Path-integral theory for photoemission spectra of electron-phonon coupled system and anomalous isotope effect

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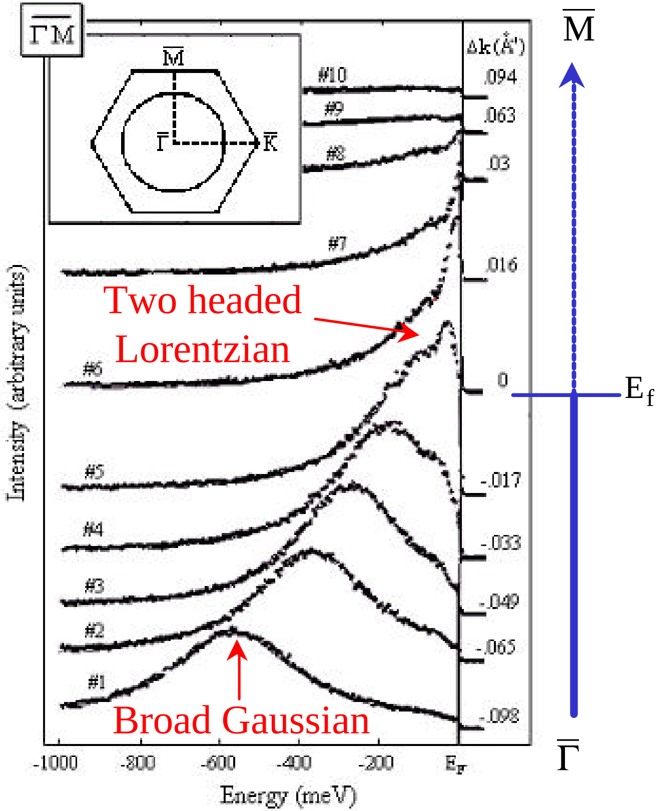
Outline

- **Path-integral theory for photoemission spectra of electron-phonon coupled system**
  - **Experimental results of ARPES on e-ph coupled systems**
  - **Path-integral theory of e-ph coupled systems**
  - **Results and discussion**

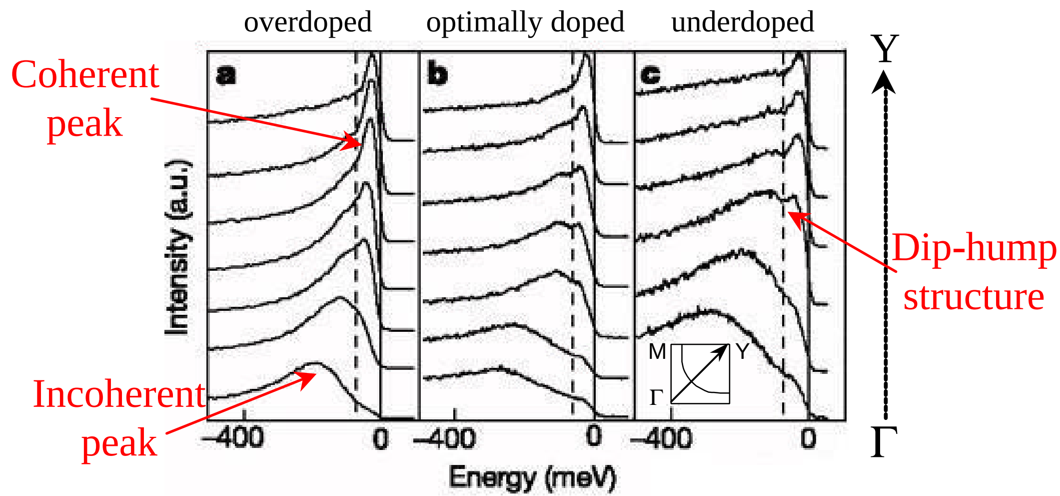
- **Theoretical study on isotope induced band shift of ARPES in Bi2212**
  - **Recent experimental discoveries of isotope effect**
  - **Theoretical explanation**

- **Summary**

Evidence of e-ph interaction from ARPES: Gaussian to Lorentzian spectral evolution



Spectral evolution from broad Gaussian to two-headed Lorentzian, observed in the ARPES of Be(0001) surface state along the ΓM symmetry line [PRL 83, 592 (1999)].



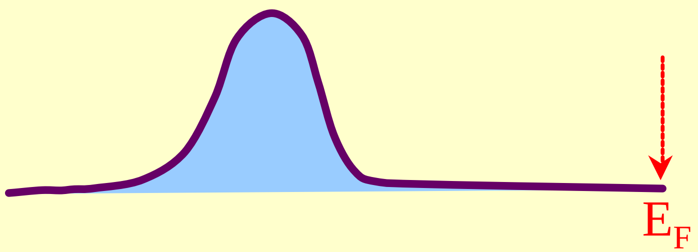
Incoherent-coherent evolution and Dip-hump structure along nodal direction (ΓY), in the ARPES of $Bi_2Sr_2CaCu_2O_8$ (Bi2212), under various doping levels [Nature 412, 510 (2001)].

Spectral evolution from Gaussian (incoherent state) at band bottom to asymmetric two-headed Lorentzian (coherent state) near E_F is universal for the e-ph coupled systems.

Difficulty encountered by conventional theories

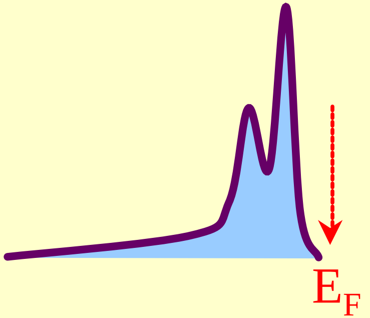
Broad Gaussian

at around band bottom

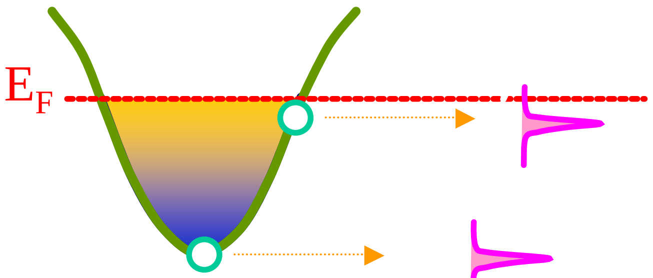


Two-headed asymmetric Lorentzian

at around Fermi surface



Experimental results



Conventional theories

Experimental results cannot be explained by the mean field or perturbation theories. They predict only a single curve.

Calculate electronic spectral function by path-integral theory

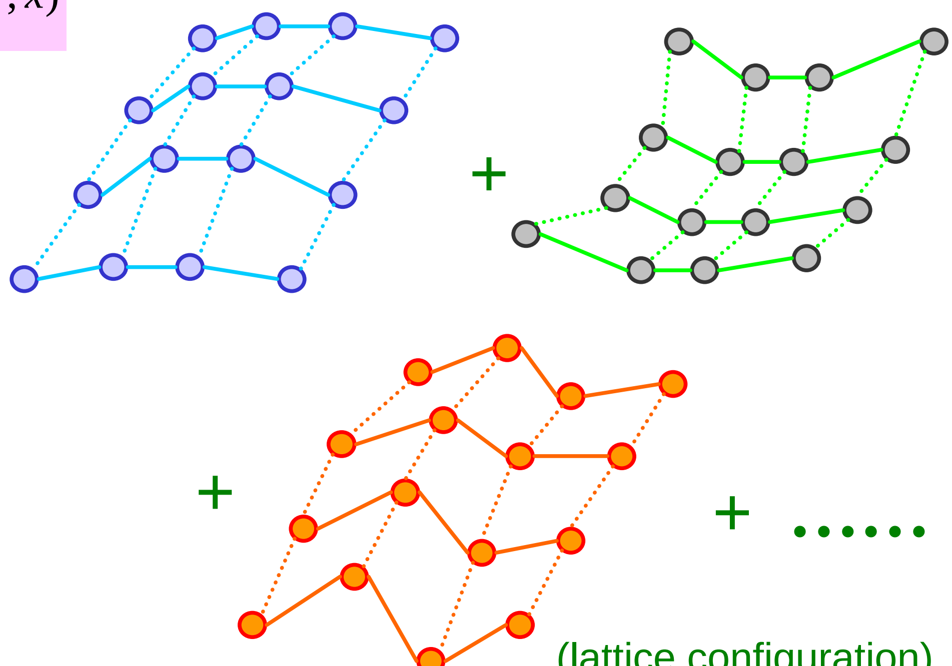
Electronic spectral function $A(w)$

$$G(t) = -\int \frac{dw}{2p} \frac{e^{-wt}}{1+e^{-bw}} A(w)$$

Electronic Green's function $G(t)$

$$G(jt, j't') = \frac{1}{Z} \int dx\, e^{-q\Phi(x)} G(jt, j't', x)$$

Path integral =



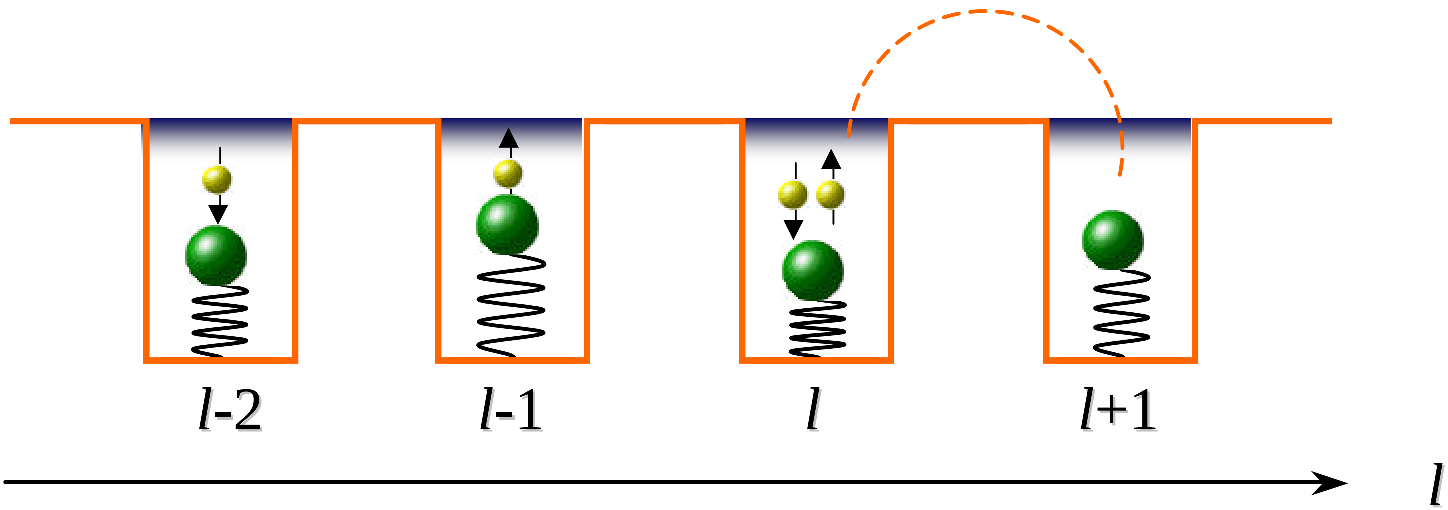
(lattice configuration)

Numerically calculated by
Quantum Monte Carlo Simulation

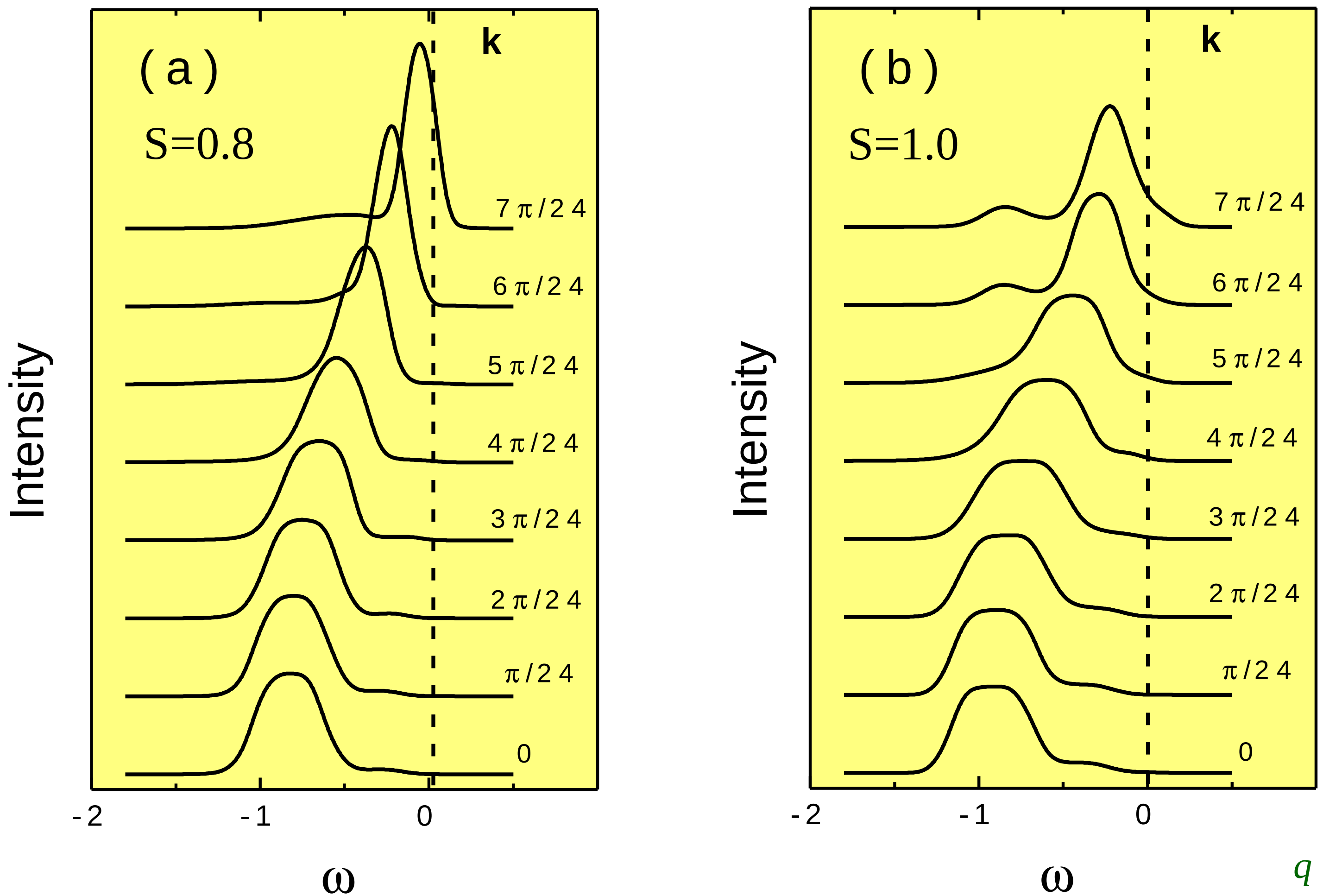
The electron-phonon coupled system (Holstein model)

$$H = -T \sum_{<l,l'>} \sum_{s} \left(a^{+}_{ls} a_{l's} + a^{+}_{l's} a_{ls} \right) - m \sum_{ls} a^{+}_{ls} a_{ls}$$

$$+ \sum_{l} \left(\frac{P_l^2}{2m} + \frac{1}{2} m w_0^2 Q_l^2 \right) - S \sum_{ls} Q_l a^{+}_{ls} a_{ls}$$



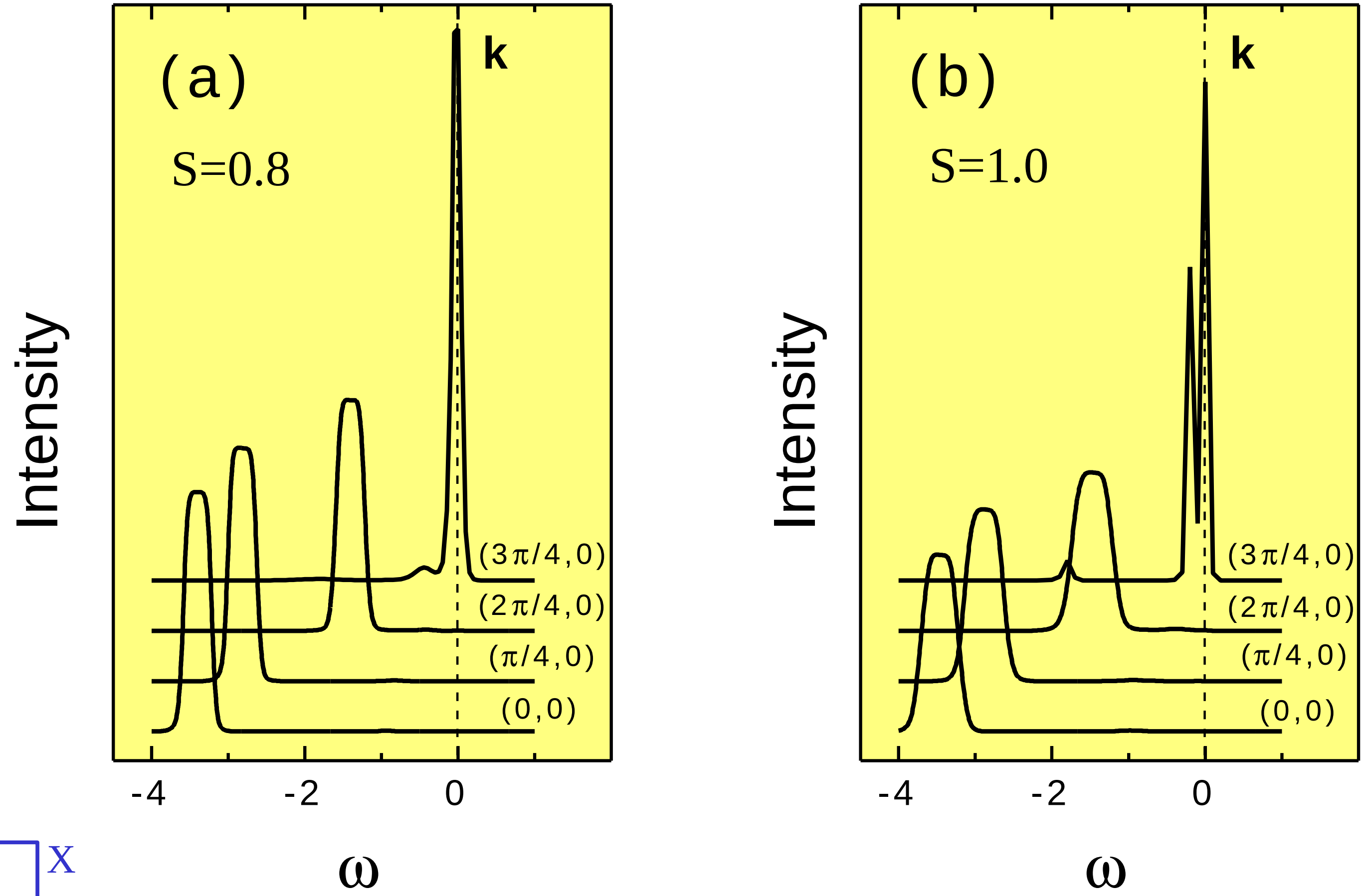
1D, dependence on coupling constant *S*

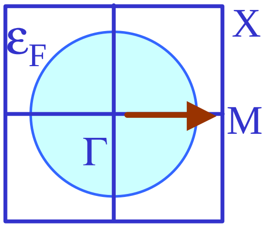


$q = 1/k_B T$

QMC results of ARPES for 1D Holstein model at 30%-filling, with S=0.8 and S=1.0. Parameters: q = 20, T = 1.0, w_0= 0.1.

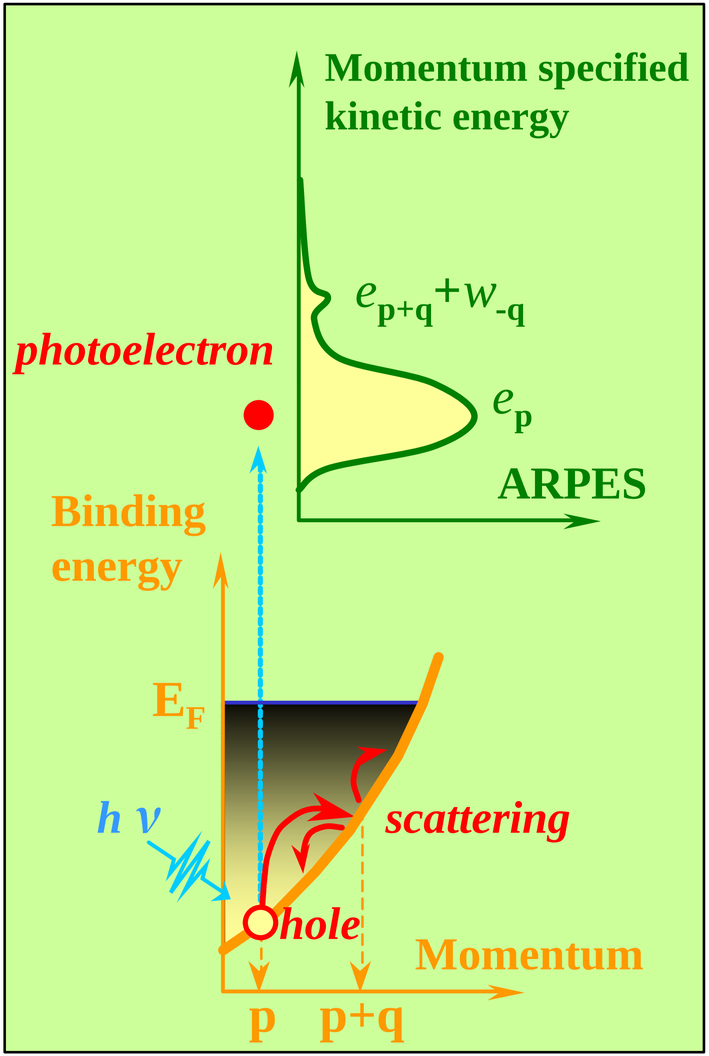
2D, dependence on coupling constant S



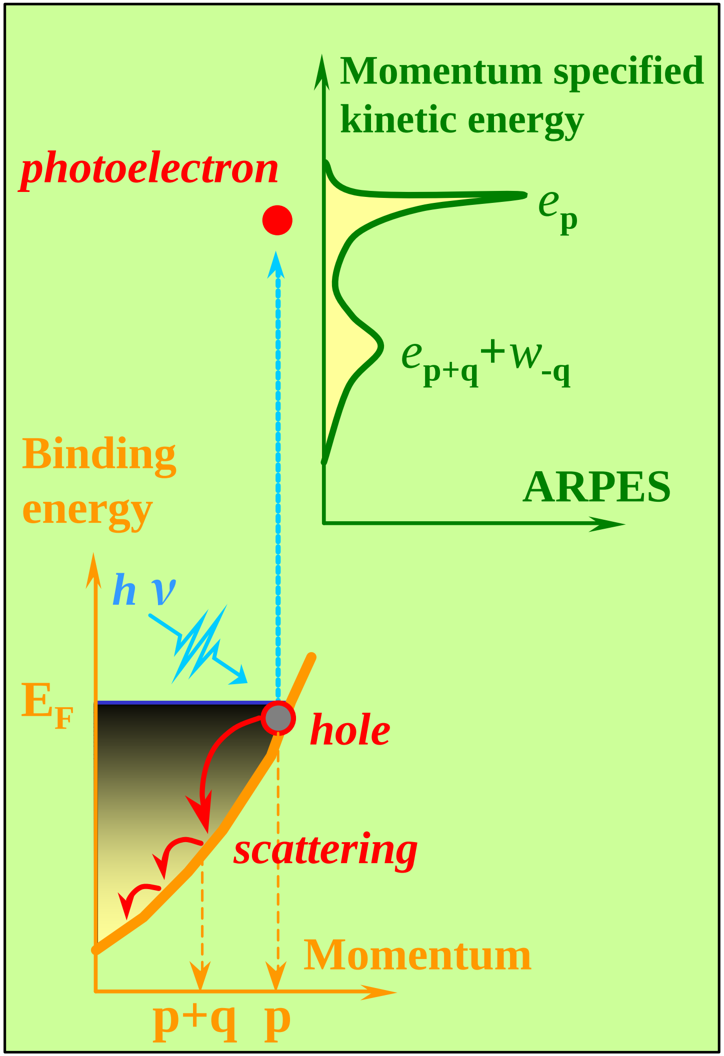


QMC results of 2D model at 36%-filling, on 8x8 square lattice. q =20, T=1.0, w_0=0.1.

Mechanism of spectral evolution: multiple e-ph scattering

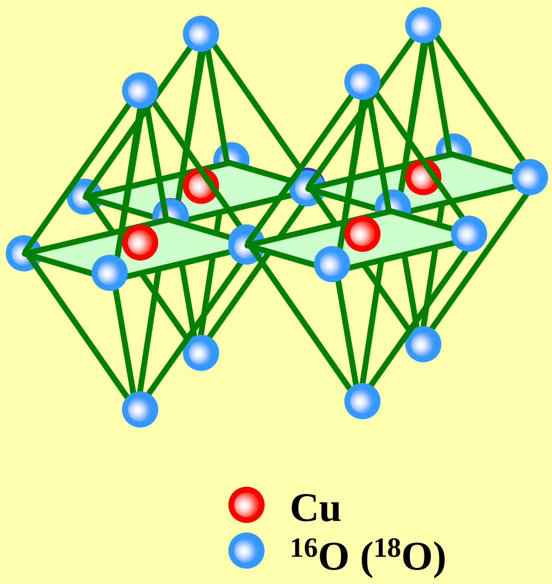


Band bottom

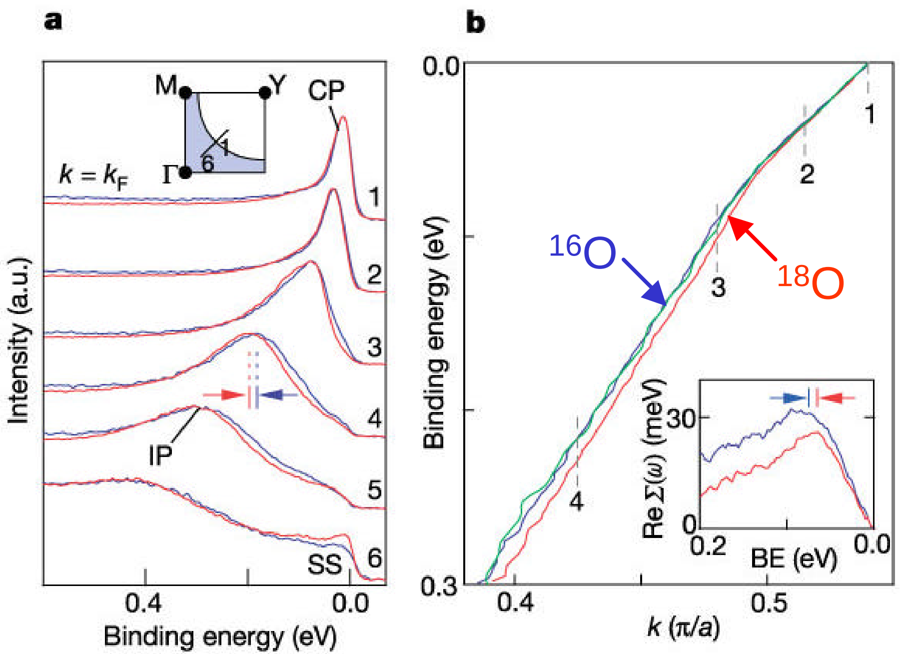


Fermi surface

Isotope effect in $Bi_2Sr_2CaCu_2O_8$ (Bi2212)



Conduction plane in cuprate superconductors



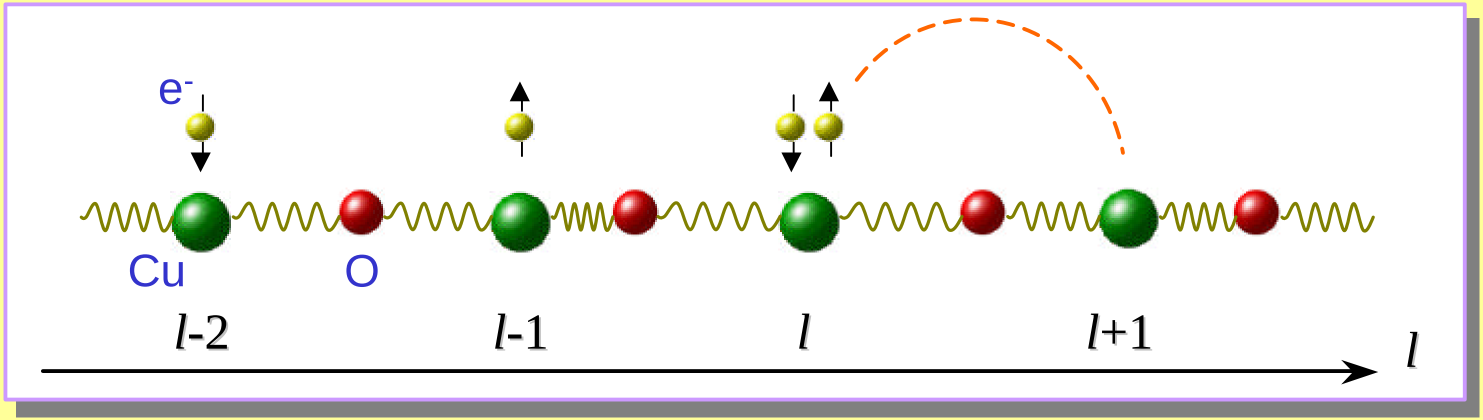
Isotope effect in the ARPES of Bi2212
G. -H. Gweon, *et al.*, Nature 430, 398 (2004).

Electron-phonon coupled model

Hamiltonian:

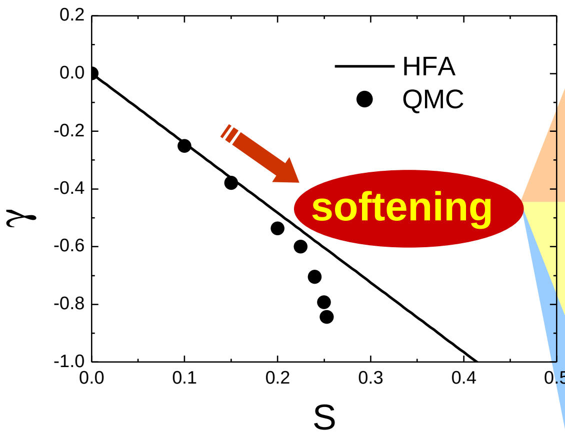
$$H = -T \sum_{<l,l'>} \sum_{s} \left(a_{ls}^{+} a_{l's} + a_{l's}^{+} a_{ls} \right) - m \sum_{ls} a_{ls}^{+} a_{ls}$$

$$+ \sum_{l} \left(\frac{P_l^2}{2m} + \frac{1}{2} m w_0^2 Q_l^2 \right) + S \sum_{ls} Q_l^2 a_{ls}^{+} a_{ls}$$

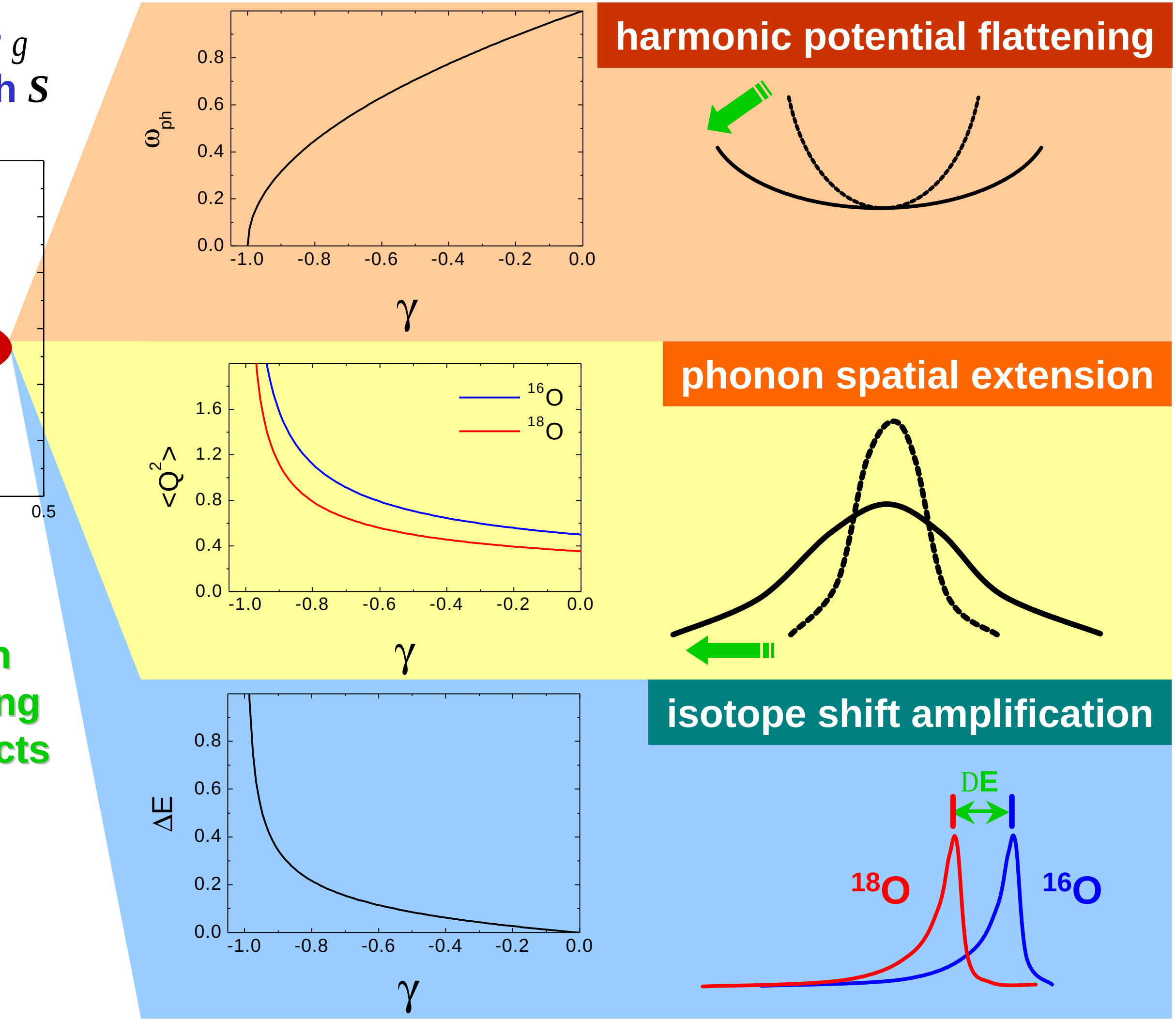


Phonon softening effect due to e-ph coupling

Phonon softening factor *g*
vs. e-ph coupling strength *S*



Strong e-ph interaction induces phonon softening and large band shift effects



Summary

✧ **We develop a path-integral theory to calculate the photoemission spectra of e-ph coupled system.**

✧ **Our calculation shows that the spectral shape is greatly modified by the e-ph scattering effect. Near the band bottom, the main peak takes a broad Gaussian form. While near the Fermi level, it is characterized by a two-headed asymmetric Lorentzian form.**

✧ **We also study the isotope induced band shift in the ARPES of Bi2212. We find this effect can be clarified by the quadratically coupled e-ph coupled. We show that the large band shift is connected with the phonon softening effect.**