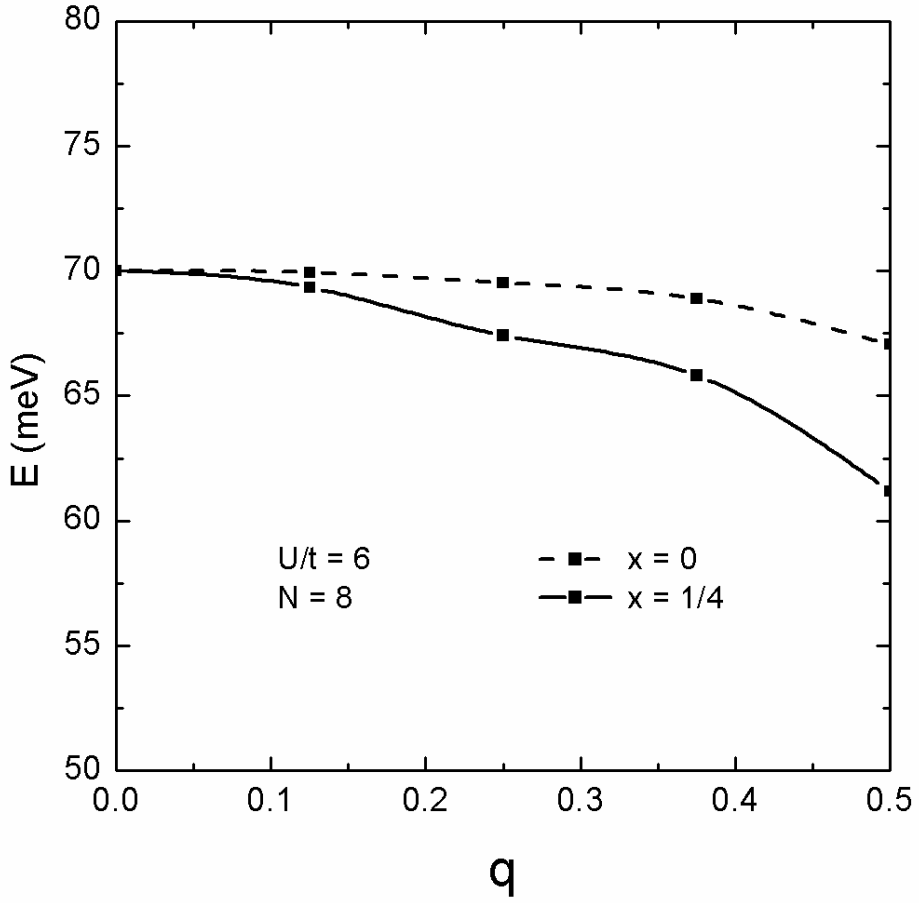
Phonon annihilation

$$B_q^{<}(\omega) = \sum_n |\langle \psi_n | b_q | \psi_0 \rangle|^2 \delta(\omega + E_n - E_0)$$

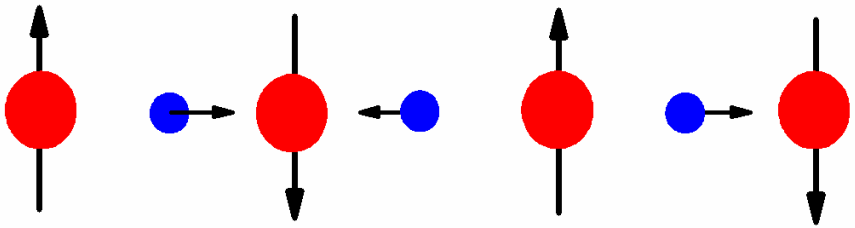

E (meV)
80
70
60
50
40
30
20
10
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
α
x = 0
x = 1/4


Phonon creation
Intensity
1.5
1.4
1.3
1.2
1.1
1.0
0.9
Phonon annihilation
Intensity
0.5
0.4
0.3
0.2
0.1
0.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
α
x = 0
x = 1/4

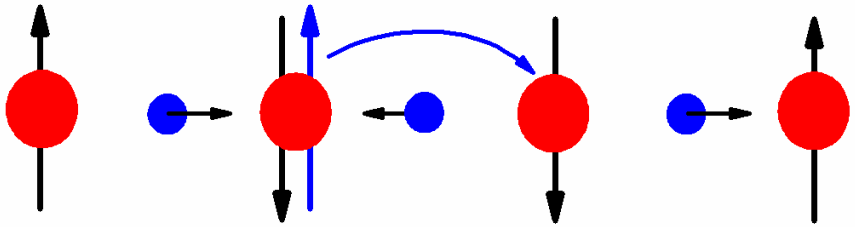

67.4
67.2
67.0
66.8
66.6
66.4
66.2
E (meV)
4
6
8
10
12
N
x = 0


80
75
70
65
60
55
50
E (meV)
0.0
0.1
0.2
0.3
0.4
0.5
q
U/t = 6
N = 8
x = 0
x = 1/4

x = 0 Mott - insulator $\Delta \sim U$



x > 0 Metal



$$F = - m\omega^2 u$$

$$F - F' = - m\omega'^2 u$$

$$\omega' < \omega$$

Charge dynamics

$$\rho_i = \langle \psi_0 | n_i | \psi_0 \rangle = \langle \psi_0 | (n_{i,\uparrow} + n_{i,\downarrow}) | \psi_0 \rangle$$

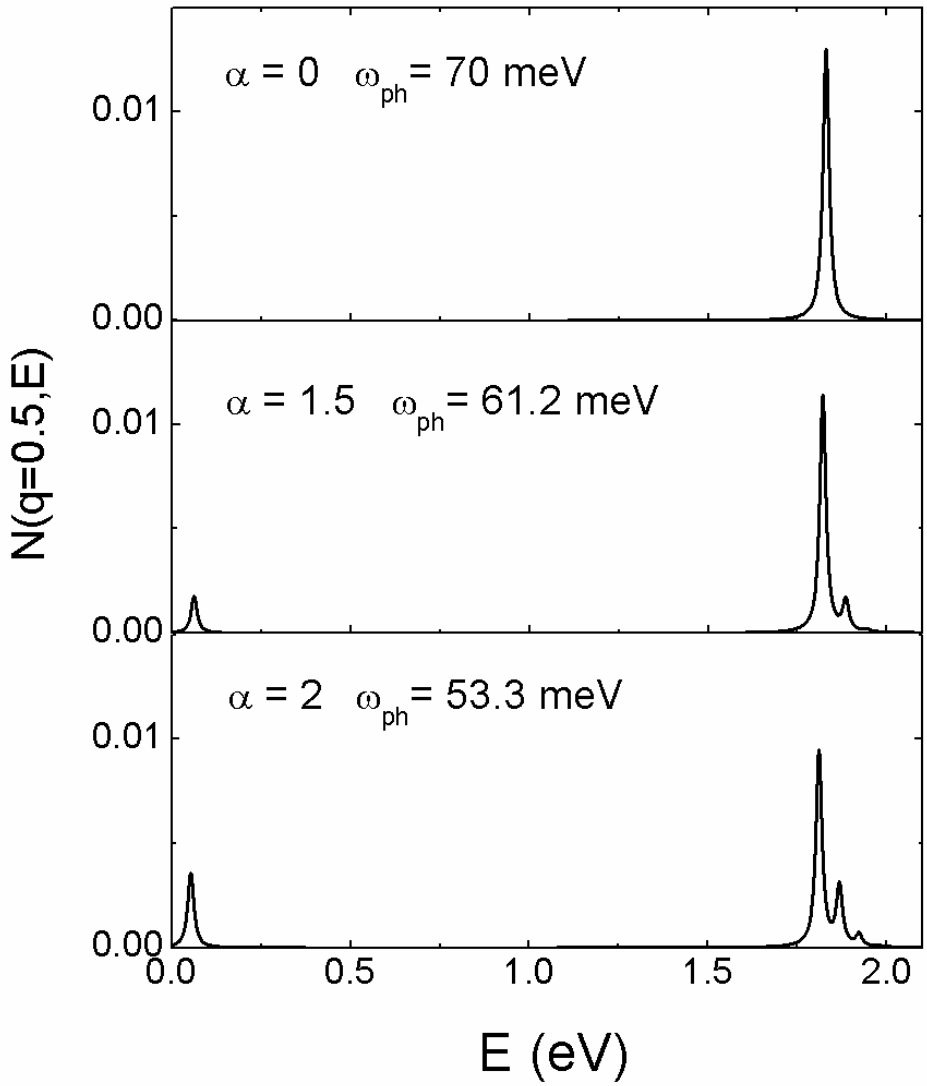
Charge-charge correlation function

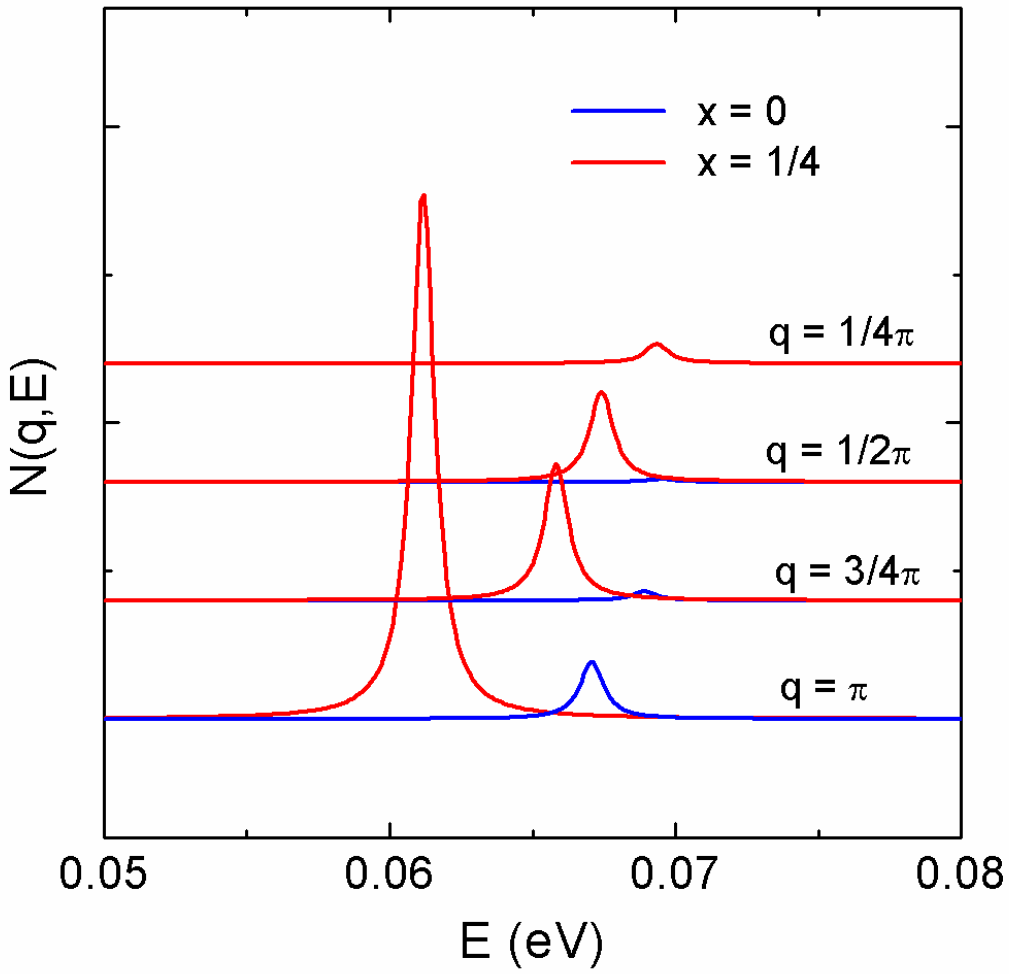
$$N_{ij} = \langle \psi_0 | n_i n_j | \psi_0 \rangle$$

$$N_q = \frac{1}{\sqrt{N}} \sum_i n_i e^{iqR_i}$$

$$N(q) = \langle \psi_0 | N_q N_{-q} | \psi_0 \rangle = \frac{1}{N} \sum_{ij} e^{iqr_{ij}} \langle \psi_0 | n_i n_j | \psi_0 \rangle$$

$$N(q,\omega) = \sum_n |\langle \psi_0 | N_q | \psi_n \rangle|^2 \delta(\omega - E_n + E_0)$$


α = 0 ω_ph = 70 meV
α = 1.5 ω_ph = 61.2 meV
α = 2 ω_ph = 53.3 meV
0.01
0.00
0.0
0.5
1.0
1.5
2.0
N(q=0.5,E)
E (eV)


x = 0
x = 1/4
q = 1/4π
q = 1/2π
q = 3/4π
q = π
N(q,E)
0.05
0.06
0.07
0.08
E (eV)

Spin dynamics

$$\hat{s}_i^z = \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow})$$

$$s_i^z = \langle \psi_0 | \hat{s}_i^z | \psi_0 \rangle$$

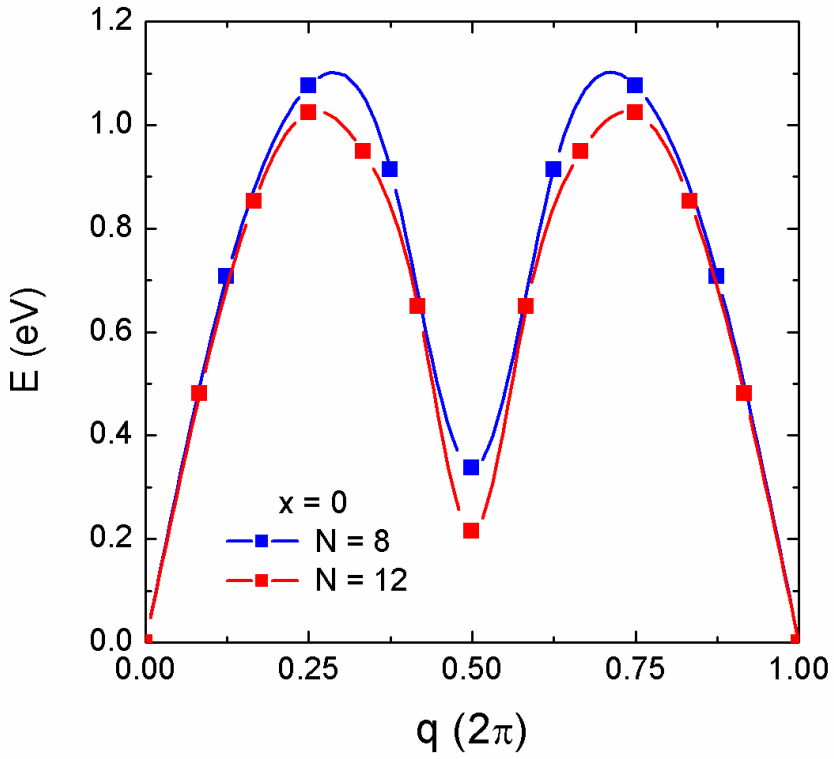
Spin-spin correlation function

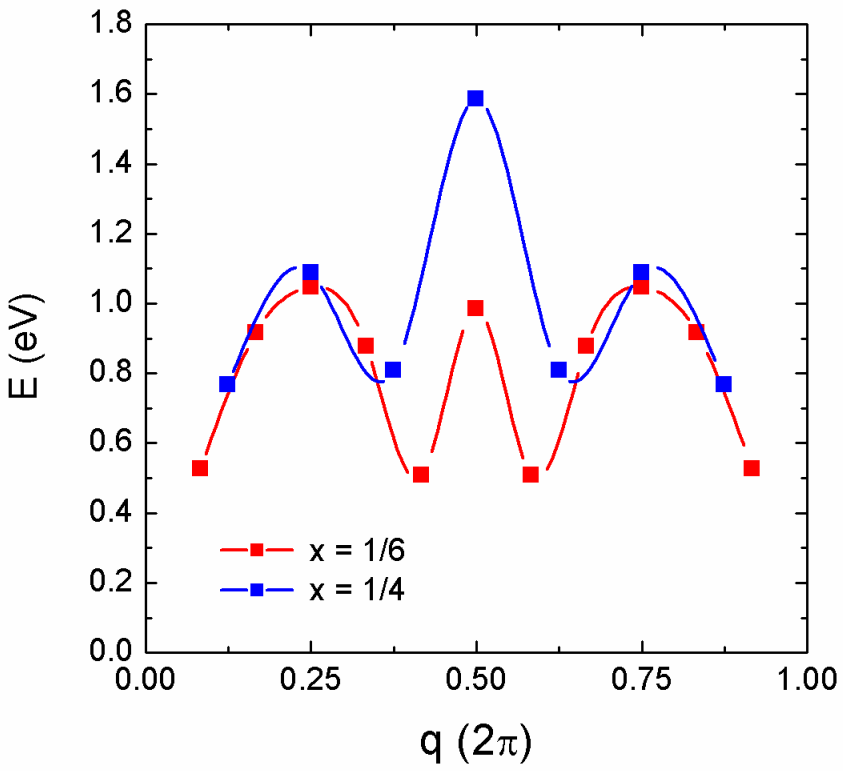
$$S_{ij} = \langle \psi_0 | s_i^z s_j^z | \psi_0 \rangle$$

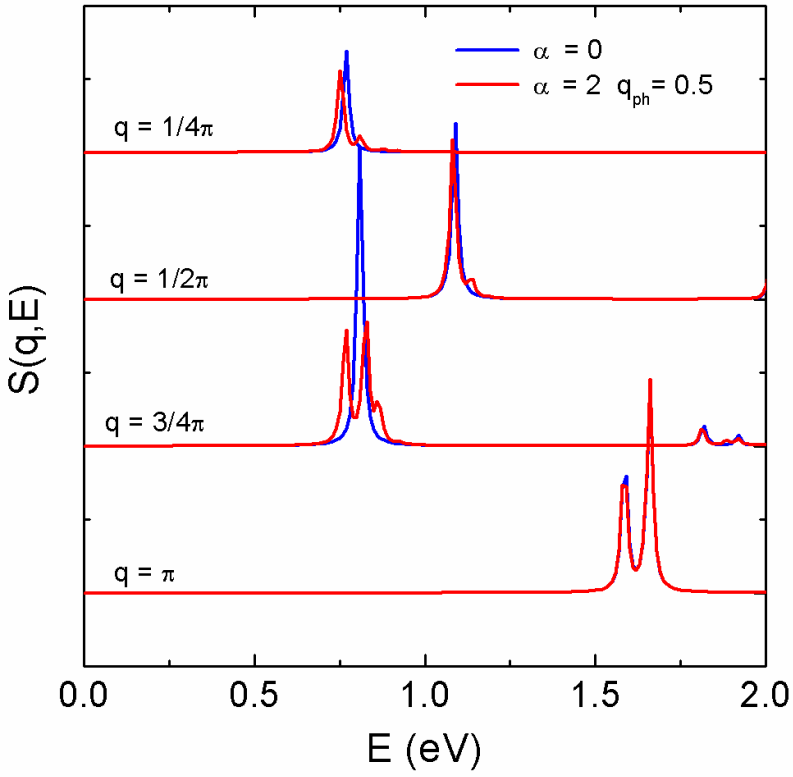
$$S_q = \frac{1}{\sqrt{N}} \sum_i s_i^z e^{iqR_i}$$

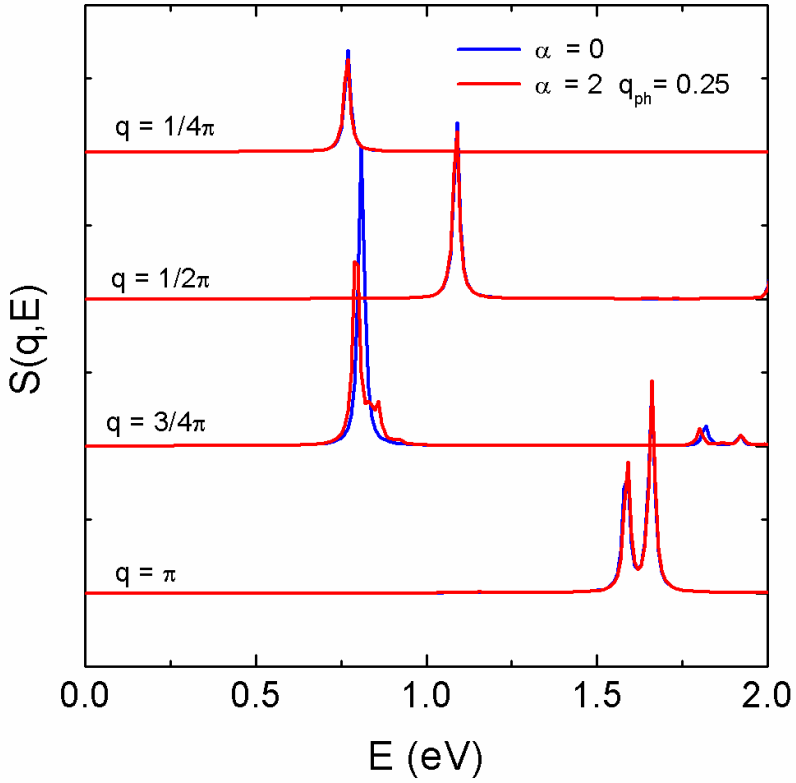
$$S(q) = \langle \psi_0 | S_q S_{-q} | \psi_0 \rangle = \frac{1}{N} \sum_{ij} e^{iqr_{ij}} \langle \psi_0 | s_i^z s_j^z | \psi_0 \rangle$$

$$S(q,\omega) = \sum_n |\langle \psi_0 | S_q | \psi_n \rangle|^2 \delta(\omega - E_n + E_0)$$


E (eV)
q (2π)
x = 0
N = 8
N = 12
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.00
0.25
0.50
0.75
1.00


E (eV)
q (2π)
x = 1/6
x = 1/4
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0.00
0.25
0.50
0.75
1.00


α = 0
α = 2 q_ph = 0.5
q = 1/4π
q = 1/2π
q = 3/4π
q = π
S(q,E)
0.0
0.5
1.0
1.5
2.0
E (eV)


α = 0
α = 2 q_ph = 0.25
q = 1/4π
q = 1/2π
q = 3/4π
q = π
S(q,E)
0.0
0.5
1.0
1.5
2.0
E (eV)

Optical conductivity

$$J_x(q=0,\omega) = \sigma(\omega) E_x(q=0,\omega)$$

$$\sigma(\omega) = D\delta(\omega) + \frac{e^2\pi}{N} \sum_{n>0} \frac{|\langle \psi_n | j_x | \psi_0 \rangle|^2}{E_n - E_0} \delta(\omega - E_n + E_0)$$

$$j_x = -it \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} - c^\dagger_{i+1,\sigma} c_{i,\sigma})$$

$$D = \frac{e^2\pi}{2N} \langle T \rangle - \frac{2e^2\pi}{N} \sum_{n>0} \frac{|\langle \psi_n | j_x | \psi_0 \rangle|^2}{E_n - E_0}$$

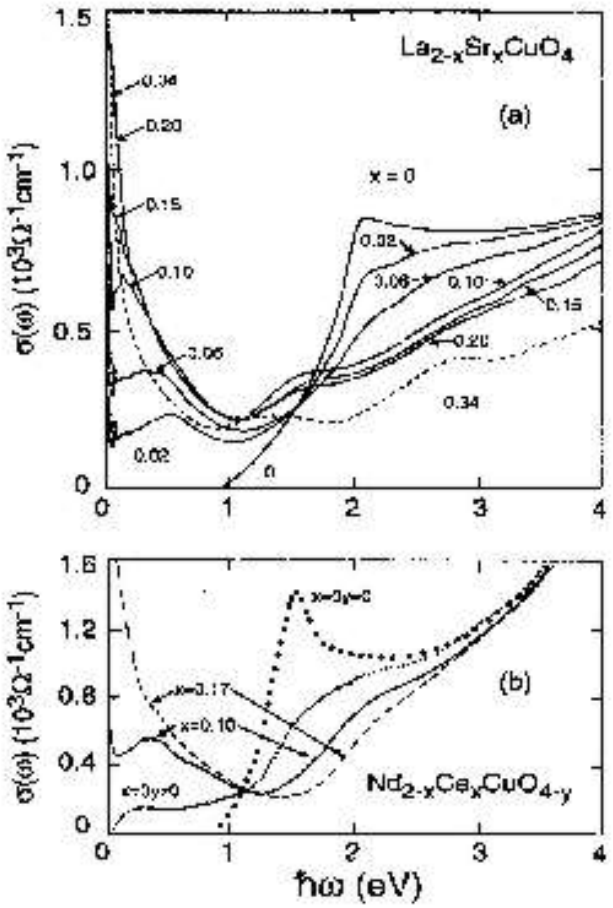
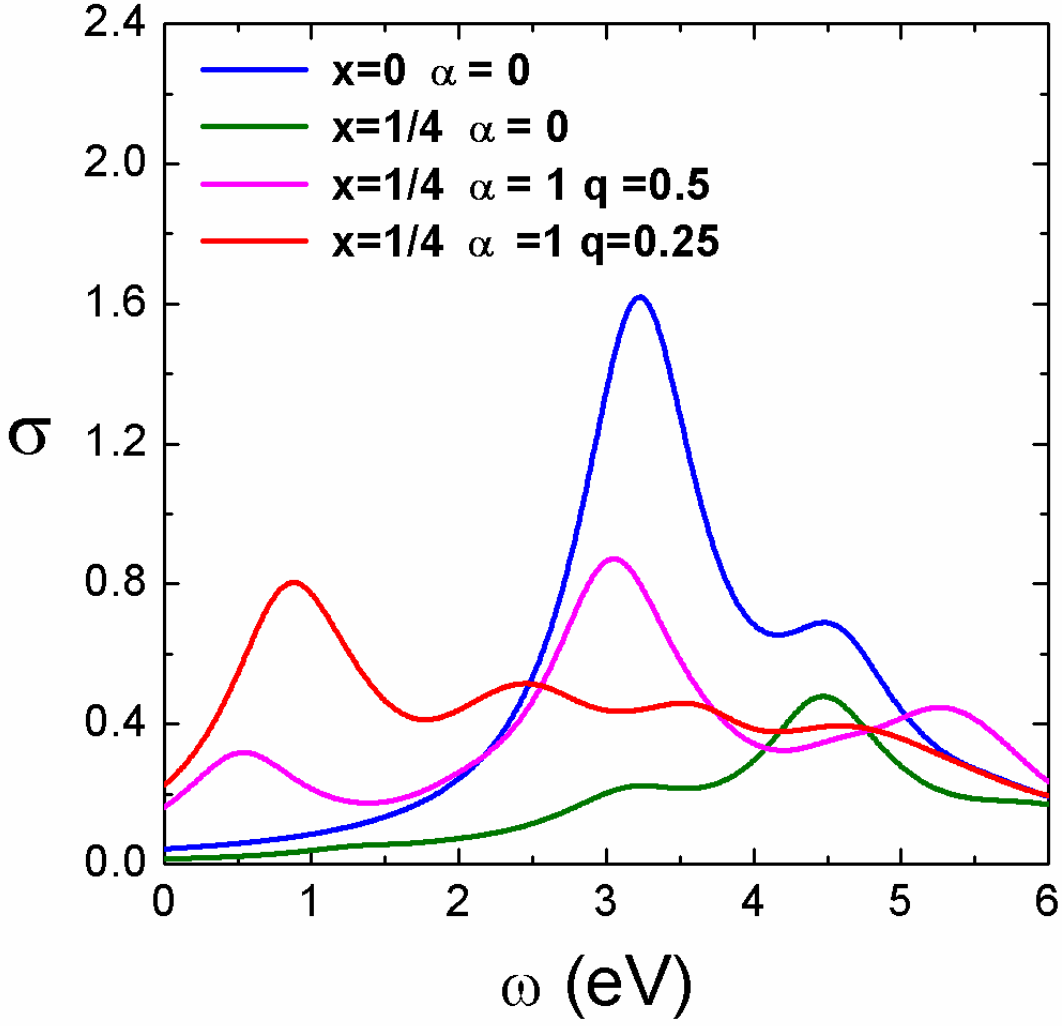


FIG. 37. (a) Optical conductivity of $La_{2-x}Sr_xCuO_4$ at 300 K vs energy. Data are shown parametric with the Sr concentration x, in the interval $0 \le x \le 0.34$ (from Uchida *et al.*, 1991). (b) Optical conductivity of $Nd_{2-x}Ce_xCuO_{4-y}$ (at room temperature) vs energy, parametric with Ce concentrations between 0.0 and 0.20 (from Uchida *et al.*, 1991).


x=0 α = 0
x=1/4 α = 0
x=1/4 α = 1 q =0.5
x=1/4 α =1 q=0.25
σ
ω (eV)
0.0
0.4
0.8
1.2
1.6
2.0
2.4
0
1
2
3
4
5
6

Conclusions

1. The exact diagonalization Lanczos method is a powerful technique for studying strongly correlated electron-phonon systems.

2. Calculations show that the ionic, Holstein-type, electron-phonon interaction may at least partly explain q-dependence of phonon softening in the cuprates.

3. Optical bond-stretching phonon induces a dynamic charge transfer between ions - vibronic state.

4. Magnetic interactions and spin dynamics in the cuprates are strongly modified by the electron-phonon interaction.

5. The midinfrared band observed in doped cuprates by optical conductivity measurements can be partly explain as a result of electron-phonon coupling.