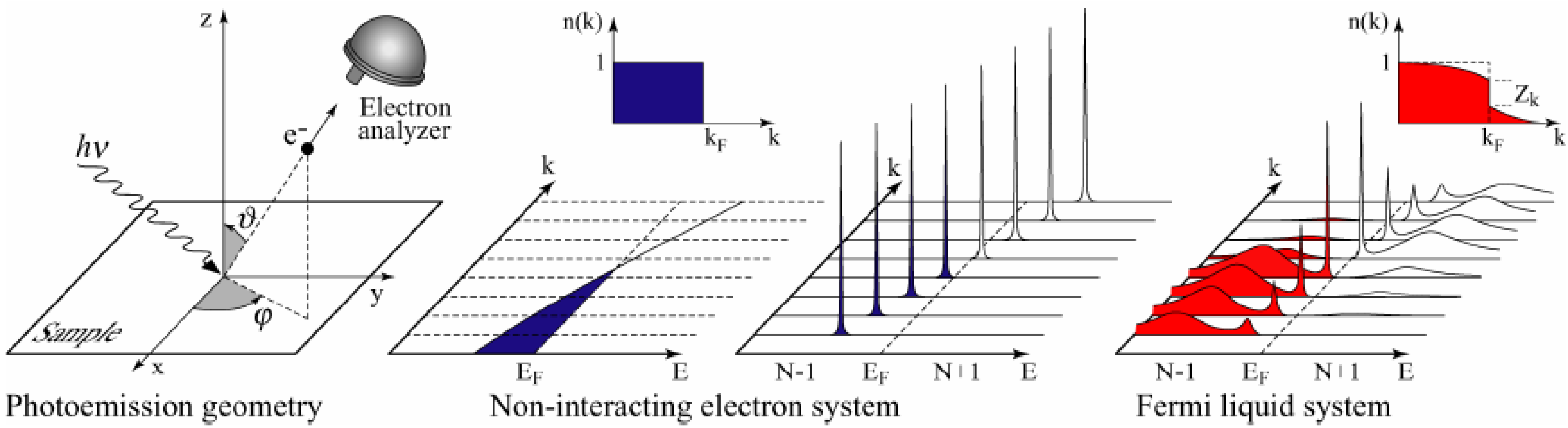
The one-particle spectral function

A. Damascelli, Z. Hussain, Z.-X Shen, Rev. Mod. Phys. **75**, 473 (2003)



Photoemission intensity: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\ A(k,\omega)$

Single-particle spectral function

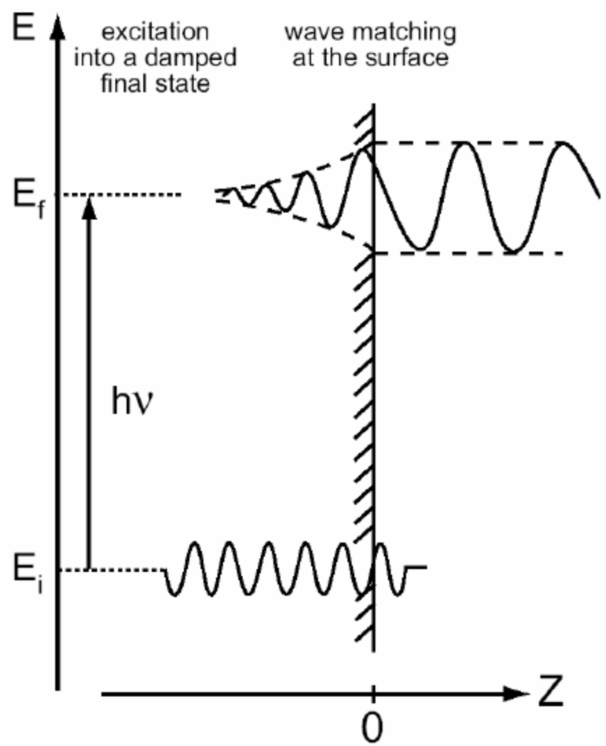
$$A(\mathbf{k},\omega)=-\frac{1}{\pi}\frac{\Sigma''(\mathbf{k},\omega)}{[\omega-\epsilon_{\mathbf{k}}-\Sigma'(\mathbf{k},\omega)]^2+[\Sigma''(\mathbf{k},\omega)]^2}$$

$\Sigma(k,\omega)$: the "self-energy" captures the effects of interactions

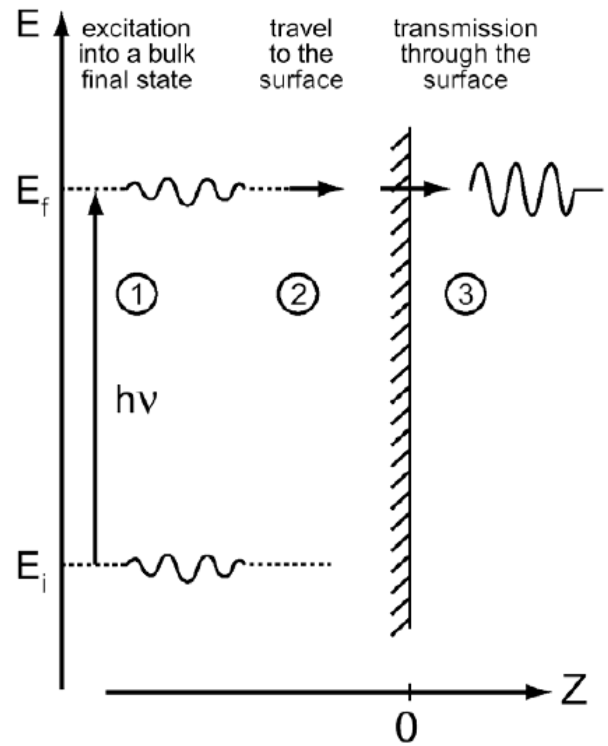
光电子谱信号

Photoemission Intensity $I(k,\omega)$ $\Big\}$ $w_{fi} \propto |\langle \Psi_f^N | \mathbf{A}\cdot\mathbf{p} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu)$

One-step model



Three-step model



光电子谱信号

$$\left.\begin{array}{l}\textbf{Photoemission}\\ \textbf{Intensity}\ \ I(k,\omega)\end{array}\right\}\ w_{fi} \propto |\langle \Psi_f^N | \mathbf{A}\cdot\mathbf{p} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu)$$

$$\left.\begin{array}{l}\textbf{Photoemission}\\ \textbf{Intensity}\ \ I(k,\omega)\end{array}\right\}\ w_{fi} \propto |\langle \phi_f^{\mathbf{k}} | \mathbf{A}\cdot\mathbf{p} | \phi_i^{\mathbf{k}} \rangle \langle \Psi_m^{N-1} | \Psi_i^{N-1} \rangle|^2 \delta(\omega - h\nu)$$

Ψ_f^N: **Sudden approximation** $\rightarrow$ $\Psi_f^N = \mathcal{A}\, \phi_f^{\mathbf{k}}\, \Psi_f^{N-1}$

Ψ_i^N: **One Slater determinant** $\rightarrow$ $\Psi_i^N = \mathcal{A}\, \phi_i^{\mathbf{k}}\, \Psi_i^{N-1}$

光电子谱信号

$$\left.\begin{array}{l}\textbf{Photoemission}\\ \textbf{Intensity } I(k,\omega)\end{array}\right\} \quad w_{fi} \propto |\langle\phi_f^{\mathbf{k}}|\mathbf{A}\cdot\mathbf{p}|\phi_i^{\mathbf{k}}\rangle\langle\Psi_m^{N-1}|\Psi_i^{N-1}\rangle|^2\delta(\omega-h\nu)$$

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Ψ_i^N: **One Slater determinant** $\rightarrow$ $\Psi_i^N=\mathcal{A}\,\phi_i^{\mathbf{k}}\,\Psi_i^{N-1}$

Photoemission intensity: $I(\mathbf{k},E_{kin})=\sum_{f,i} w_{f,i}$

$$I(\mathbf{k},E_{kin})\propto\sum_{f,i}|M_{f,i}^{\mathbf{k}}|^2\sum_m|c_{m,i}|^2\delta(E_{kin}+E_m^{N-1}-E_i^N-h\nu)$$

$$|M_{f,i}^{\mathbf{k}}|^2\equiv|\langle\phi_f^{\mathbf{k}}|\mathbf{A}\cdot\mathbf{p}|\phi_i^{\mathbf{k}}\rangle|^2 \qquad |c_{m,i}|^2=|\langle\Psi_m^{N-1}|\Psi_i^{N-1}\rangle|^2$$

In general $\Psi_i^{N-1}=c_{\mathbf{k}}\Psi_i^N$ **NOT orthogonal** Ψ_m^{N-1}

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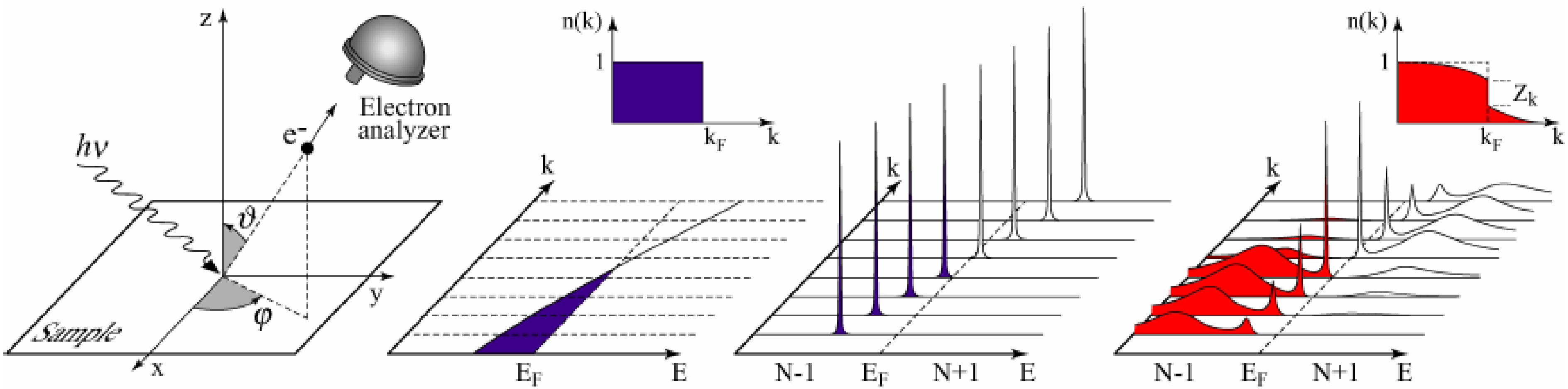

Photoemission geometry — Non-interacting electron system — Fermi liquid system

Photoemission intensity: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\,A(k,\omega)$

Non-interacting

$$A(\mathbf{k},\omega)=\delta(\omega-\epsilon_k)$$

No Renormalization

Infinite lifetime

Fermi Liquid

$$A(\mathbf{k},\omega)=Z_{\mathbf{k}}\frac{\Gamma_{\mathbf{k}}/\pi}{(\omega-\varepsilon_{\mathbf{k}})^2+\Gamma_{\mathbf{k}}^2}+A_{inc}$$

$$m^*>m \qquad |\varepsilon_{\mathbf{k}}|<|\epsilon_{\mathbf{k}}|$$

$$\tau_{\mathbf{k}}=1/\Gamma_{\mathbf{k}}$$

$\Sigma(k,\omega)$: the "self-energy" captures the effects of interactions

Electronic structure of quantum materials studied by angle-resolved photoemission spectroscopy

Jonathan A. Sobota

Stanford Institute for Materials and Energy Sciences,
SLAC National Accelerator Laboratory,
2575 Sand Hill Road,
Menlo Park, California 94025,
USA

Yu He

Stanford Institute for Materials and Energy Sciences,
SLAC National Accelerator Laboratory,
2575 Sand Hill Road,
Menlo Park, California 94025,
USA
Department of Physics,
University of California,
Berkeley, California 94720,
USA

Zhi-Xun Shen

Stanford Institute for Materials and Energy Sciences,
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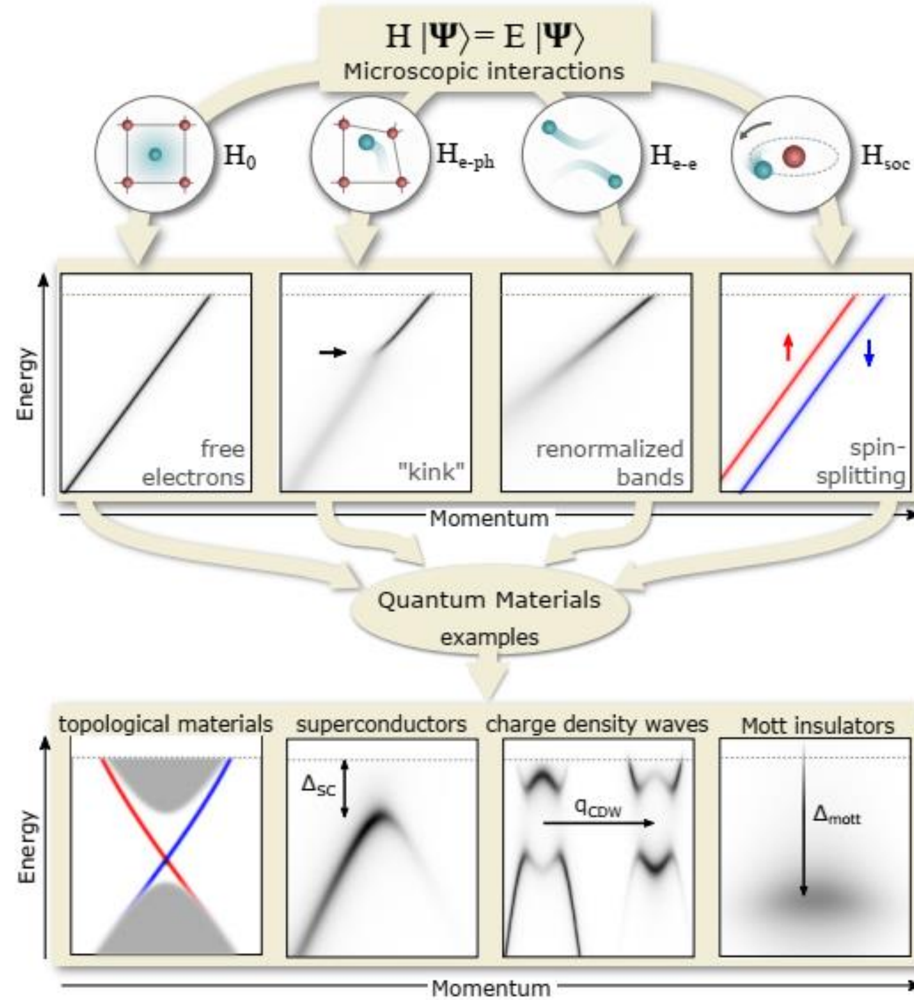
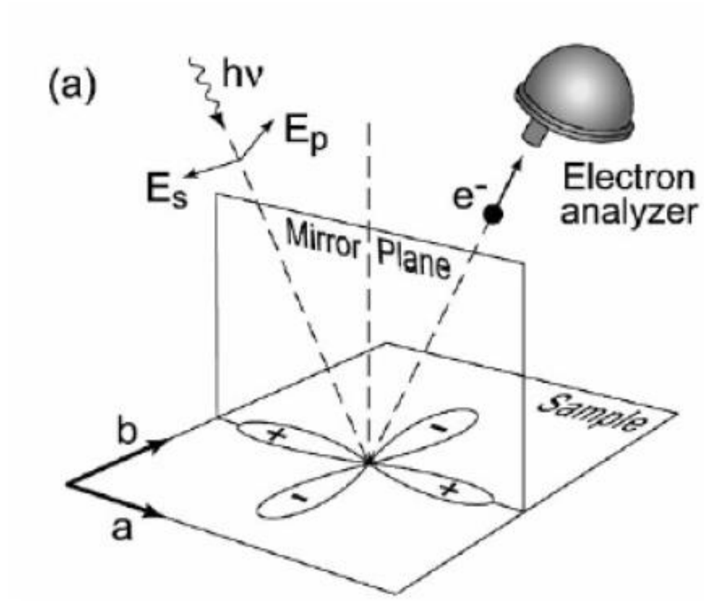
Geballe Laboratory for Advanced Materials,
Departments of Physics and Applied Physics,
Stanford University,
Stanford, California 94305,
USA

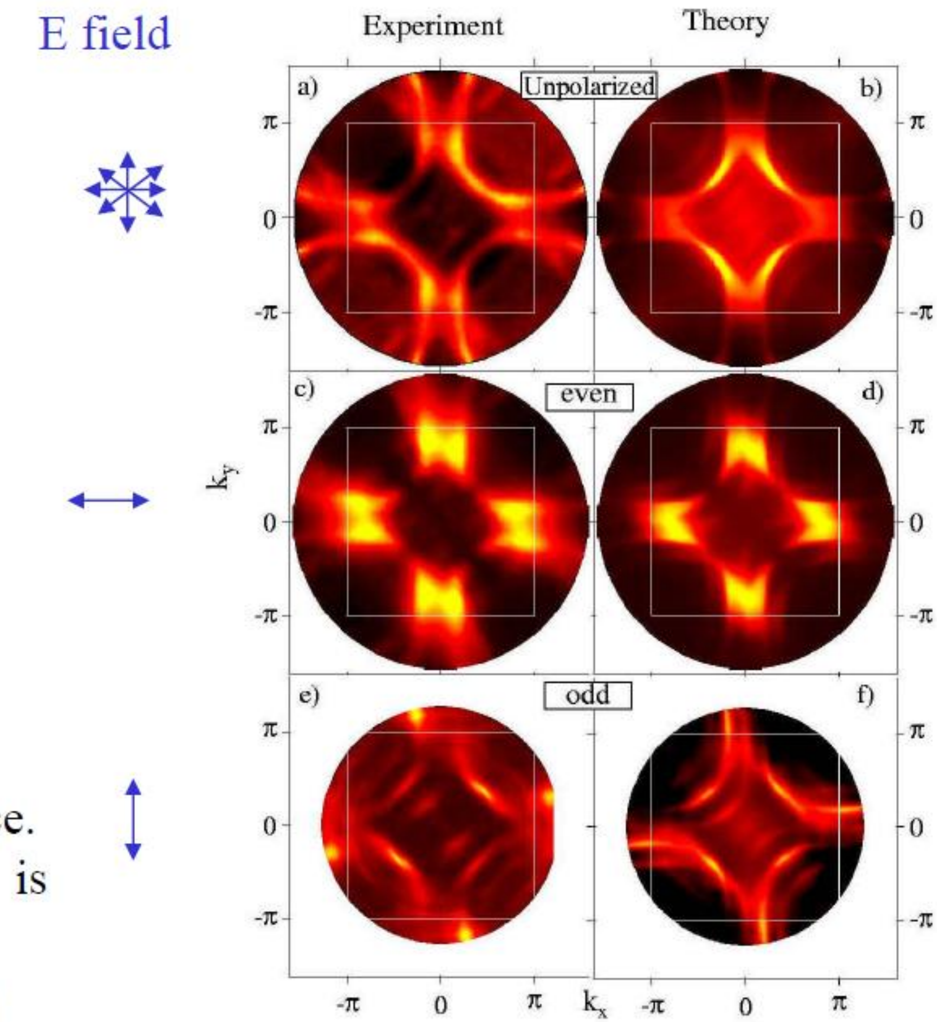


https://arxiv.org/abs/2008.02378

对称性



$$\langle \phi_f^{\mathbf{k}} | \mathbf{A}\cdot\mathbf{p} | \phi_i^{\mathbf{k}} \rangle \begin{cases} \phi_i^{\mathbf{k}} \ \text{even} \ \ \langle + | + | + \rangle \Rightarrow \mathbf{A} \ \text{even} \\ \phi_i^{\mathbf{k}} \ \text{odd} \ \ \langle + | - | - \rangle \Rightarrow \mathbf{A} \ \text{odd}. \end{cases}$$

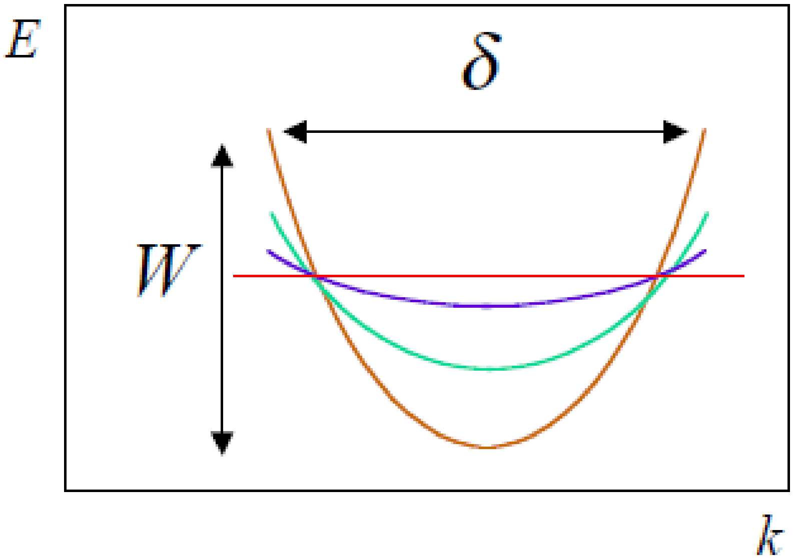


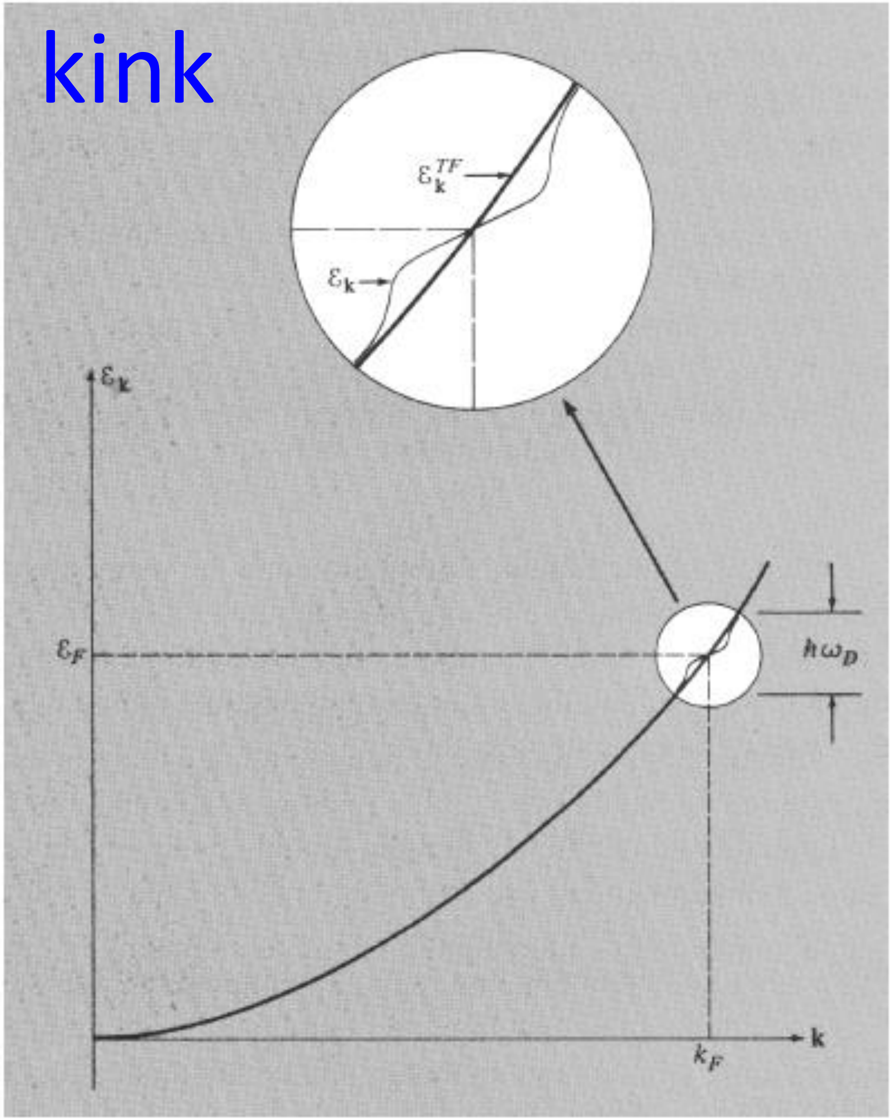
The matrix element is integrated over all space. The integration axis of interest here is perpendicular to a chosen mirror plane.
If net odd symmetry, then the matrix element integrates to exactly zero.

电子-电子/电子-声子相互作用

$$E = \frac{m^* v^2}{2} = \frac{\hbar^2 k^2}{2m^*}$$

$$\boxed{m^* = \frac{0.946\,\delta[\text{Å}^{-1}]^2}{W[\text{eV}]}}$$





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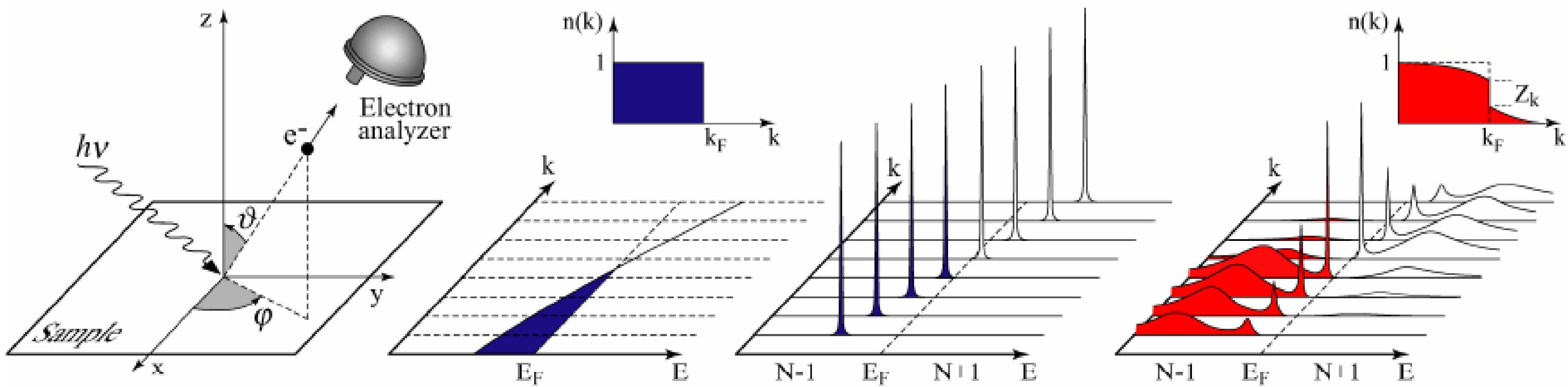

Photoemission geometry   Non-interacting electron system   Fermi liquid system

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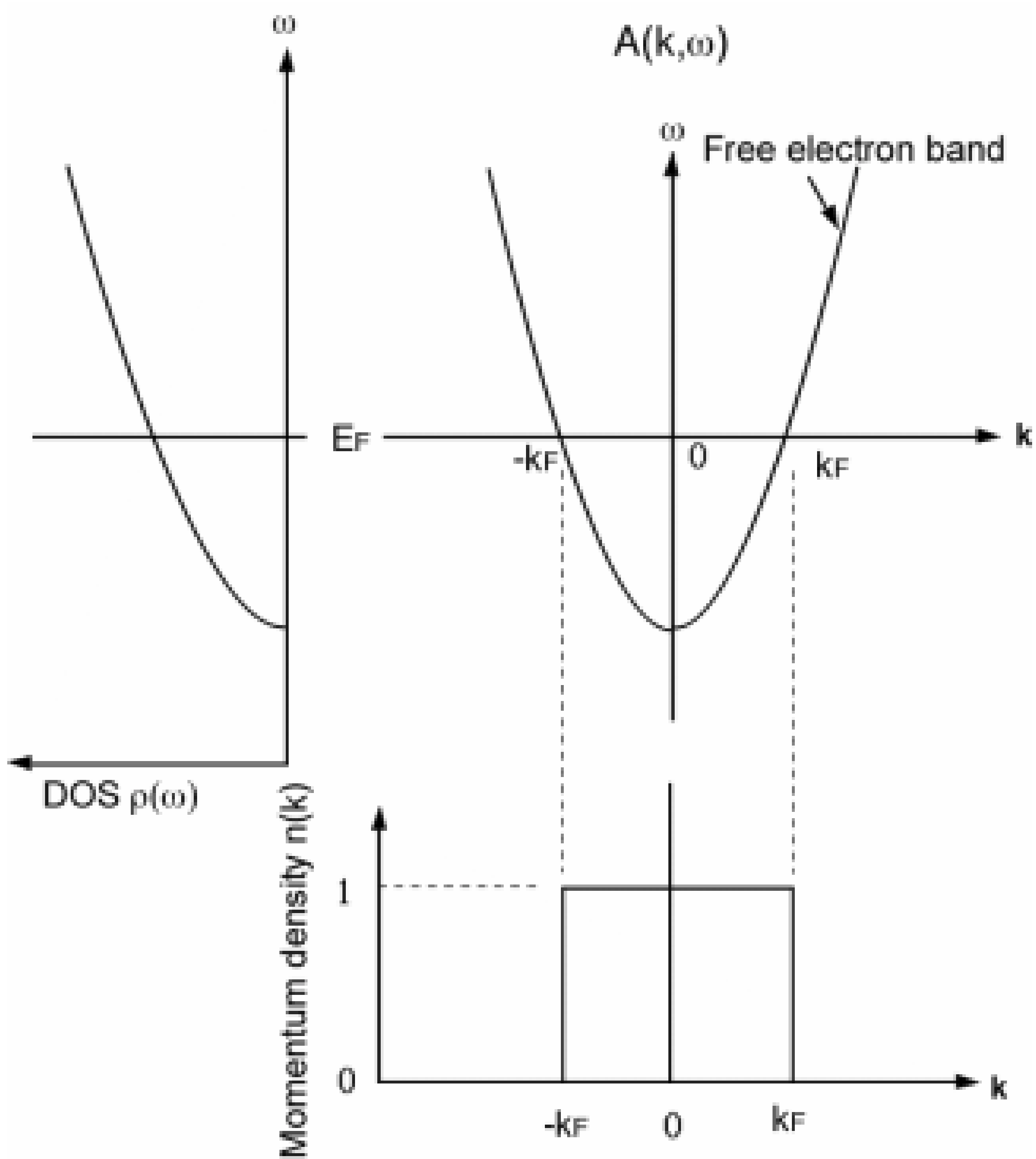
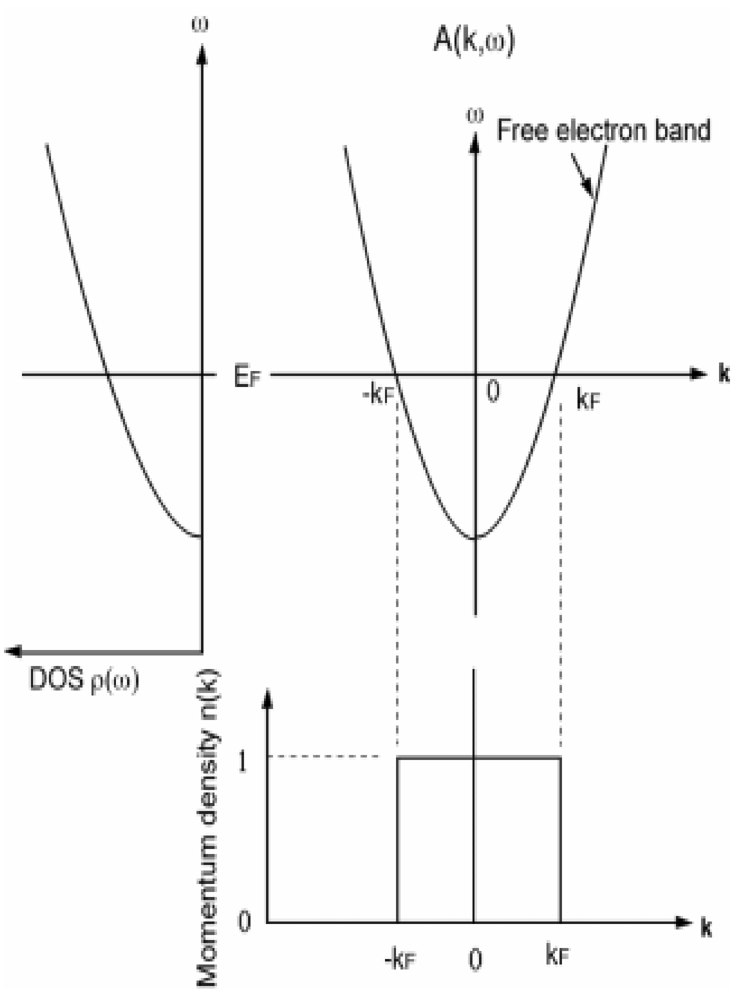
$\Sigma(k,\omega)$: the "self-energy" captures the effects of interactions

近自由电子能带色散、态密度、n(k)

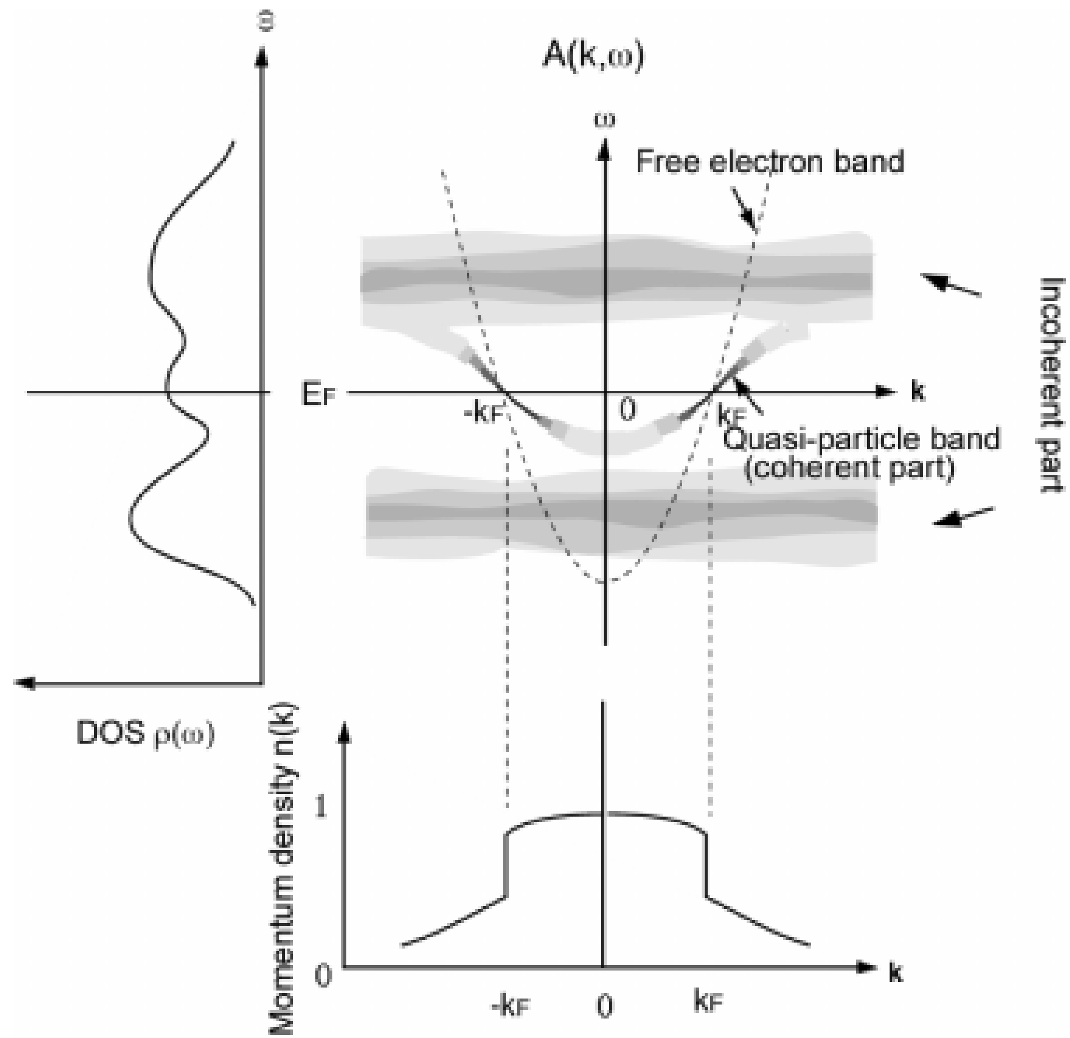


电子关联效应
单粒子谱函数、能带色散、态密度、n(k)

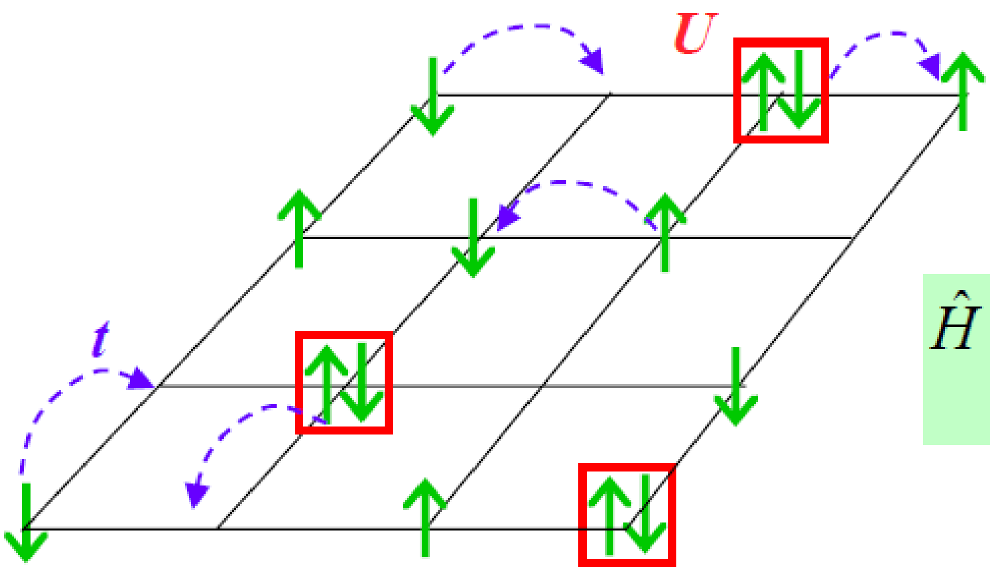
近自由电子



关联电子系统



Hubbard model



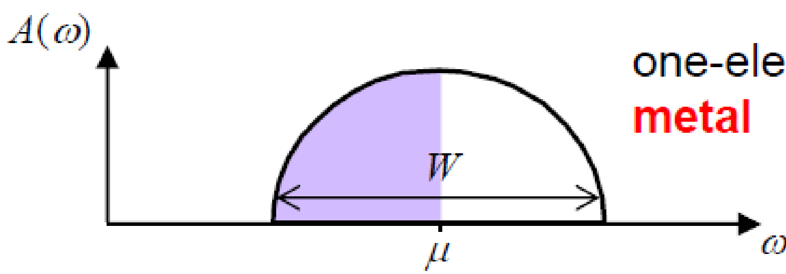
kinetic energy,
itinerancy

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\downarrow} n_{i\uparrow}$$

local Coulomb energy,
localization

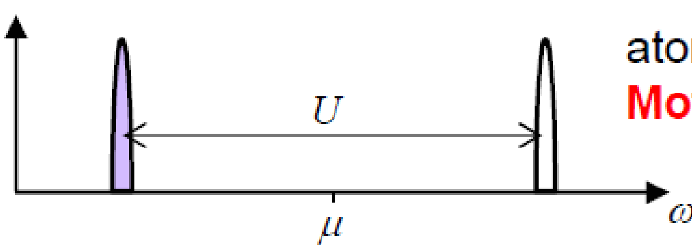
$W \sim t$

$U/W << 1$



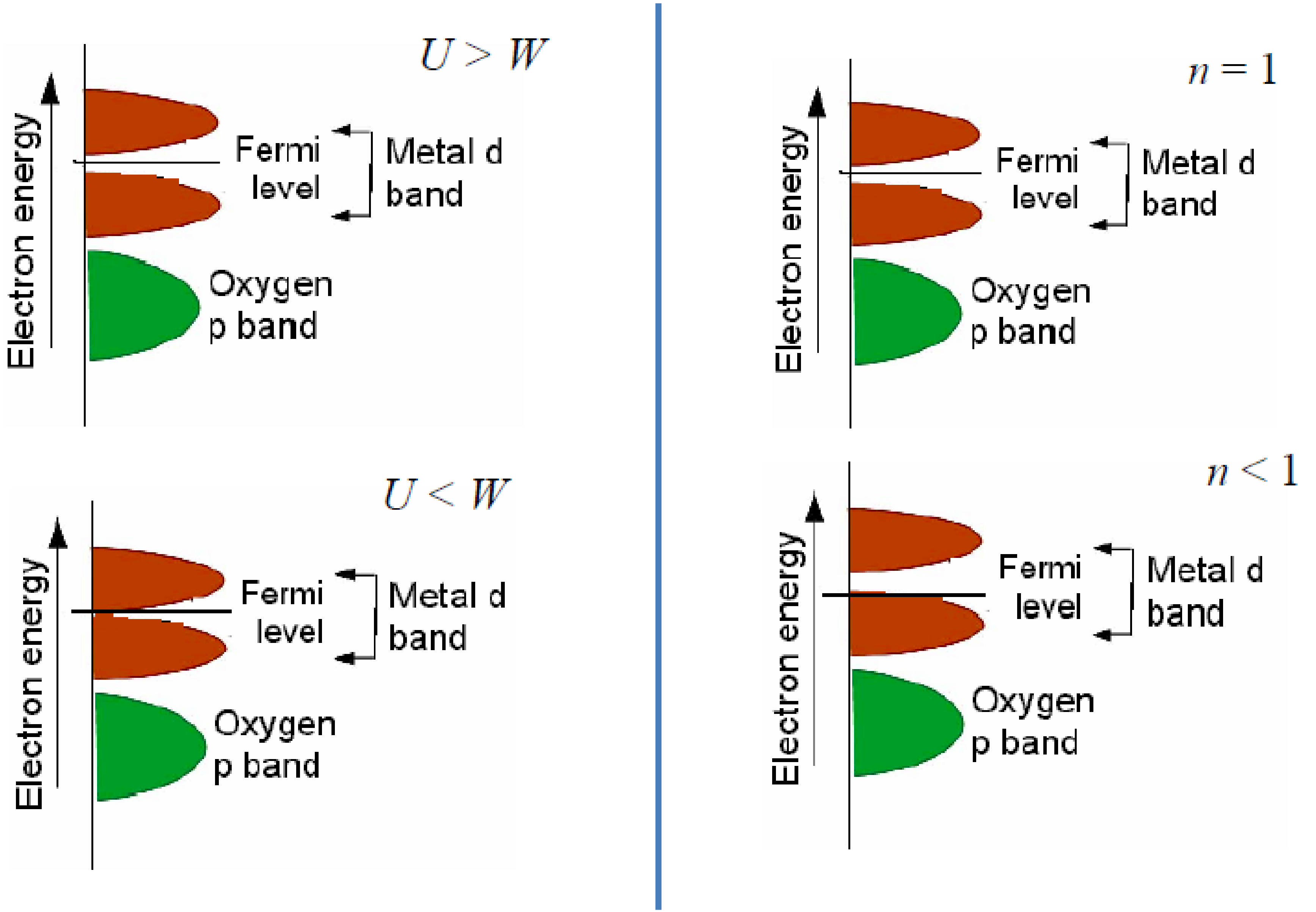
one-electron conduction band:
metal

$U/W >> 1$

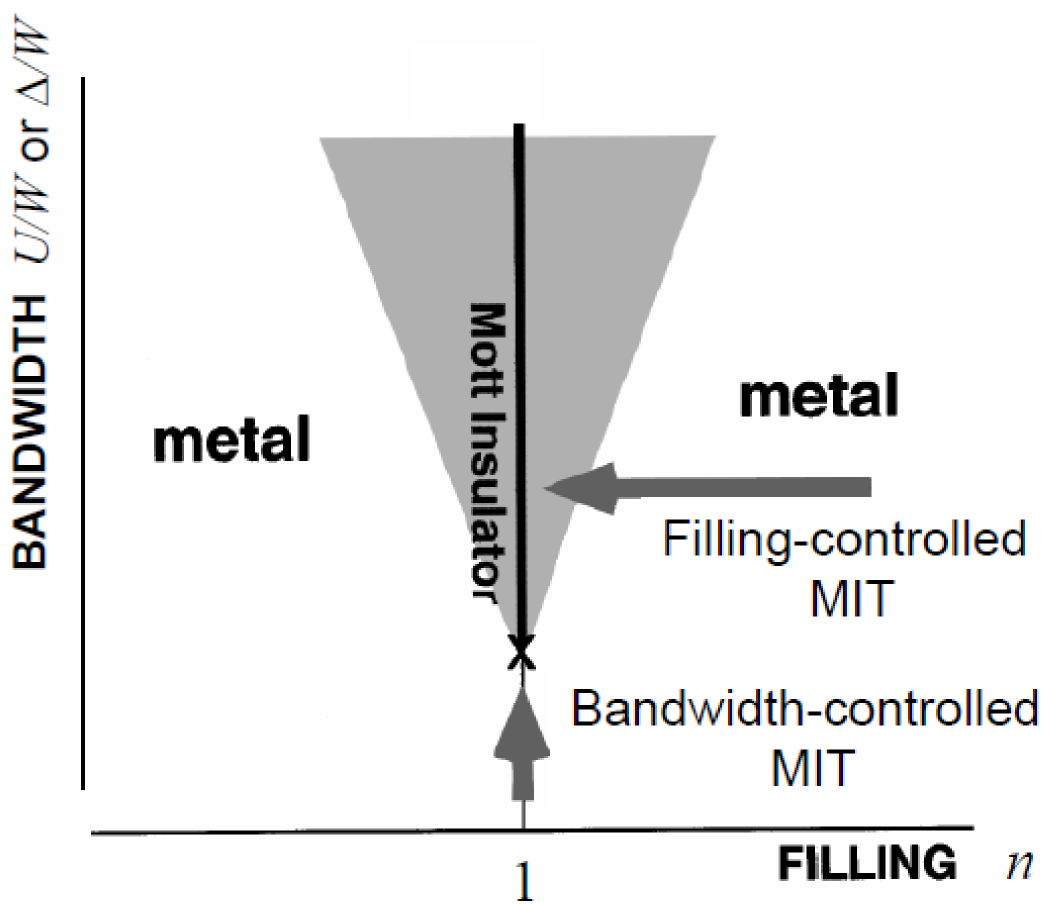


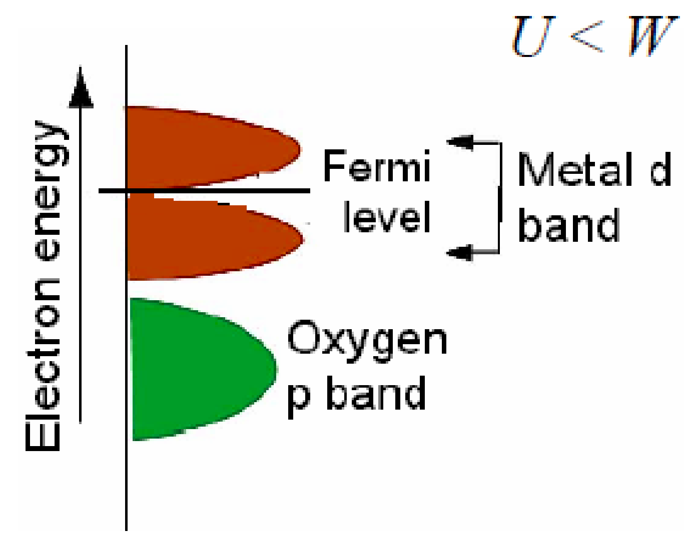
atomic limit:
Mott insulator

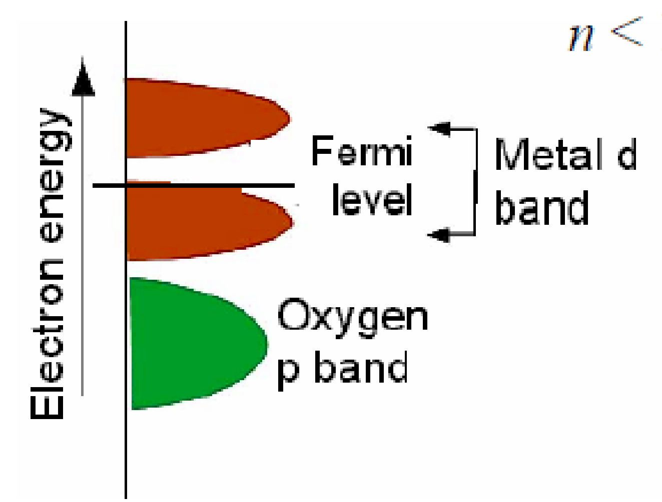
Metal-insulator transition in Hubbard model



载流子掺杂与能带带宽调节金属-绝缘体转变







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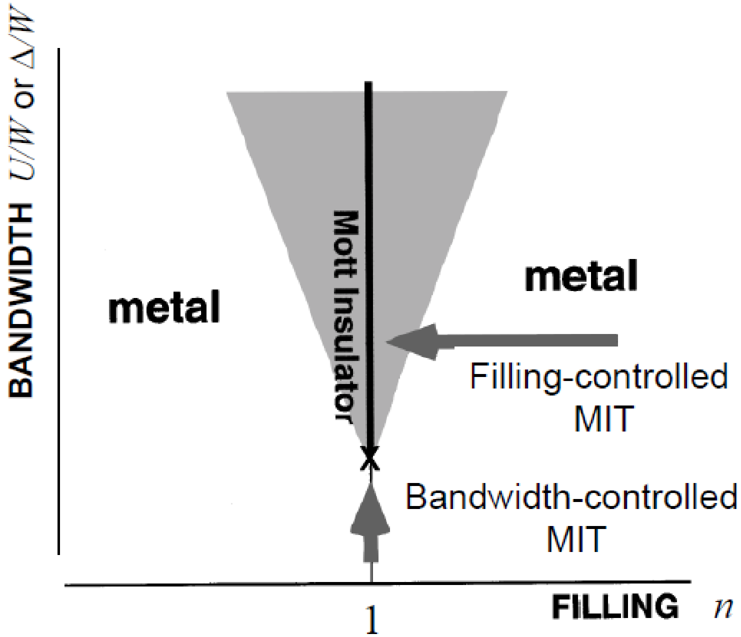
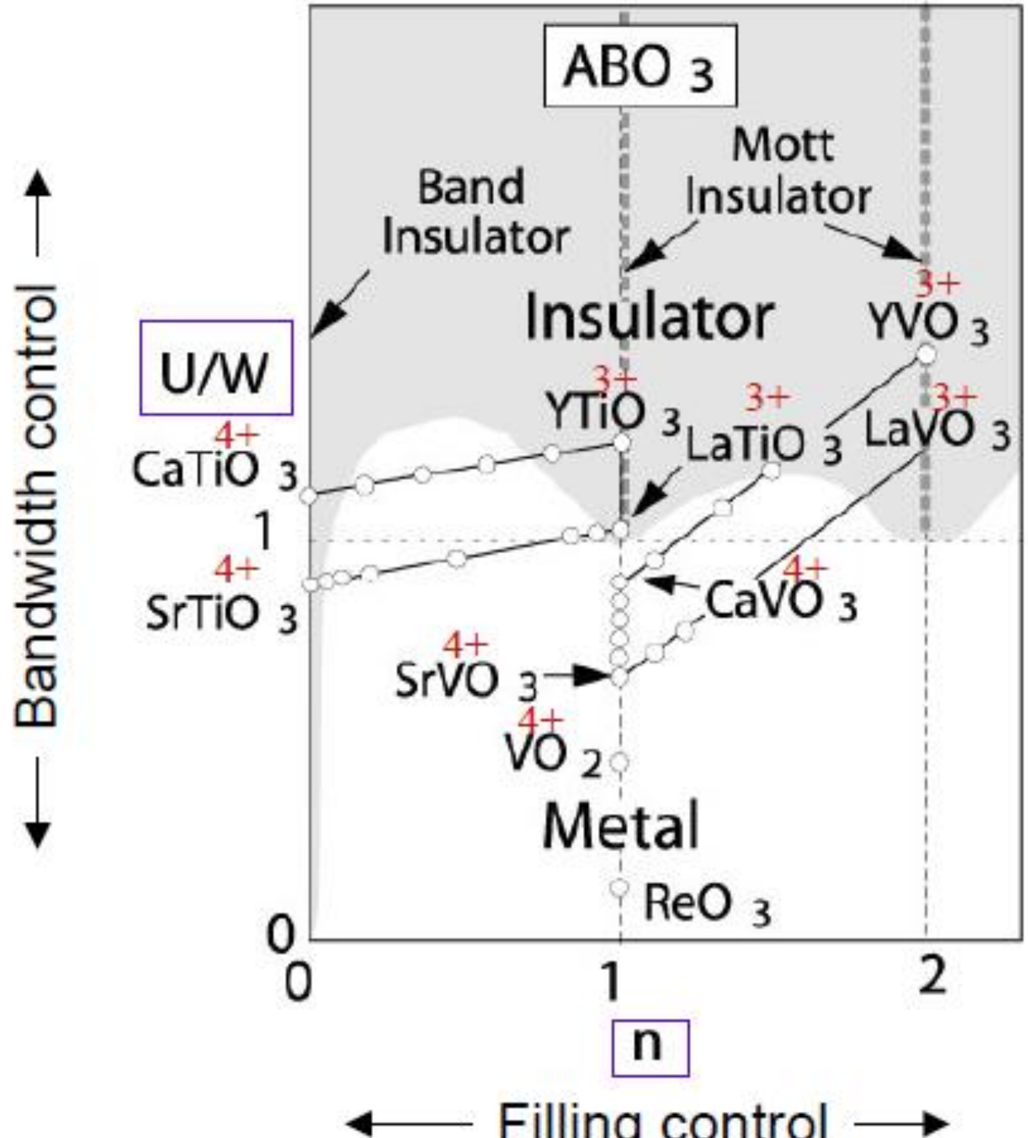
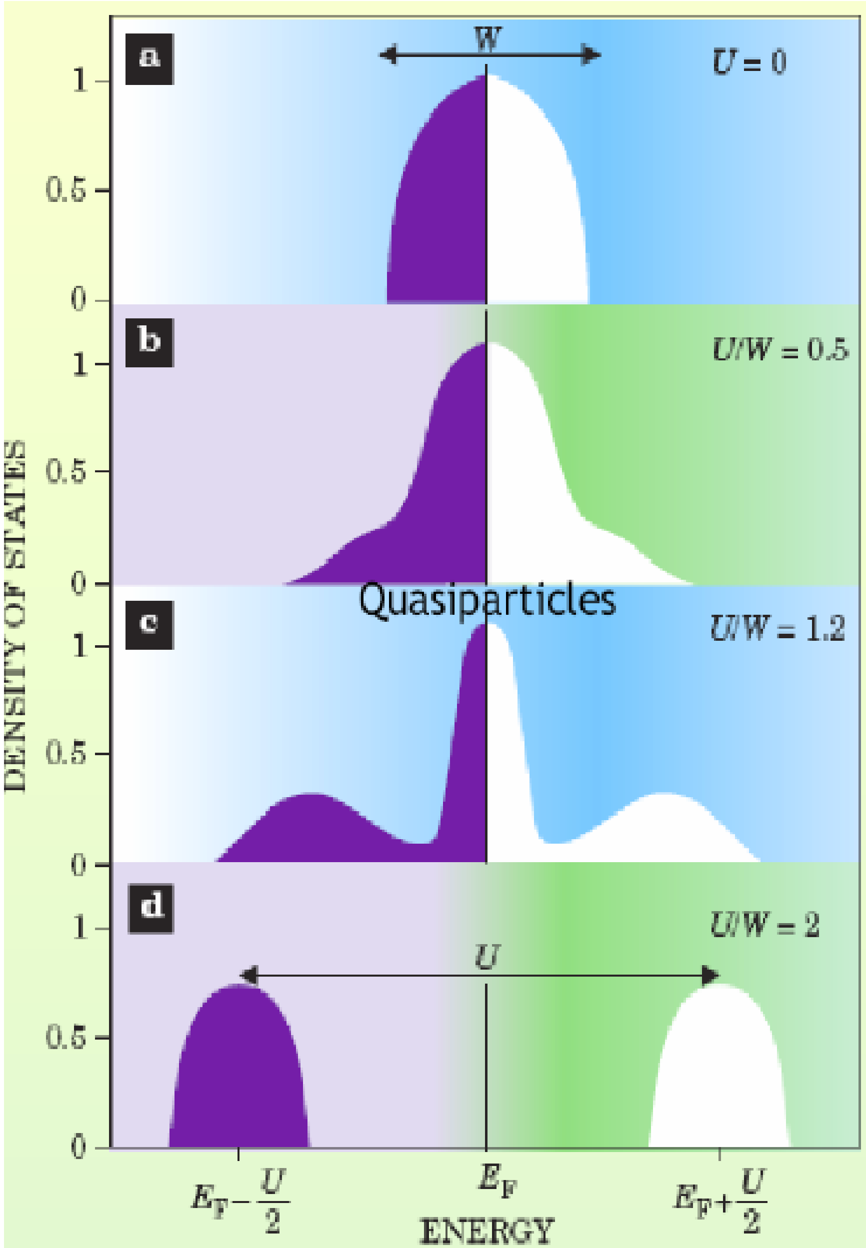
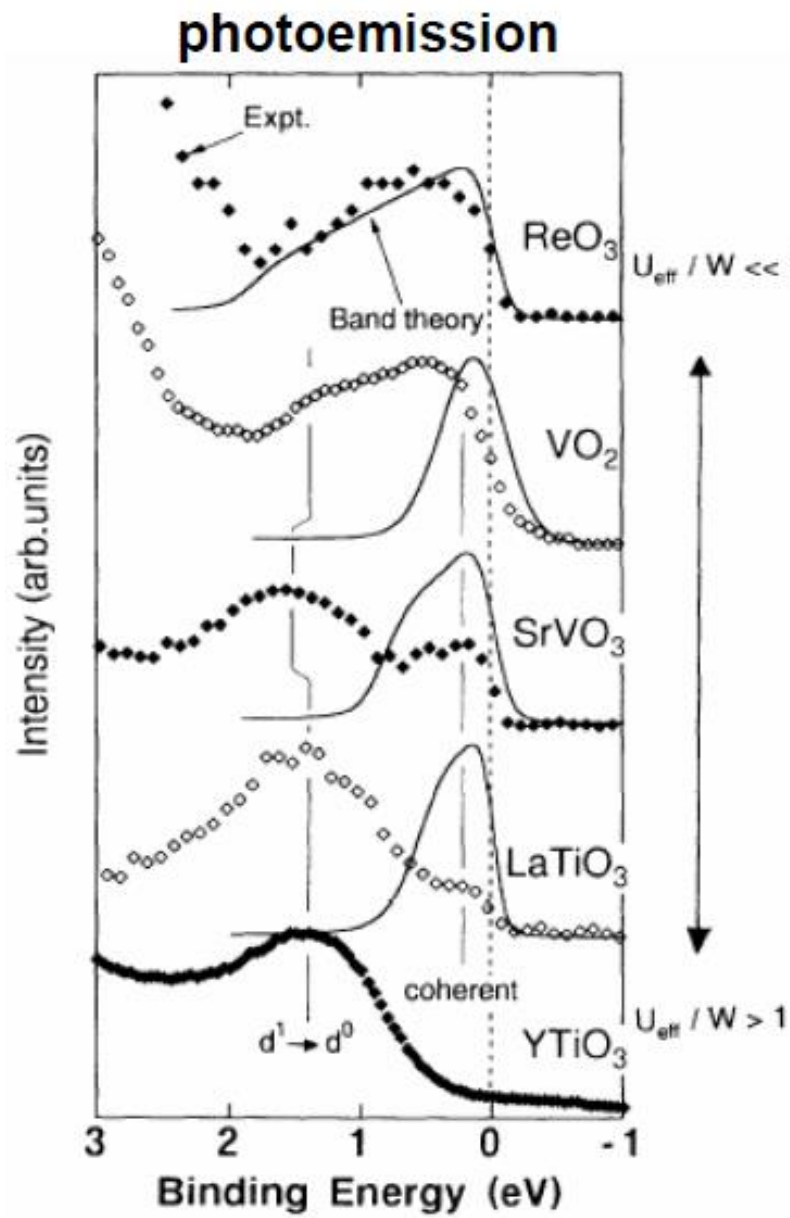


Fujimori



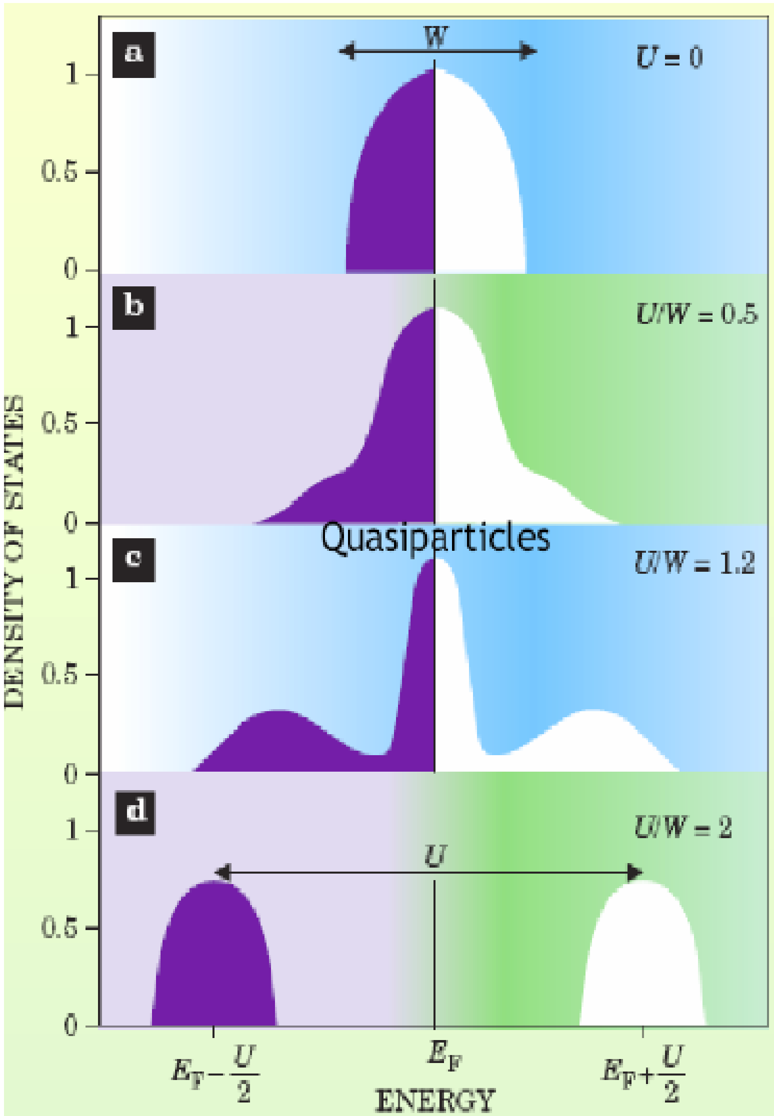
能带带宽调节金属-绝缘体转变



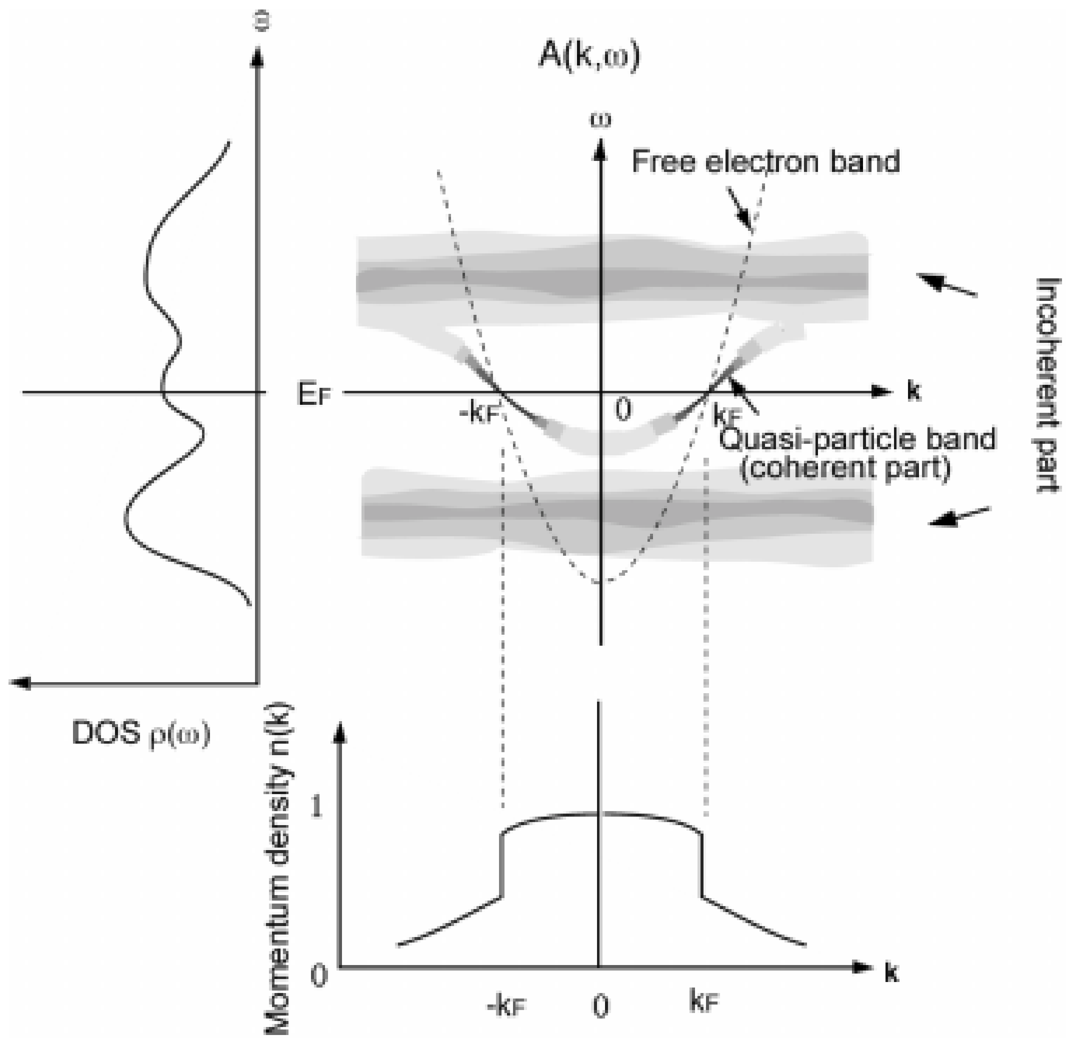


A. Fujimori et al., PRL 1992

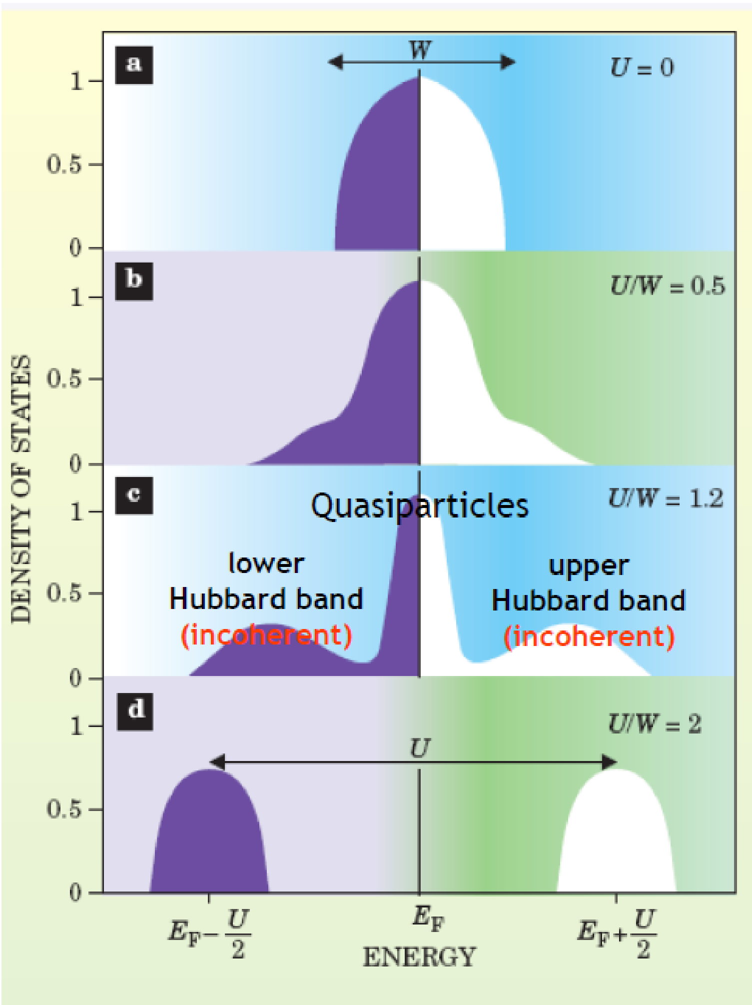
能带带宽调节金属-绝缘体转变

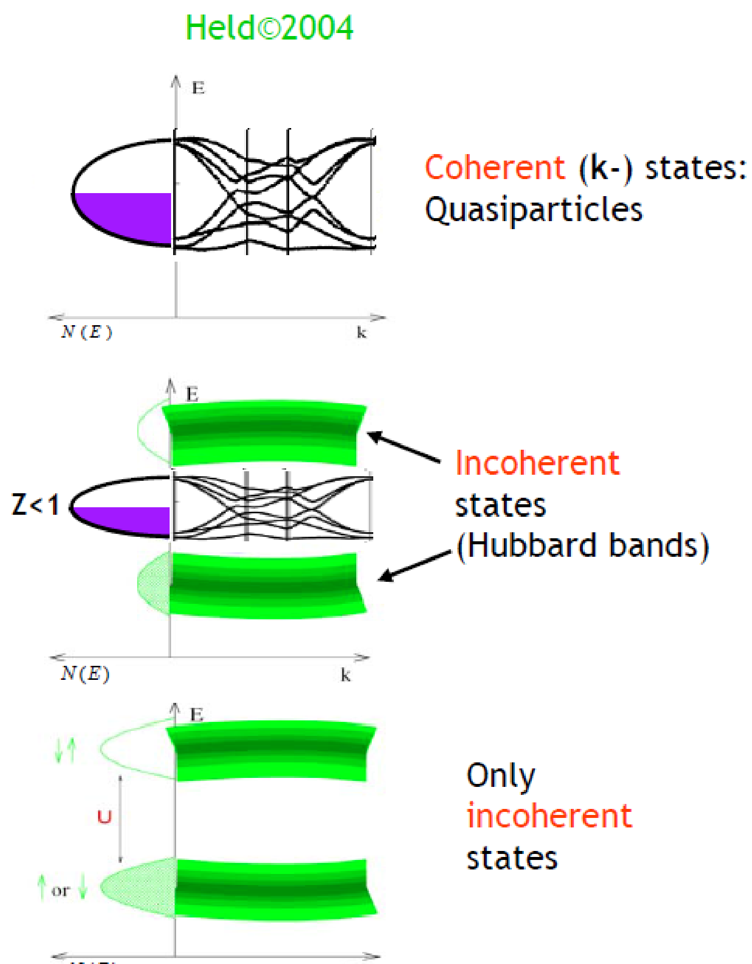


关联电子系统



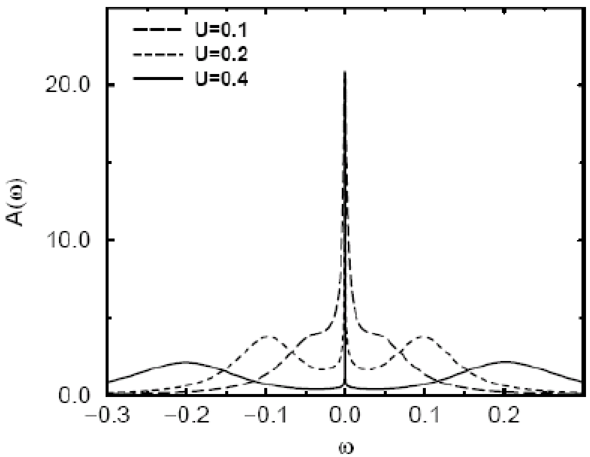
DMFT: Mott-Hubbard metal-insulator transition



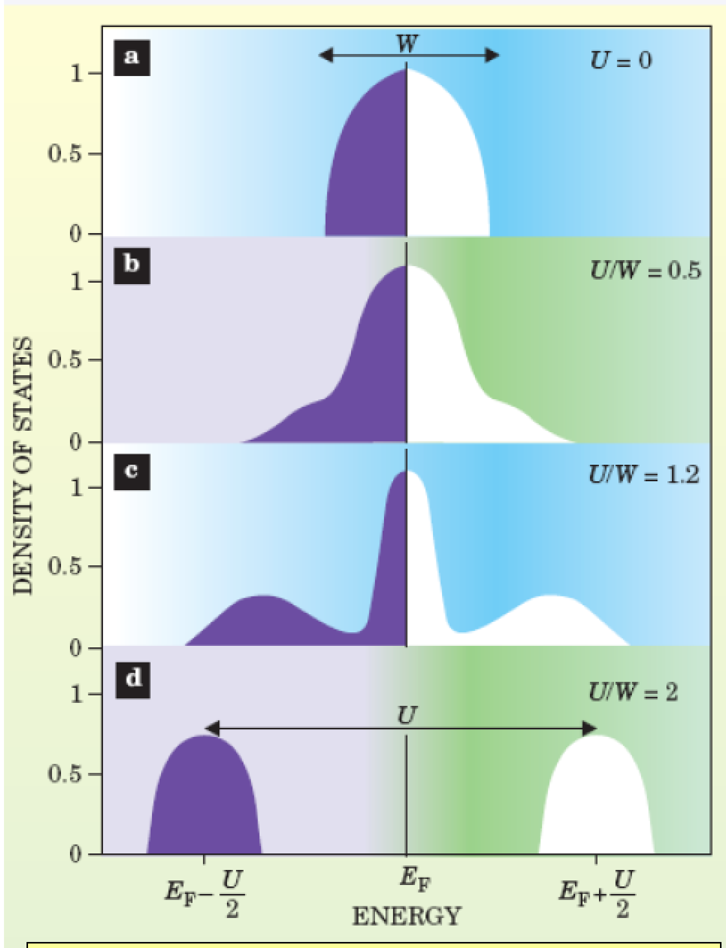


Correlations lead to transfer of spectral weight

Characteristic three-peak structure



Single-impurity Anderson model



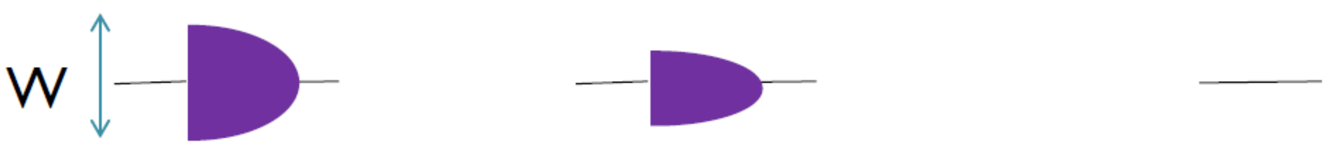
Two types of electrons

Only one type of electron

Mott-Hubbard vs Brinkman-Rice transition

The Mott-Hubbard transition (insulator) Uc=W

The Brinkman-Rice transition (metallic) Uc=2W



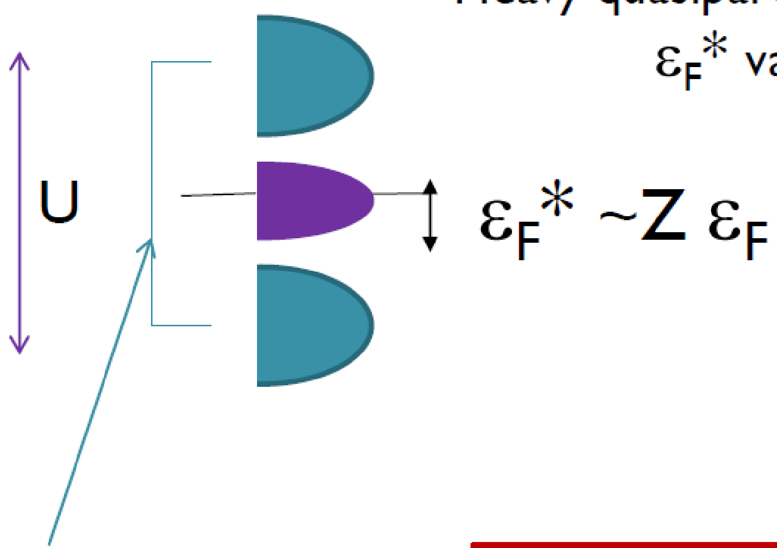
Heavy quasiparticle
(reduced K.E.)
Reduced quasiparticle residue

Quasiparticle disappears

$$\varepsilon_F^* \sim Z\, \varepsilon_F$$

E. Bascones

Mott-Hubbard + Brinkman-Rice transition



Heavy quasiparticle which disappears when $\varepsilon_F{}^*$ vanishes at $U_{c2} > U_{c1}$

Gap U-W between the Hubbard bands opens at U_{c1}=W=2D

- Density of States: Quasiparticle and Hubbard Bands three peak structure.

- Two energy scales: $\varepsilon_F{}^*$ and the gap between the Hubbard bands

E. Bascones

如何调节U/W

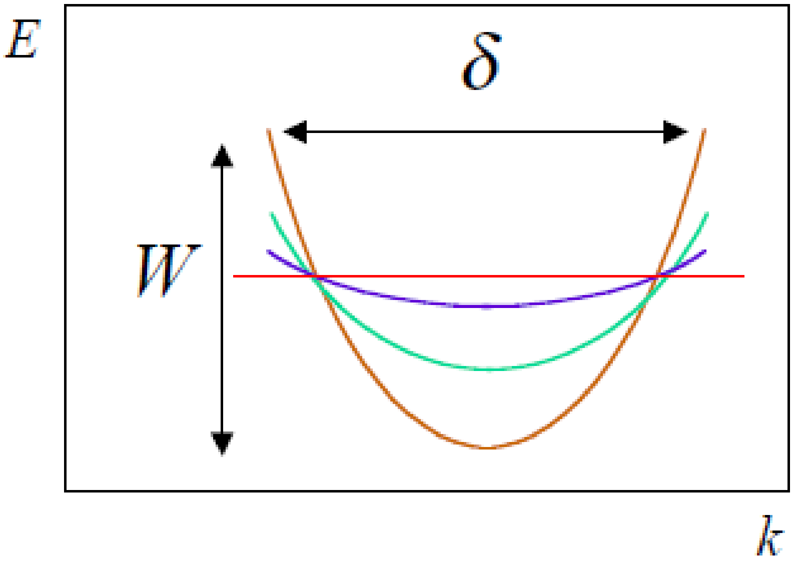
考虑原子尺度下的电荷、自旋、轨道、晶格等量子维度。

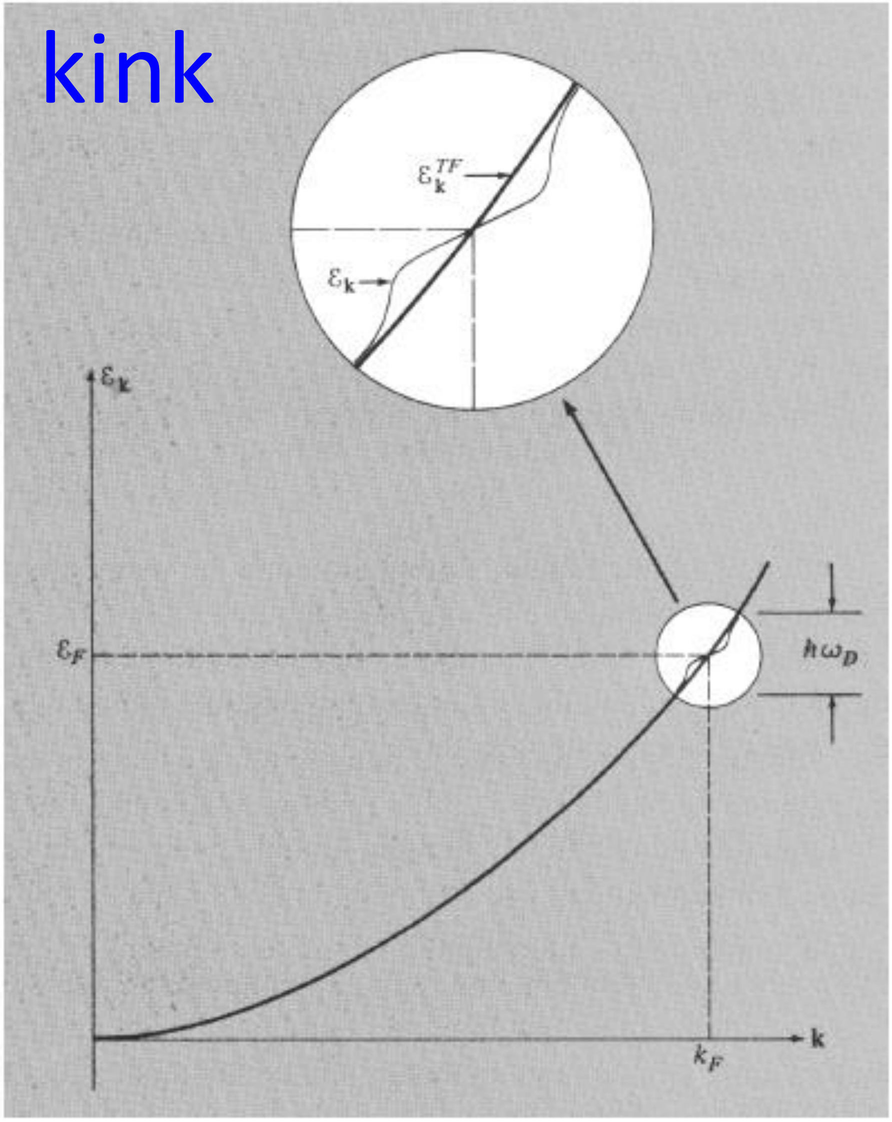
- 电荷：浓度、波的局域化。。。
- 自旋：自旋维度的影响。。。
- 轨道：重叠、轨道序。。。
- 晶格：维度、Jahn-Teller效应、晶胞拓展。。

电子-电子/电子-声子相互作用

$$E=\frac{m^* v^2}{2}=\frac{\hbar^2 k^2}{2m^*}$$

$$\boxed{m^*=\frac{0.946\,\delta[\text{Å}^{-1}]^2}{W[\text{eV}]}}$$





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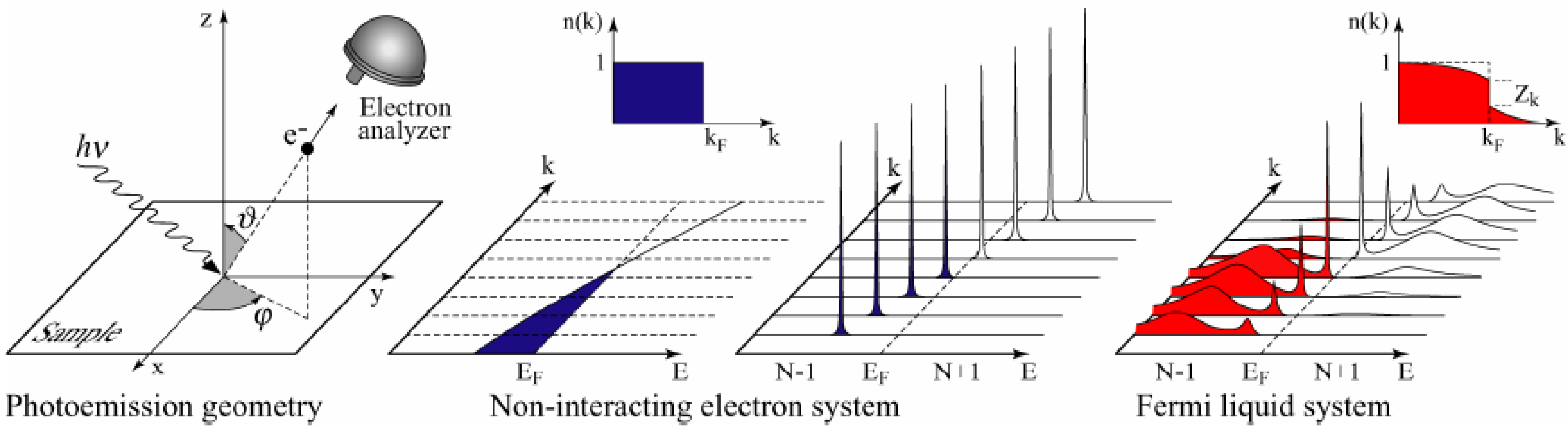

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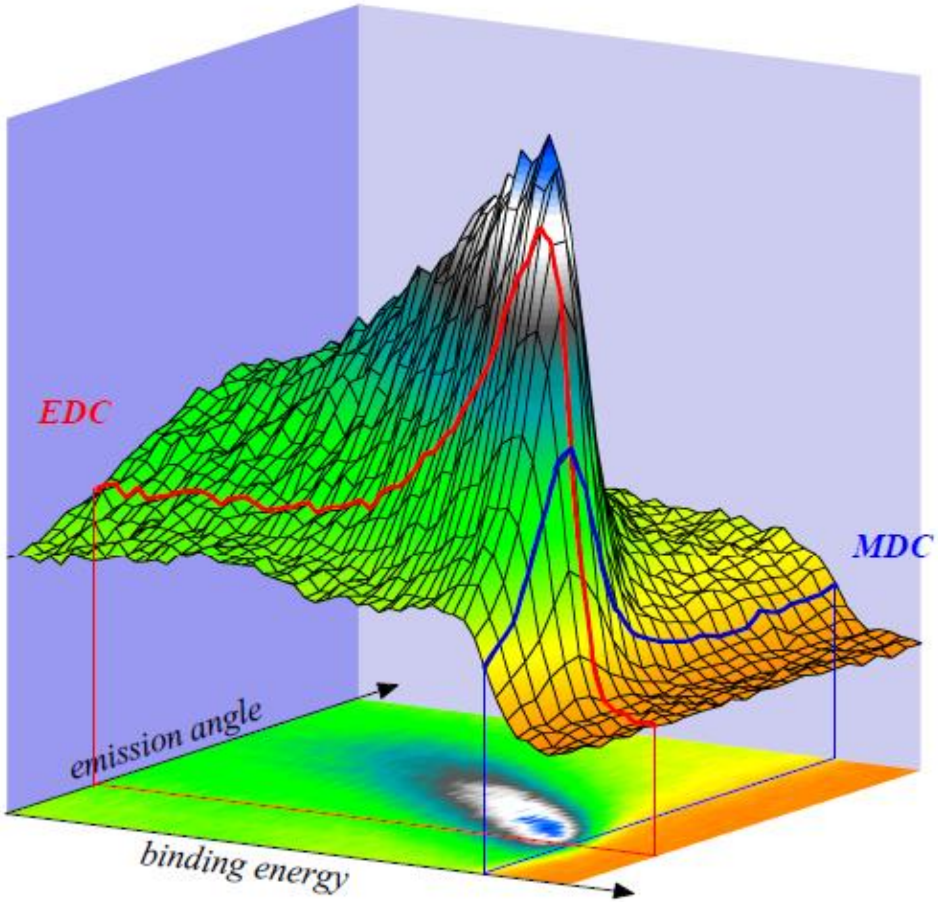
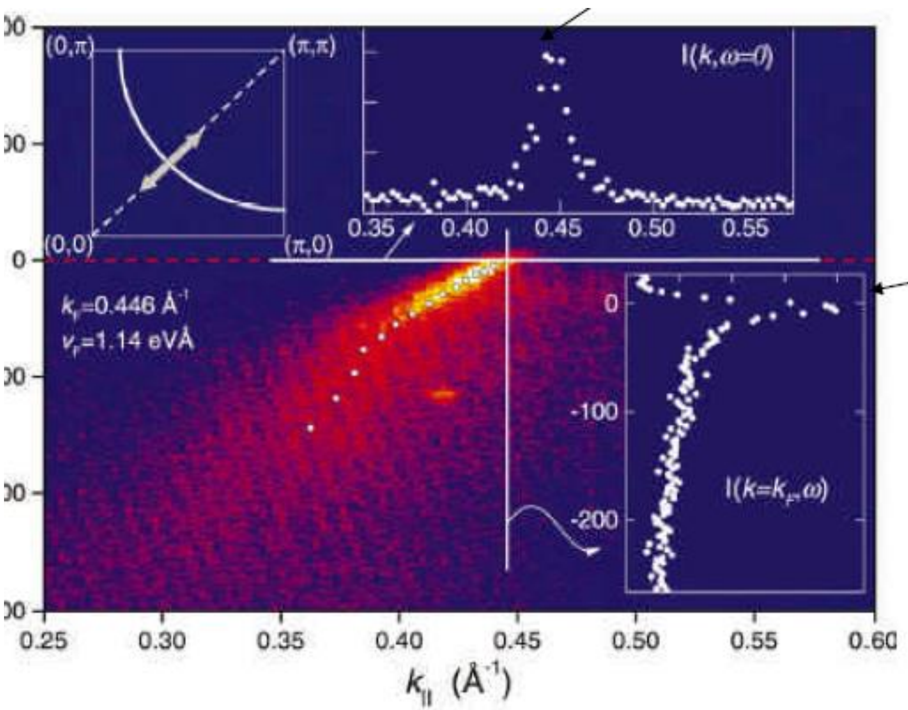
$\Sigma(k,\omega)$: the "self-energy" captures the effects of interactions

EDC 和 MDC



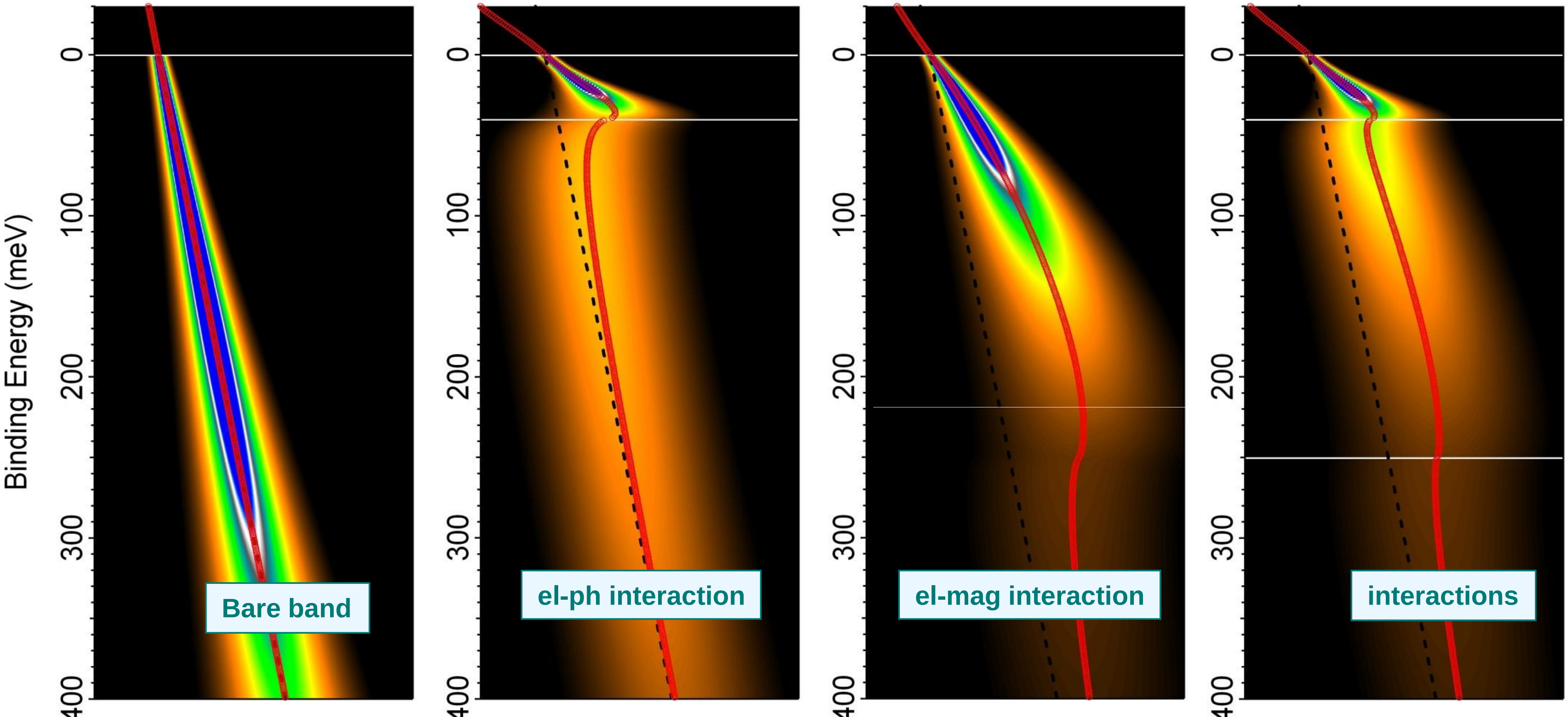
EDC
MDC
emission angle
binding energy



(0,π)
(π,π)
(0,0)
(π,0)
I(k,ω=0)
0.35
0.40
0.45
0.50
0.55
k_F=0.446 Å^-1
v_F=1.14 eVÅ
I(k=k_F,ω)
0
-100
-200
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0.60
k_∥ (Å^-1)

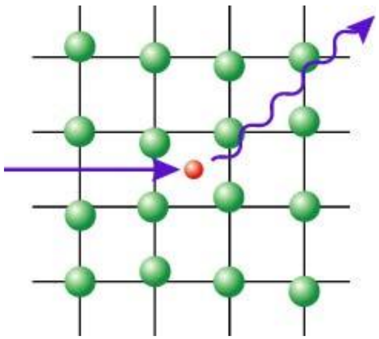
Interaction Effects in Band Dispersion

Computer simulation of Quasi-particle dispersion
Including many-body interactions



High-resolution ARPES with tunable synchrotron radiation
to determine the mass enhancement m^*/m_b

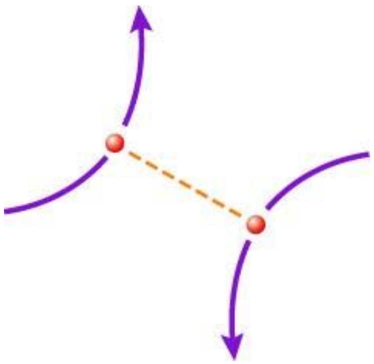
Lifetime broadening mode



electron-phonon coupling

Γ_{el-ph}

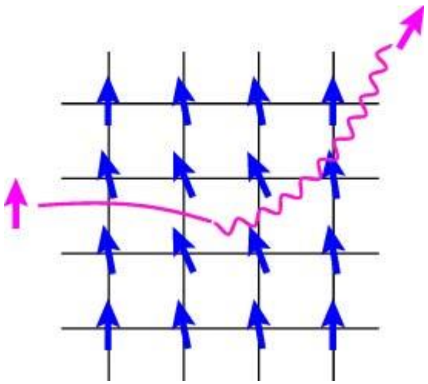
Debye temp. ~0.04 eV



electron-electron interaction

Γ_{el-el}

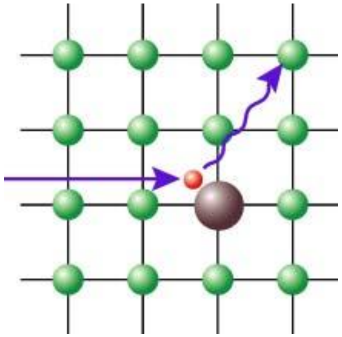
Band width 3~5 eV



electron-magnon coupling

Γ_{el-mag}

Mag. DOS ~0.4 eV for Ni, Fe



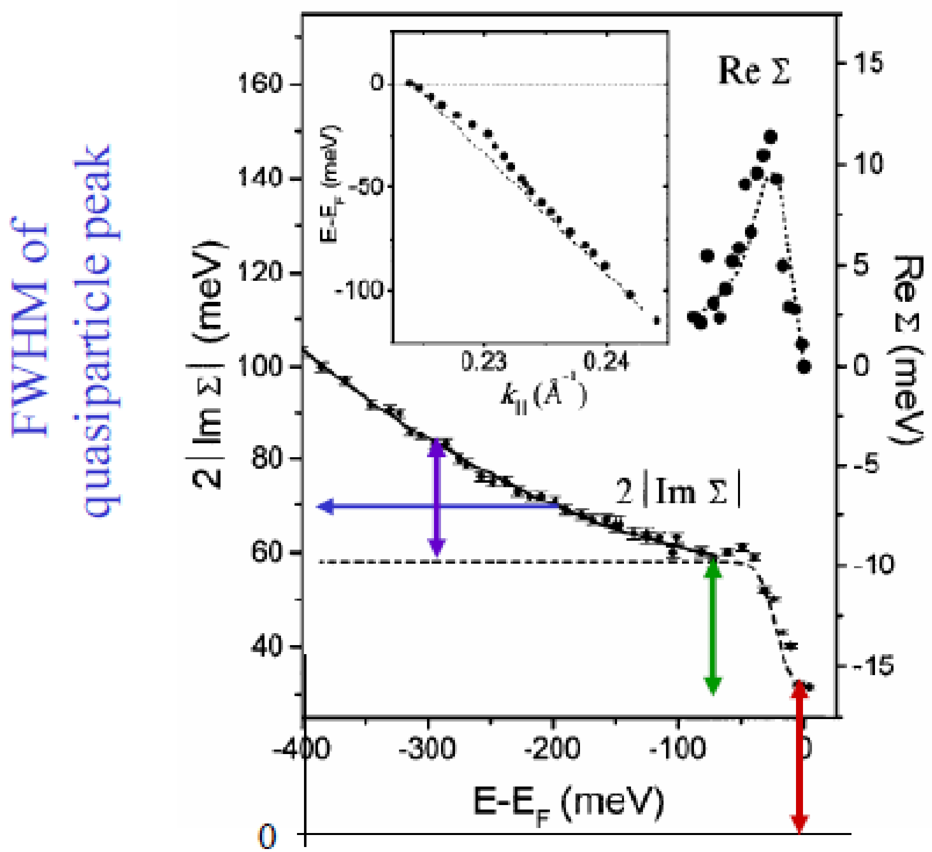
electron-impurity scattering

Γ_{el-imp}

energy indep.

$$\Delta E = \frac{\hbar}{\tau} = \Gamma_{el-ph} + \Gamma_{el-el} + \Gamma_{el-mag} + \Gamma_{el-imp} + \Gamma_0 = 2|\mathrm{Im}\Sigma|$$

自能实部与虚部



ImΣ = width of spectral peak
Measurable in the same spectra.

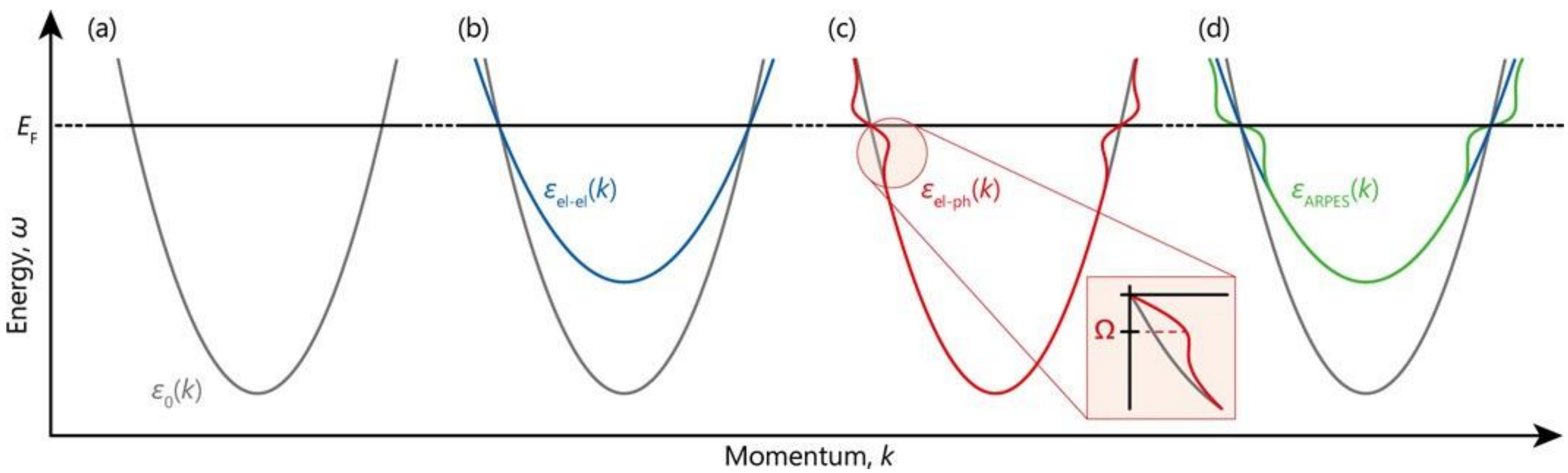
ImΣ and ReΣ related through Kramers-Kronig relations.

Electron-electron scattering

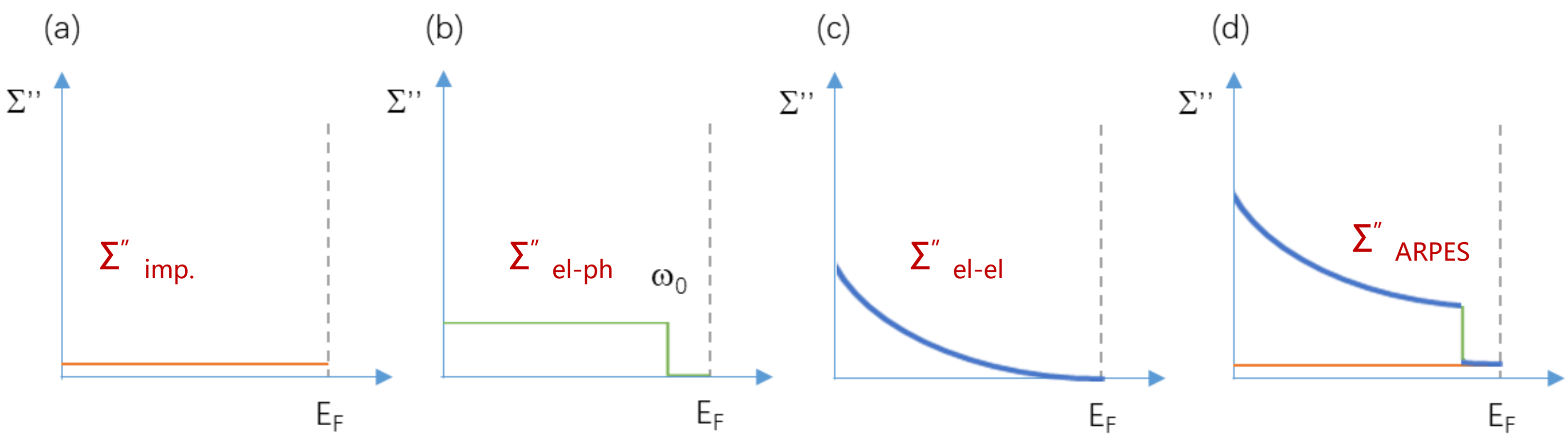
Coupling to phonons

Impurities, finite resolution, final state effects, etc.

自能实部与虚部

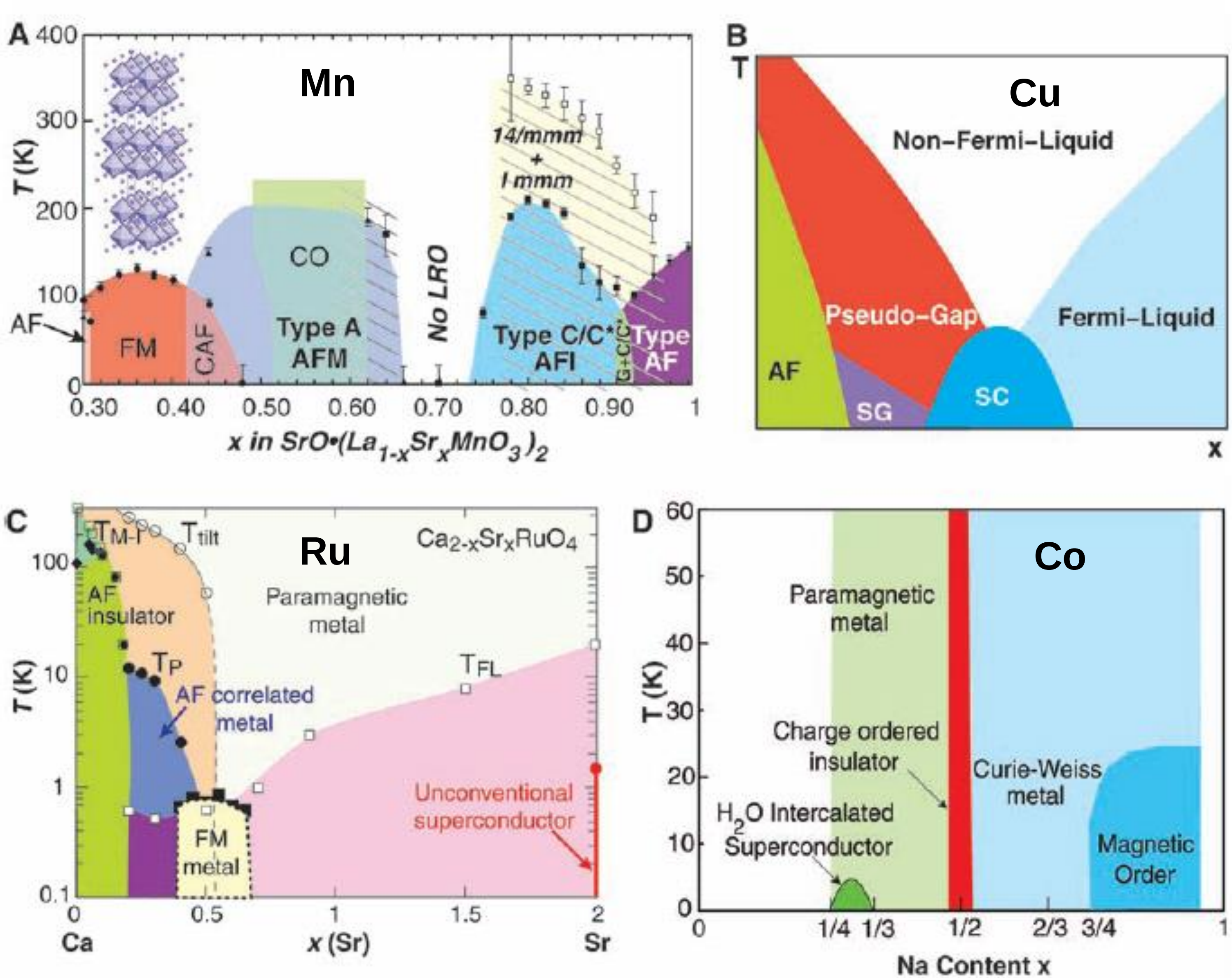


(a)
(b)
(c)
(d)
E_F
Energy, ω
$\varepsilon_0(k)$
$\varepsilon_{el-el}(k)$
$\varepsilon_{el-ph}(k)$
$\varepsilon_{ARPES}(k)$
Ω
Momentum, k

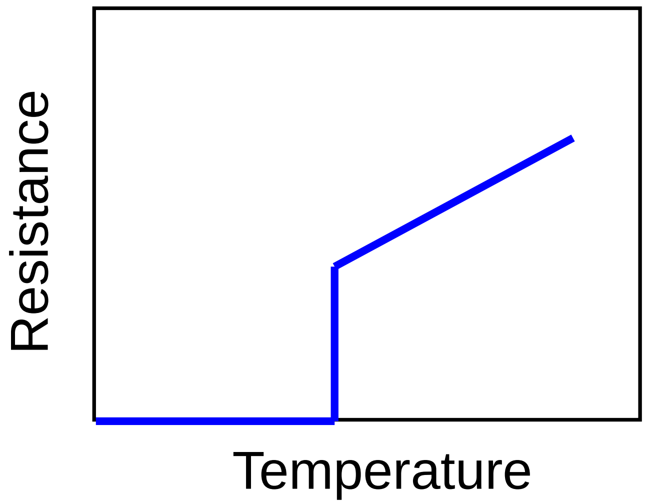
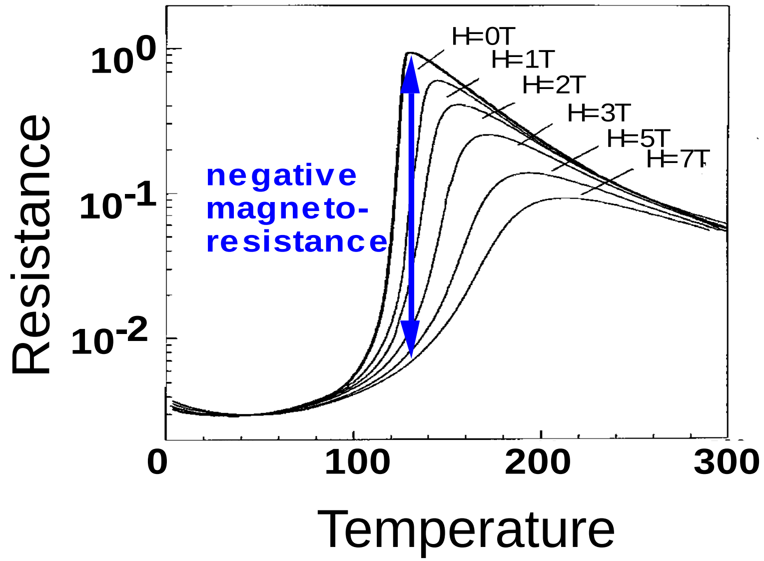


(a)
(b)
(c)
(d)
Σ''
$\Sigma''_{imp.}$
Σ''_{el-ph}
ω_0
Σ''_{el-el}
Σ''_{ARPES}
E_F

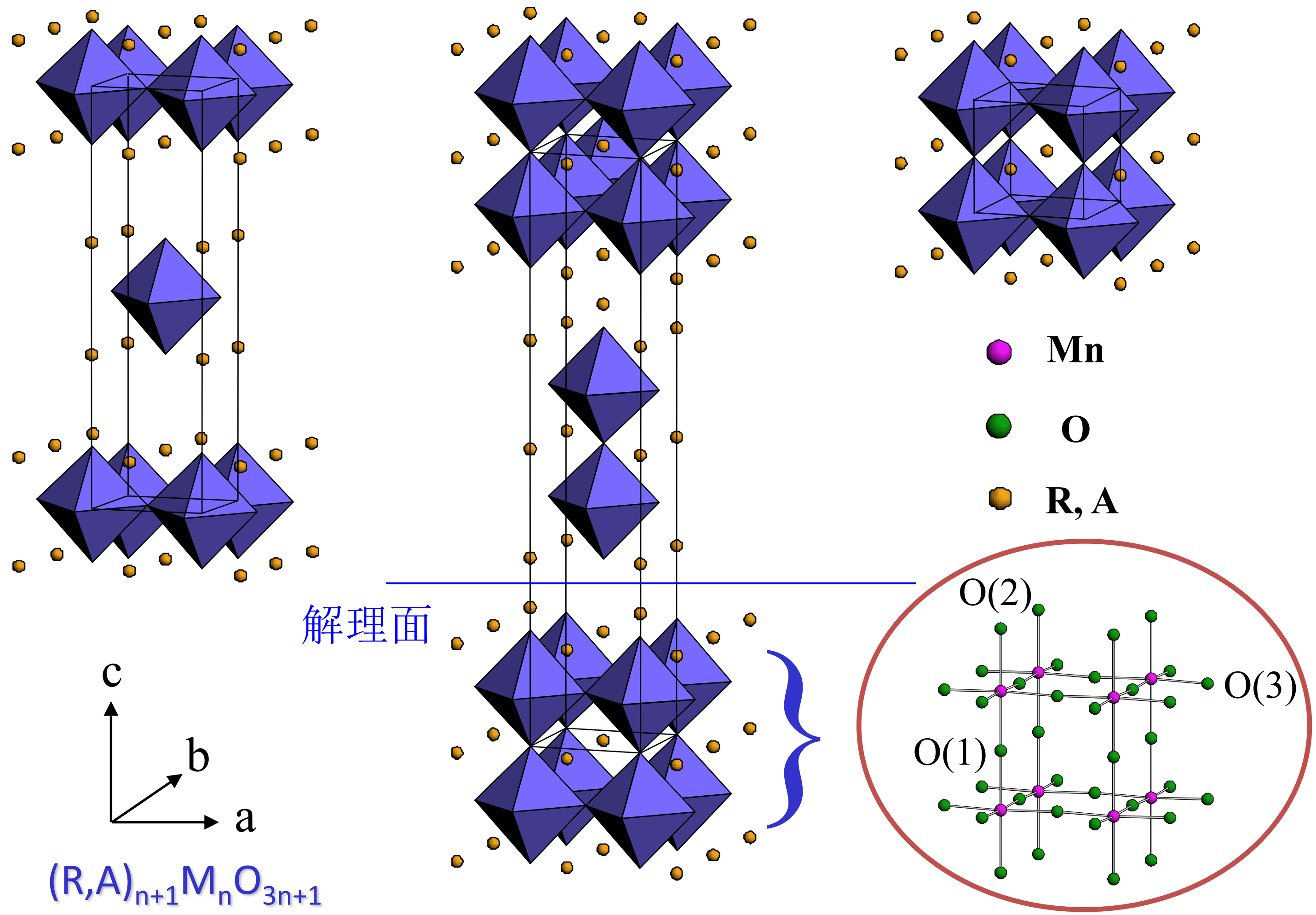
关联电子系统的特点


A
Mn
T (K)
AF
FM
CAF
CO
Type A AFM
No LRO
I4/mmm + I mmm
Type C/C* AFI
G+C/C*
Type AF
x in SrO•(La1-xSrxMnO3)2
B
T
Cu
Non-Fermi-Liquid
Pseudo-Gap
Fermi-Liquid
AF
SG
SC
x
C
Ru
Ca2-xSrxRuO4
TM-I
Ttilt
AF insulator
Paramagnetic metal
TP
AF correlated metal
TFL
FM metal
Unconventional superconductor
T (K)
Ca
x (Sr)
Sr
D
Co
T (K)
Paramagnetic metal
Charge ordered insulator
H2O Intercalated Superconductor
Curie-Weiss metal
Magnetic Order
Na Content x

典型的例子

高温超导电性 (e.g. $Bi_2Sr_2CaCu_2O_8$)	庞磁阻 (e.g. $La_{2-2x}Ca_{1+x}Mn_2O_7$)
	

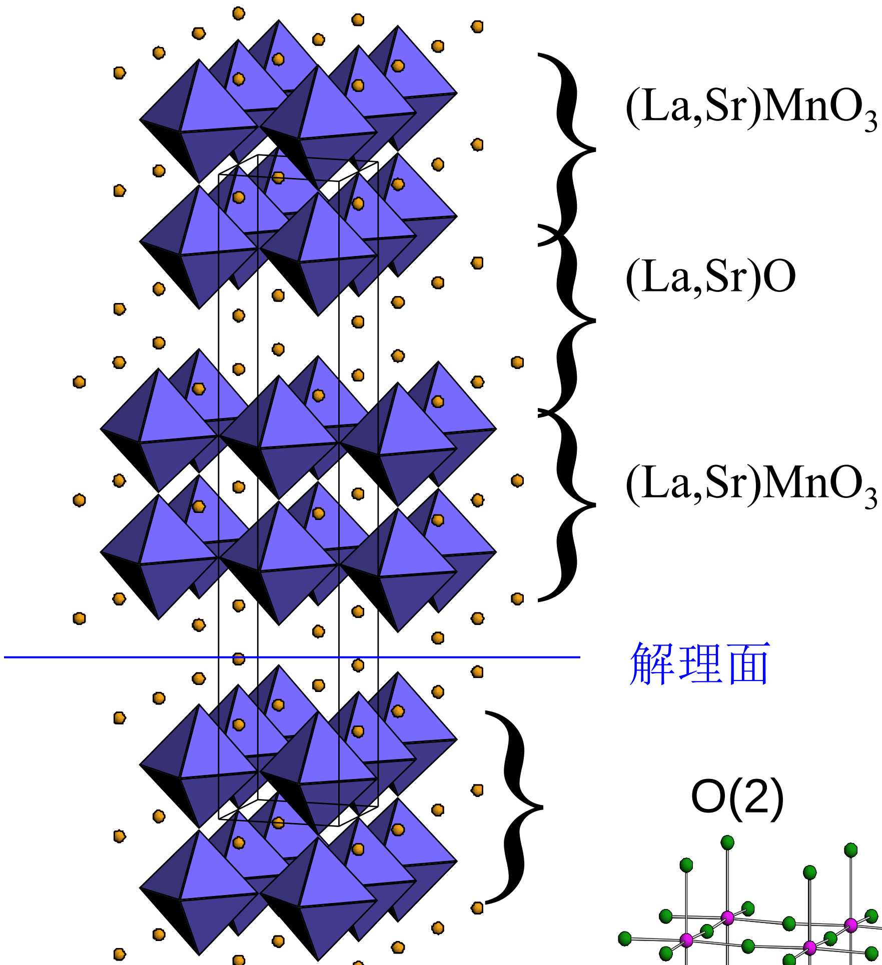
Crystal structure of manganites

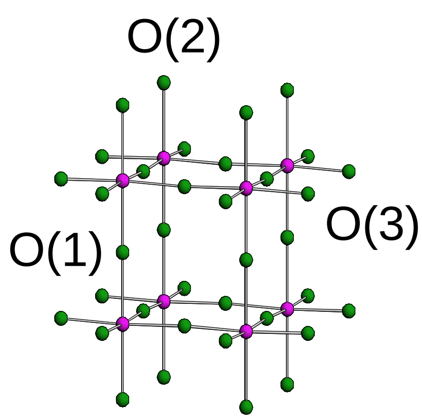


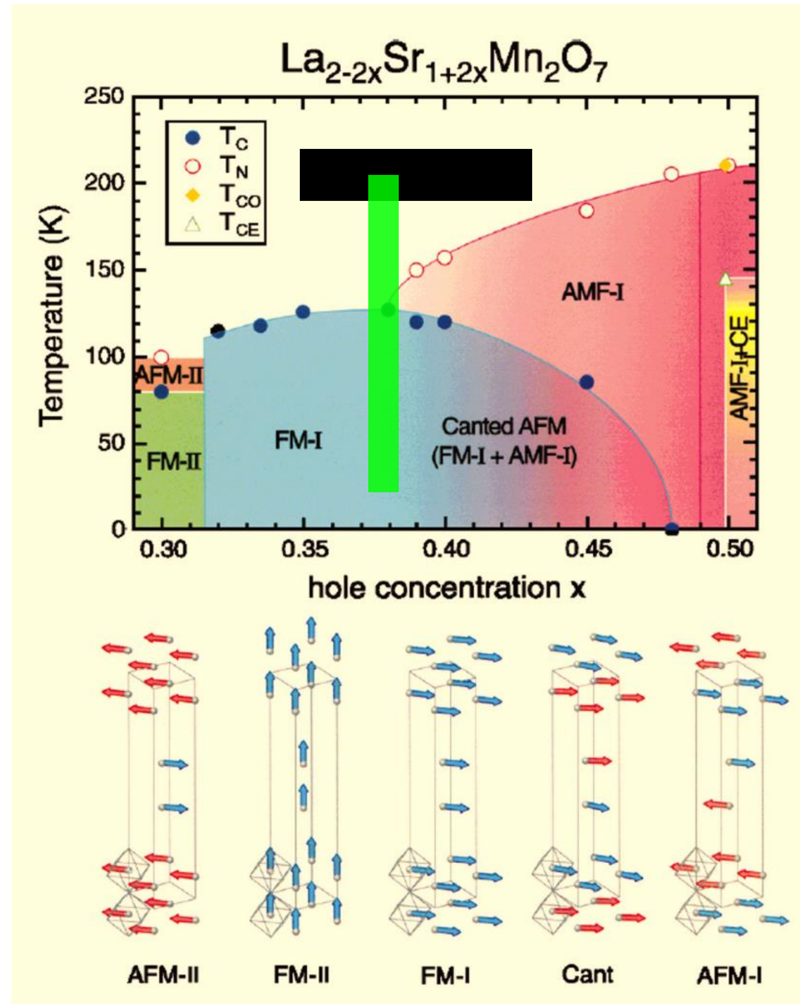
$(R,A)_{n+1}M_nO_{3n+1}$

Important physics occurs in MnO_6 octahedra and MnO_2 planes

$La_{2-2x}Sr_{1+2x}Mn_2O_7$ 的晶体结构和相图





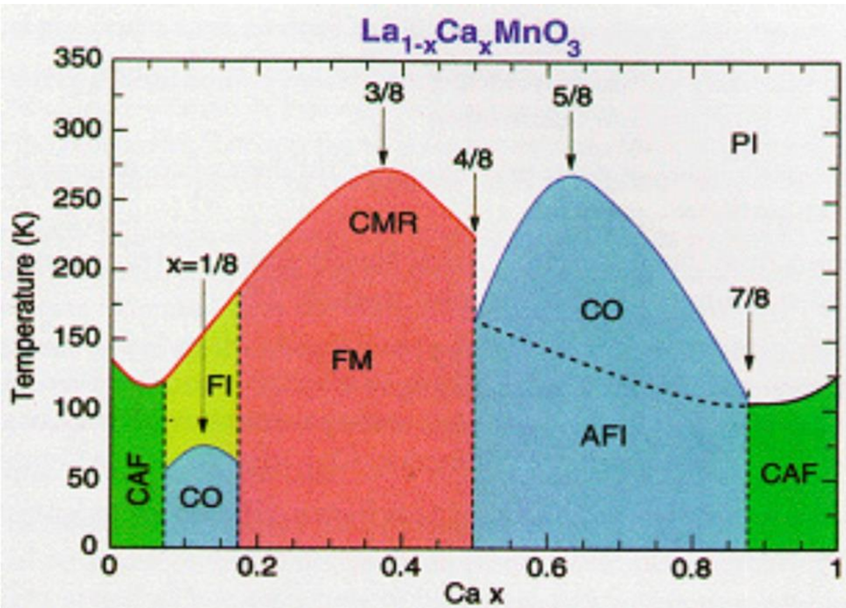


Space Group: I4/mmm
a=3.87 Å, c=20.1 Å

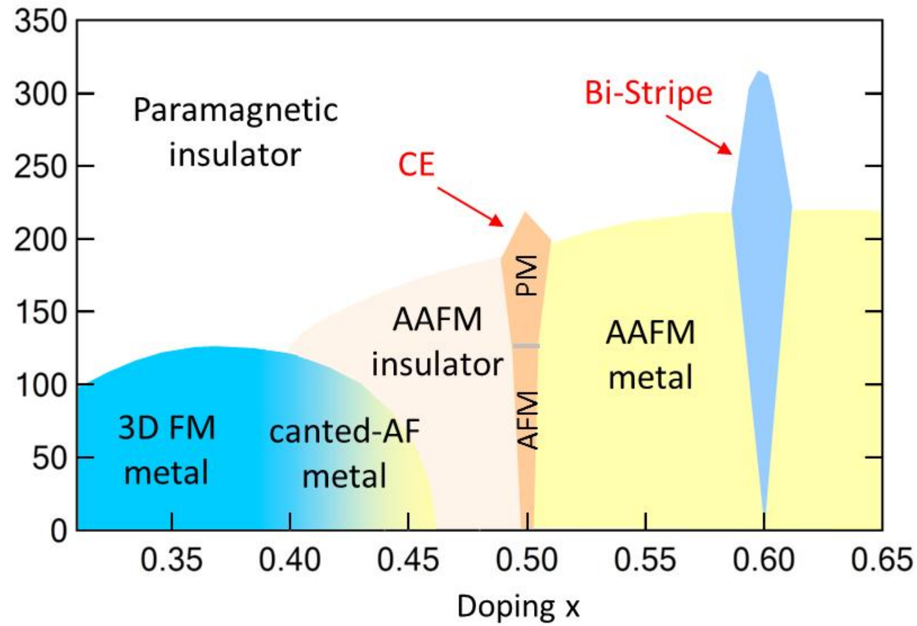
Kubota, J. Phys. Soc. Jpn. **69**, 1606 (2000).

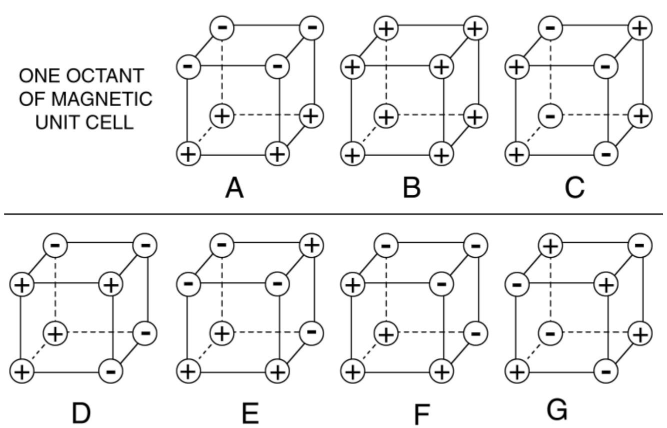
Phase diagram and magnetic structure

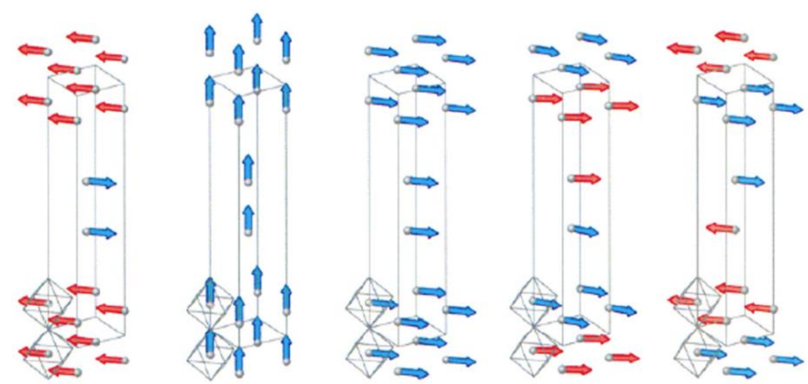
$La_{1-x}Ca_xMnO_3$



$La_{2-2x}Sr_{1+2x}Mn_2O_7$



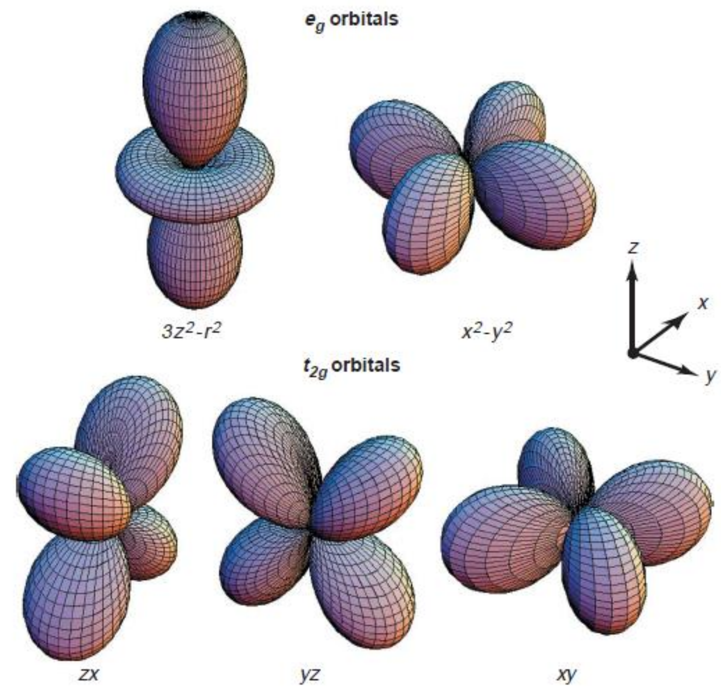


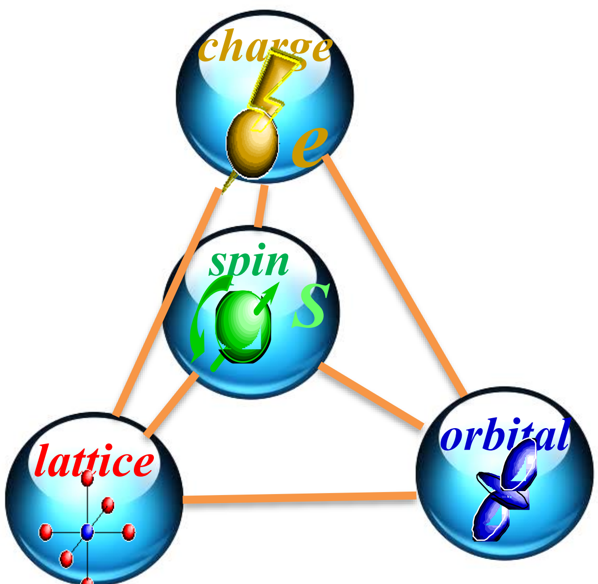


Orbital Physics in Transition-Metal Oxides

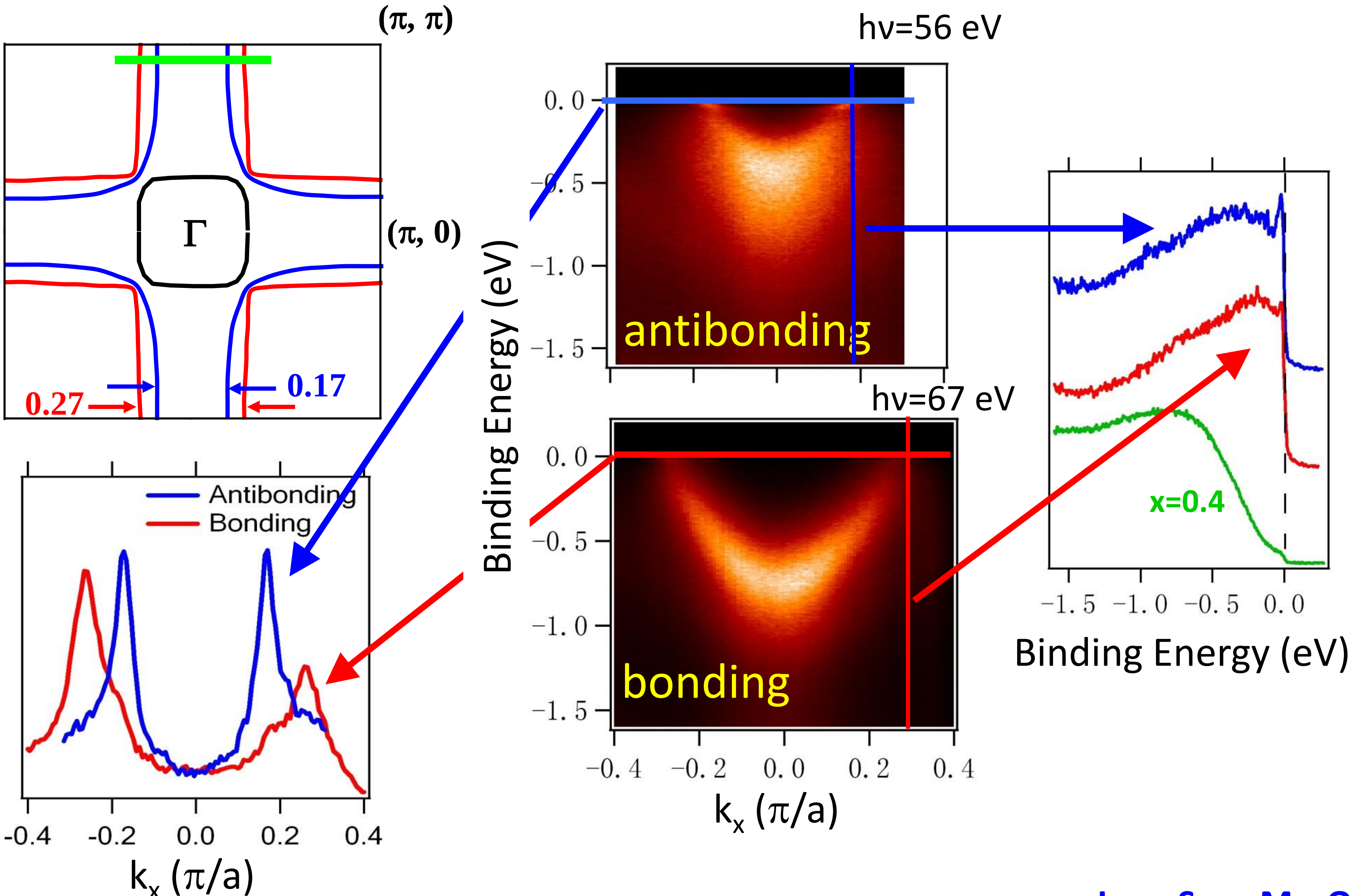
Y. Tokura[1,2] and N. Nagaosa[1]

An electron in a solid, that is, bound to or nearly localized on the specific atomic site, has three attributes: charge, spin, and orbital. The orbital represents the shape of the electron cloud in solid. In transition-metal oxides with anisotropic-shaped d-orbital electrons, the Coulomb interaction between the electrons (strong electron correlation effect) is of importance for understanding their metal-insulator transitions and properties such as high-temperature superconductivity and colossal magnetoresistance. The orbital degree of freedom occasionally plays an important role in these phenomena, and its correlation and/or order-disorder transition causes a variety of phenomena through strong coupling with charge, spin, and lattice dynamics. An overview is given here on this "orbital physics," which will be a key concept for the science and technology of correlated electrons.



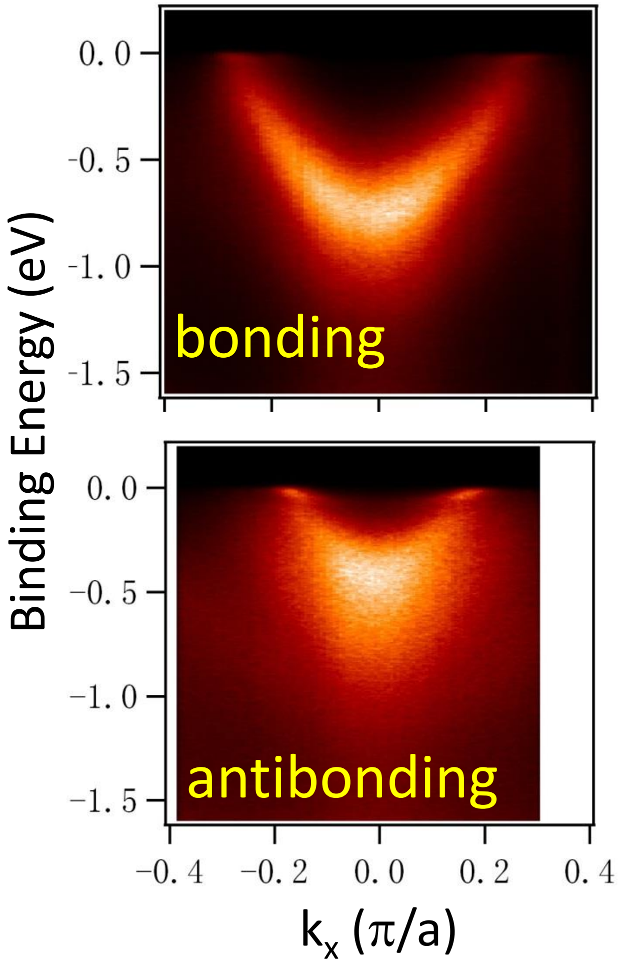


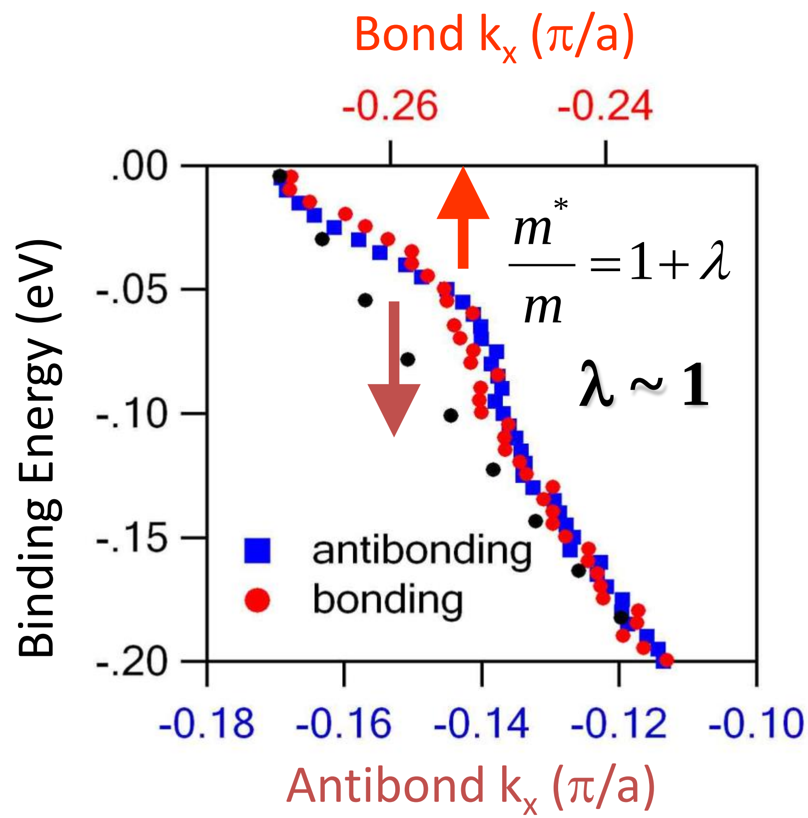
Bi-layer split band structure in x=0.36, 0.38 compounds



$La_{2-2x}Sr_{1+2x}Mn_2O_7$

Dispersions of bi-layer split bands of x=0.36, 0.38 compounds



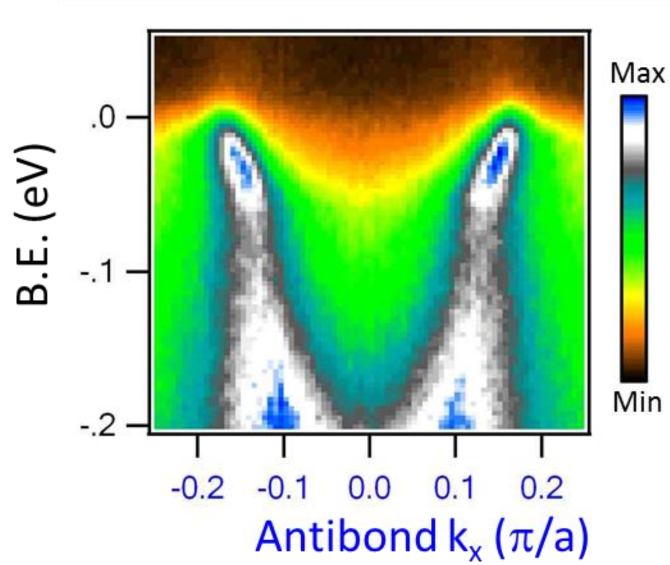


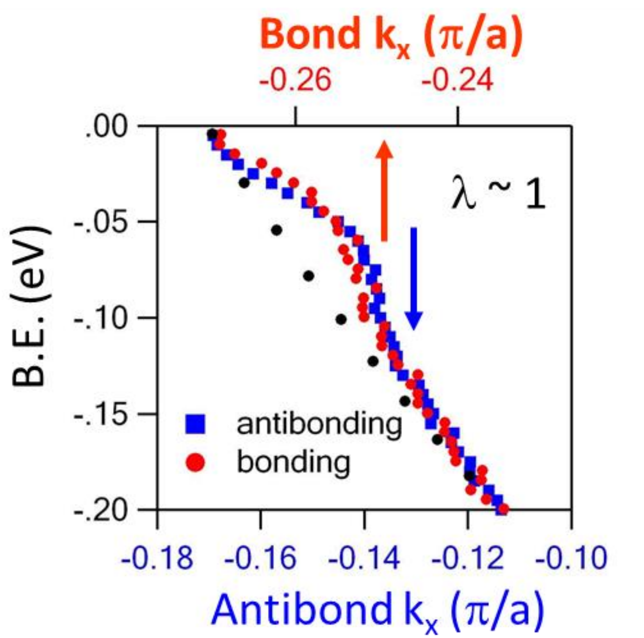
λ= 1-1.5 metal-insulator transition

specific data

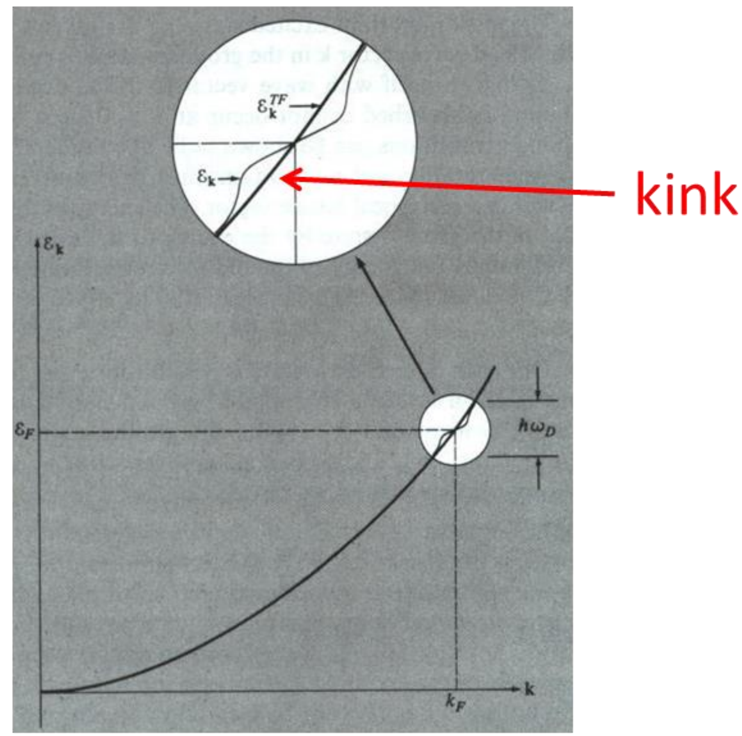
$La_{2-2x}Sr_{1+2x}Mn_2O_7$

铁磁金属态(x=0.36, 0.38)中的电子-声子耦合





Zhe Sun et al.
PRL 97, 056401 (2006)



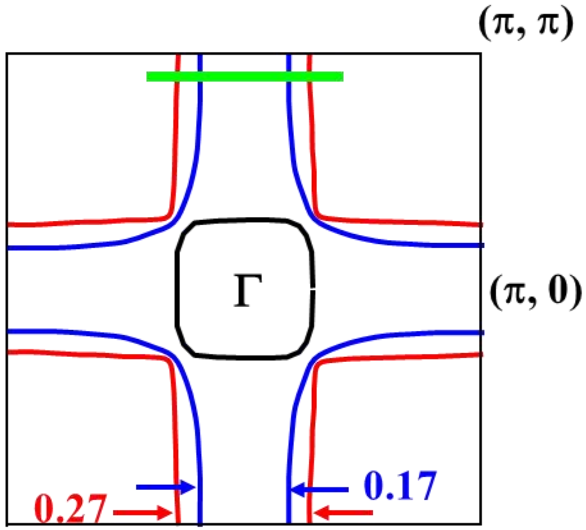
Ashcroft & Mermin, 1976

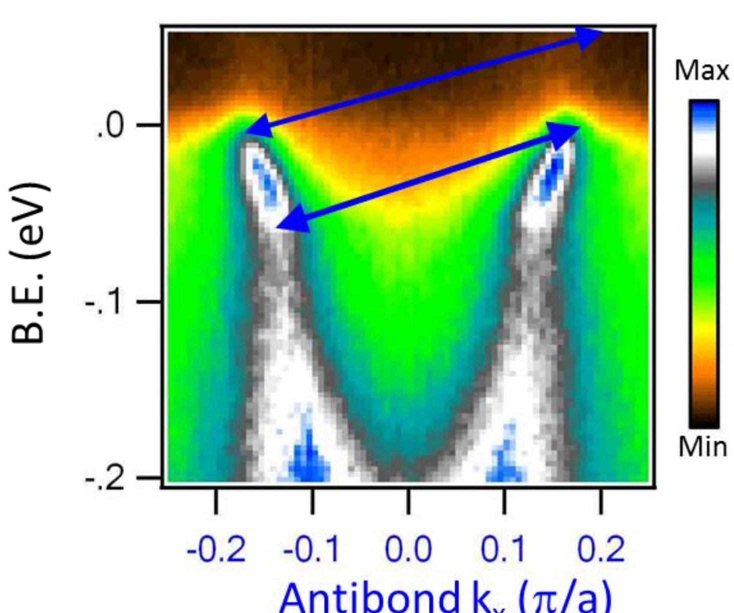
声子能级ω_D ~50-70meV

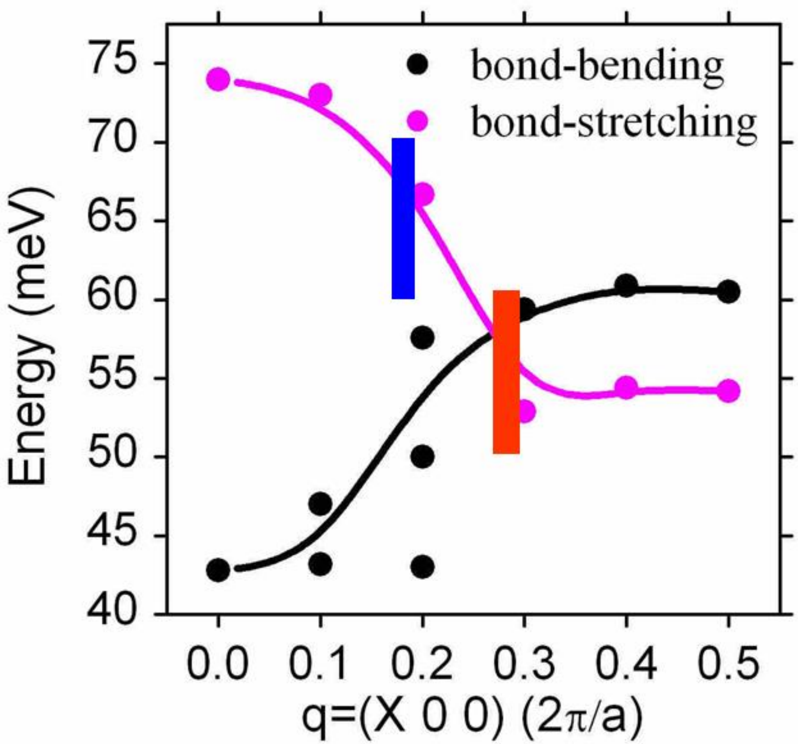
电声耦合强度 $\lambda \sim 1$

$$\frac{d\varepsilon/dk}{d\omega/dk} = 1 + \lambda$$

铁磁金属态(x=0.36, 0.38)中的电子-声子耦合







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