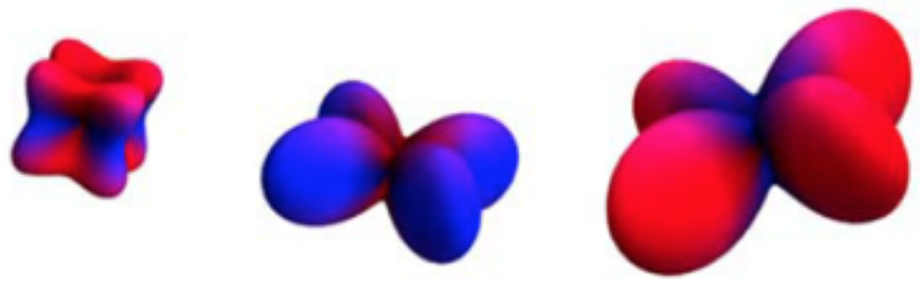
Anisotropic interactions in correlated electronic systems with strong spin-orbit coupling

Natalia Perkins

University of Minnesota

Spin Orbit Coupling School



Max Planck - UBC Summer School, Oct. 22-25 2015

Spin-Orbit Coupling vs Correlations

$3d$: $U \sim$ 3-6 eV $\lambda_{so} \sim 20$ meV

Strong correlations

Weak spin-orbit coupling

Sc	*Ti*	*V*	*Cr*	*Mn*	*Fe*	*Co*	*Ni*	*Cu*	*Zn*
Y	*Zr*	*Nb*	*Mo*	*Tc*	*Ru*	*Rh*	*Pd*	*Ag*	*Cd*
Lu	*Hf*	*Ta*	*W*	*Re*	*Os*	*Ir*	*Pt*	*Au*	*Hg*

Weak correlations

$5d$: $U \sim 1.5$ eV $\lambda_{so} \sim 0.5$ eV

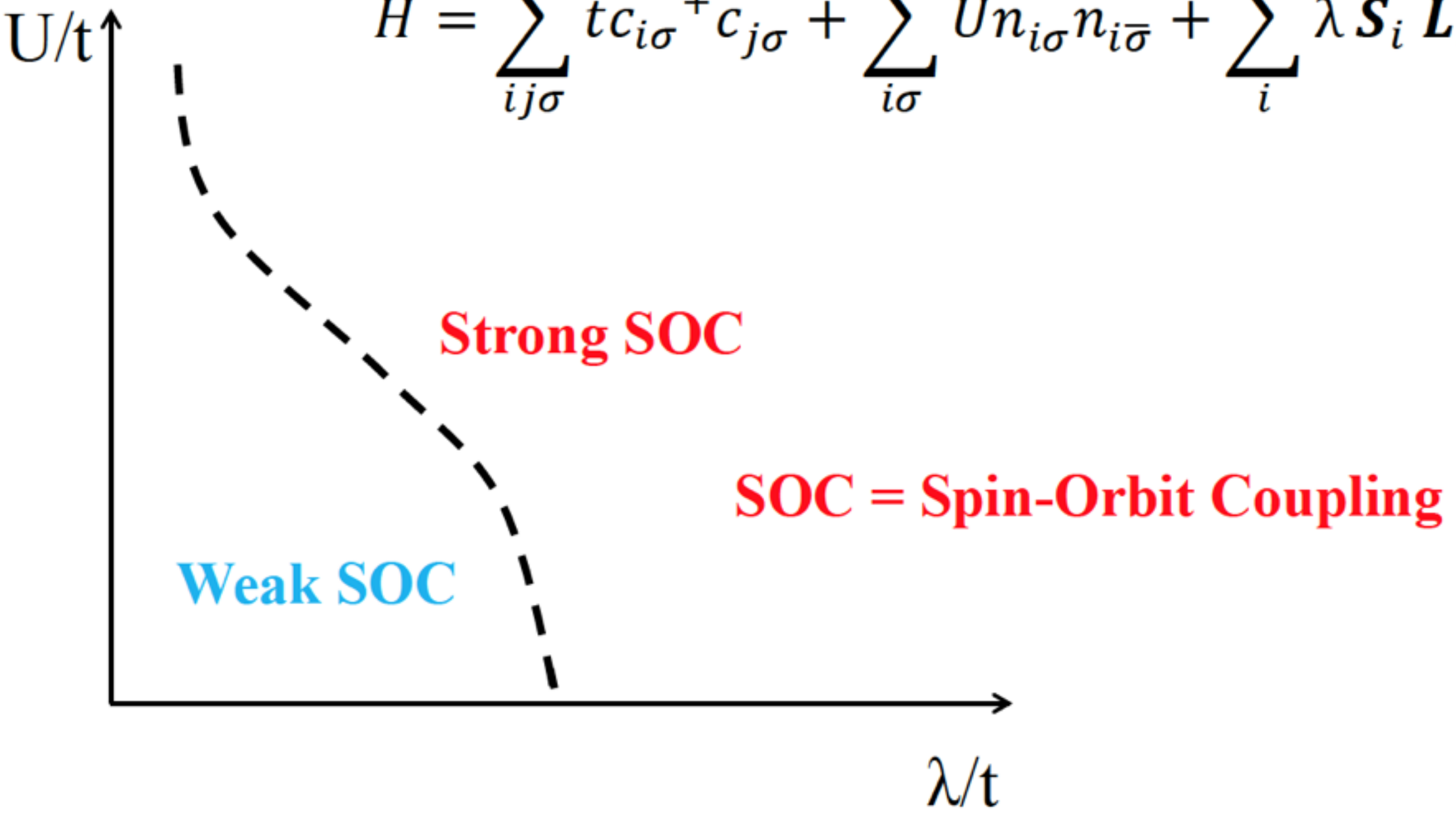
Strong spin-orbit coupling

Cu: **Z=29**

Ir: **Z=77**

Spin-Orbit Coupling vs Correlations

$$H = \sum_{ij\sigma} t c_{i\sigma}{}^{+} c_{j\sigma} + \sum_{i\sigma} U n_{i\sigma} n_{i\bar{\sigma}} + \sum_{i} \lambda \boldsymbol{S}_i \boldsymbol{L}_i$$



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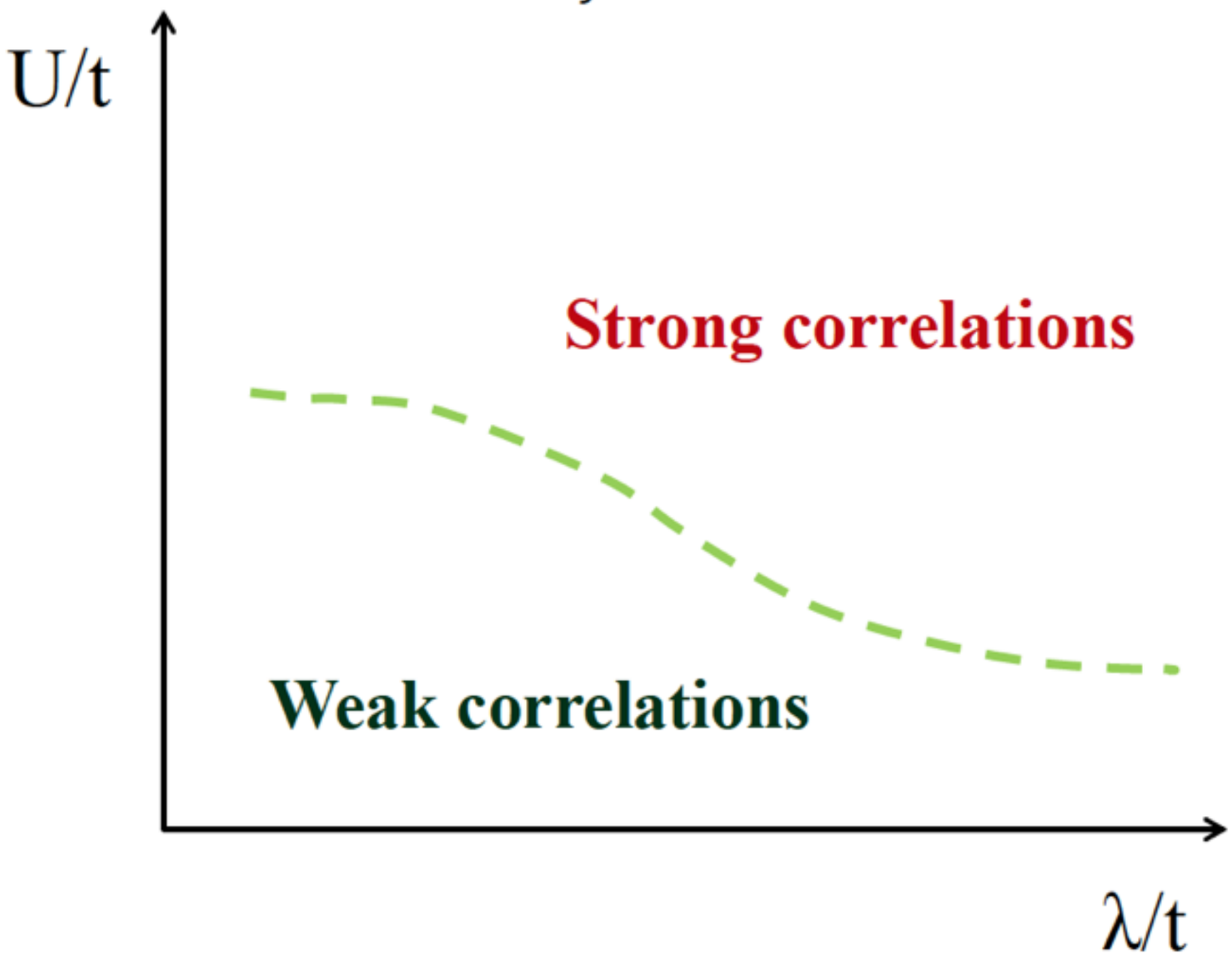

Spin-Orbit Coupling vs Correlations

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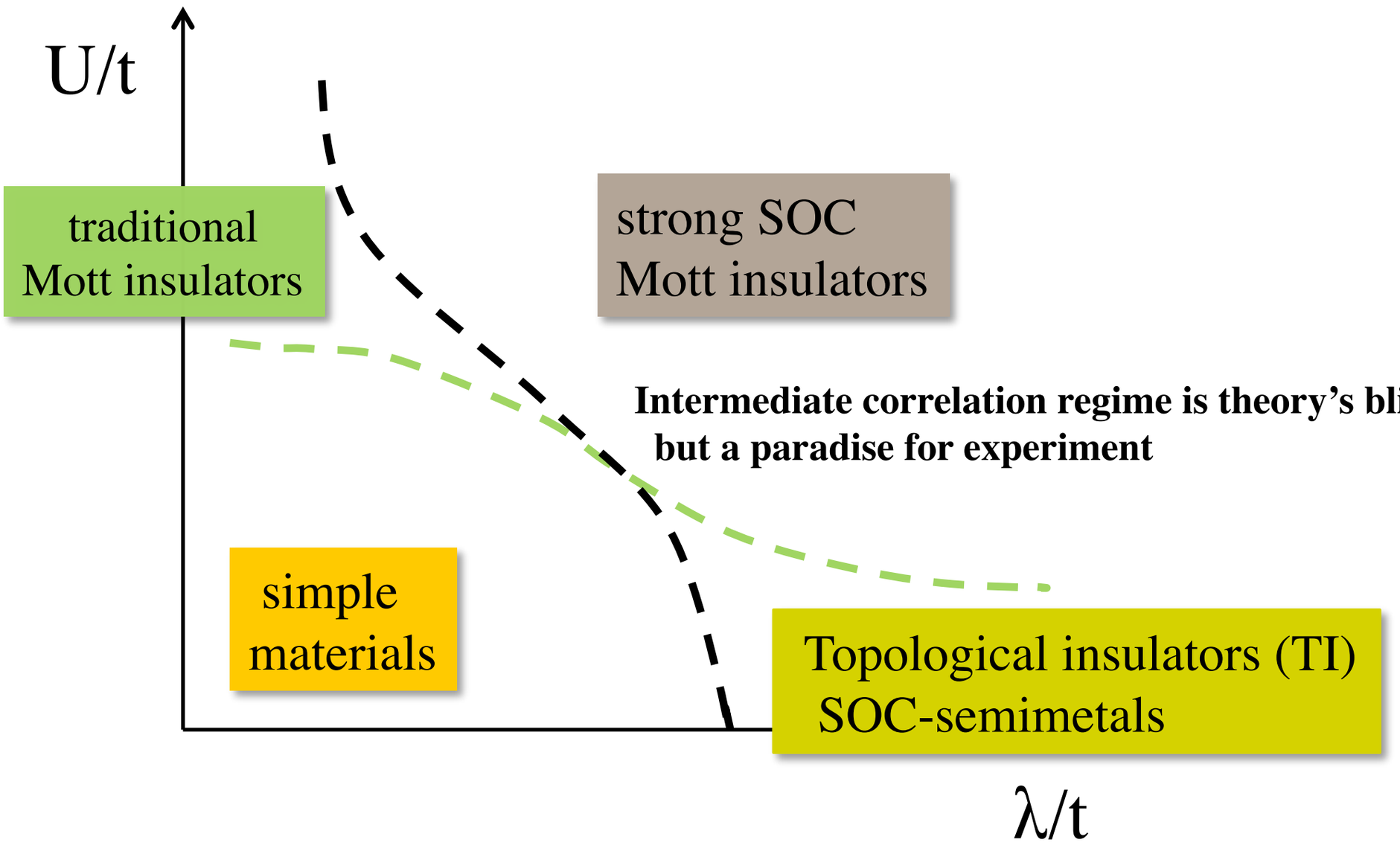
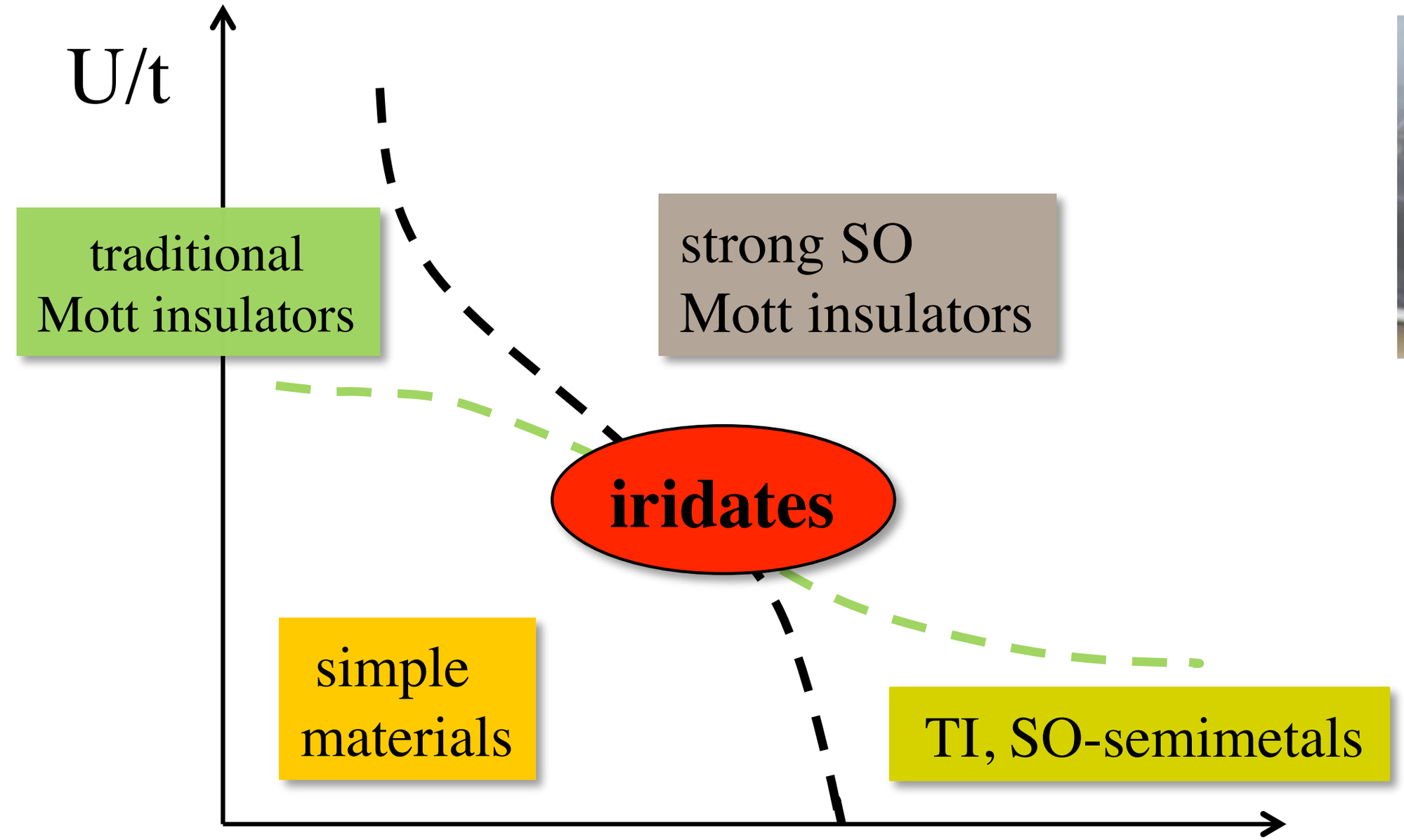
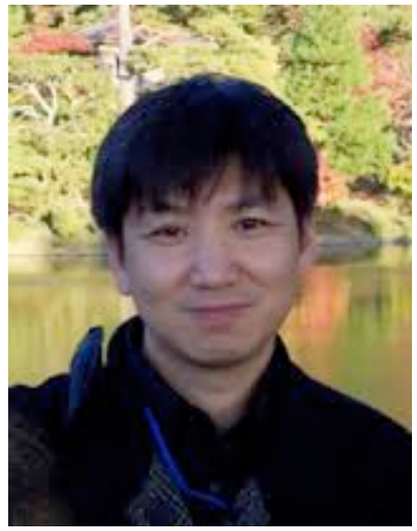
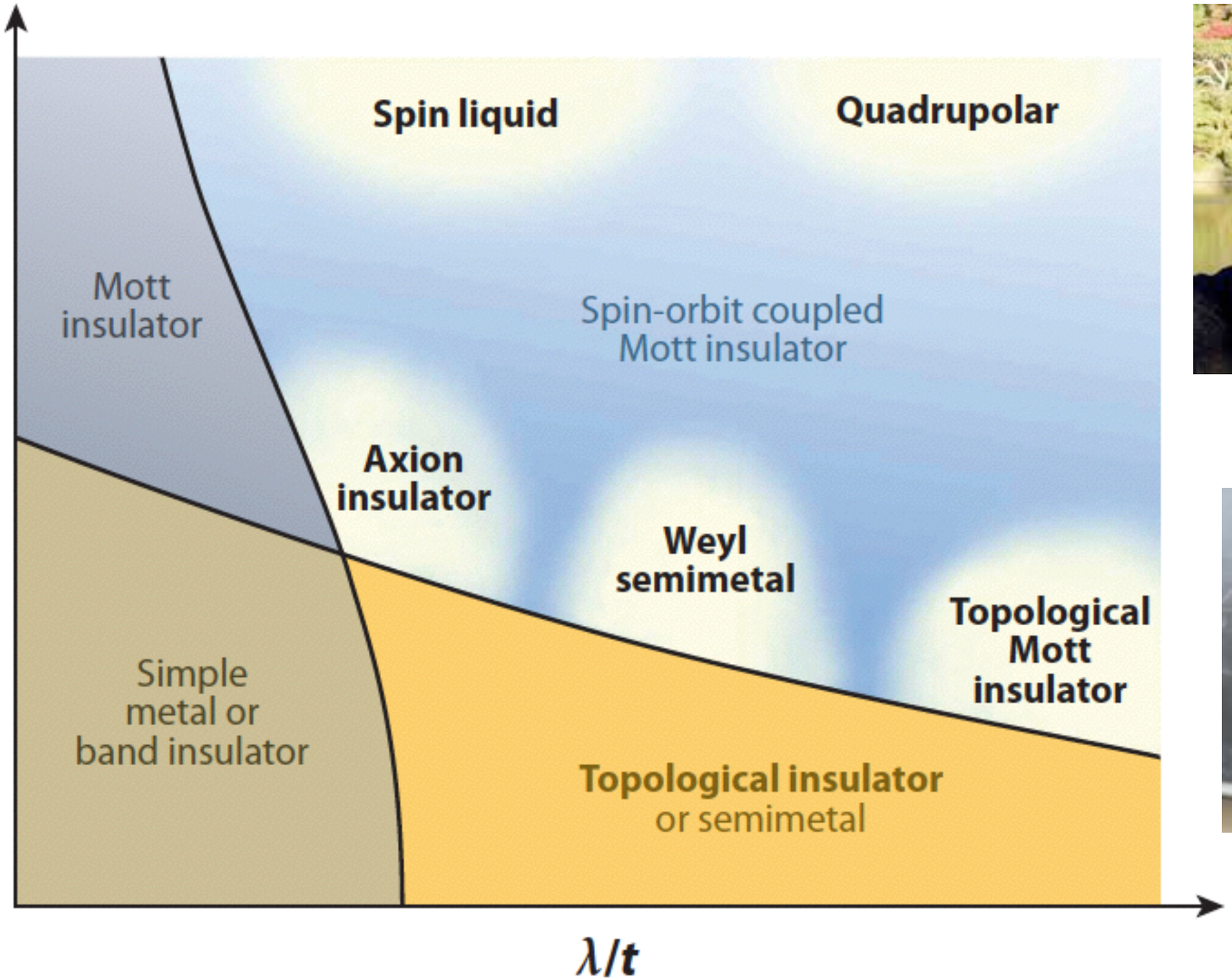


Spin-Orbit Coupling vs Correlations



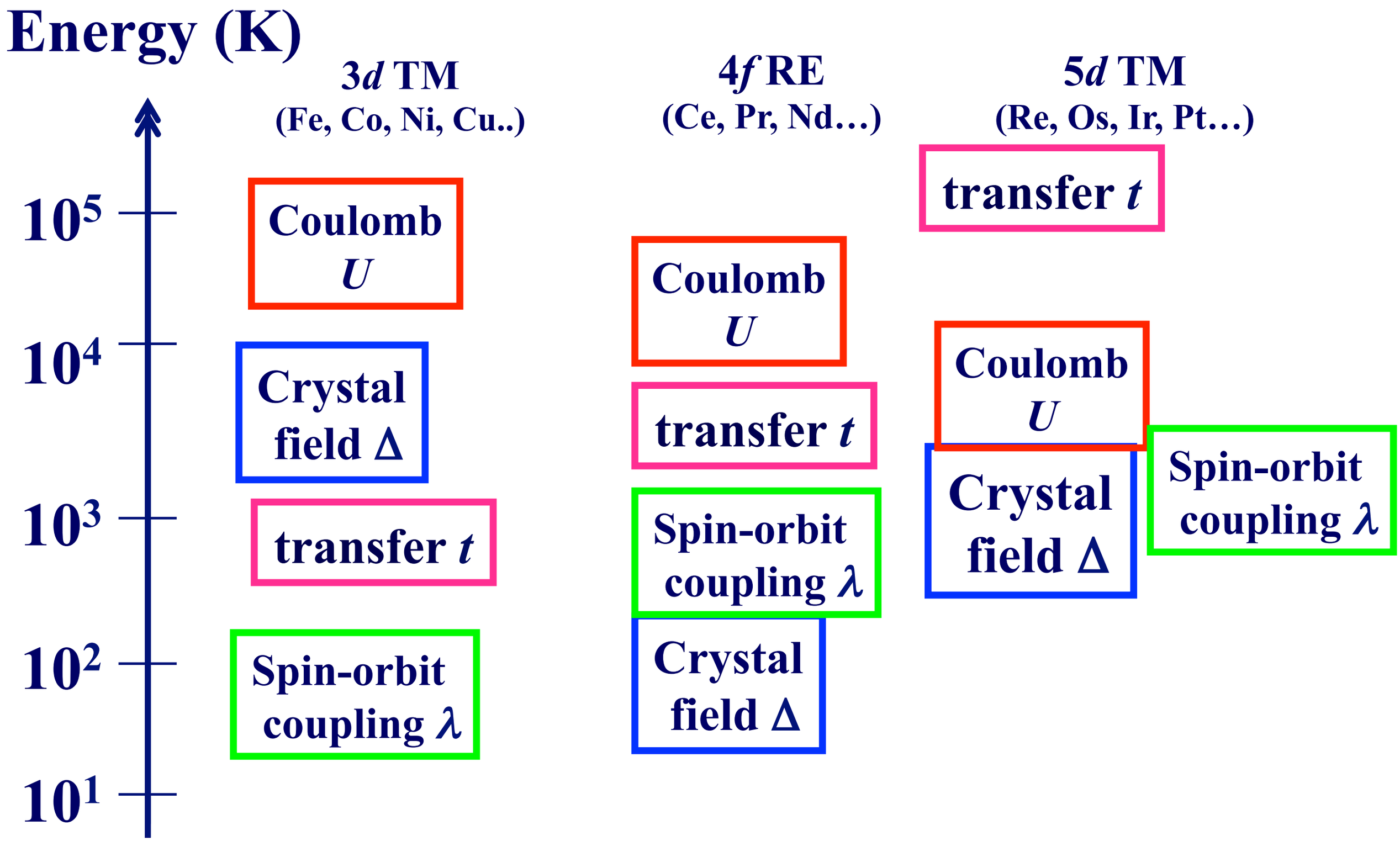
D.Pesin and L.Balents, Nature Physics (2010)





W. Witczak-Krempa, G. Chen, Y. B.Kim, L. Balents,
Annual Review of Condensed Matter Physics 2014

Energy scales



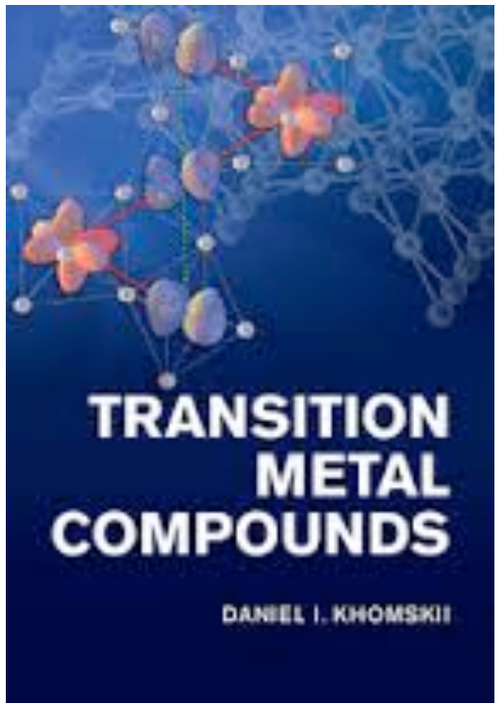
Outline

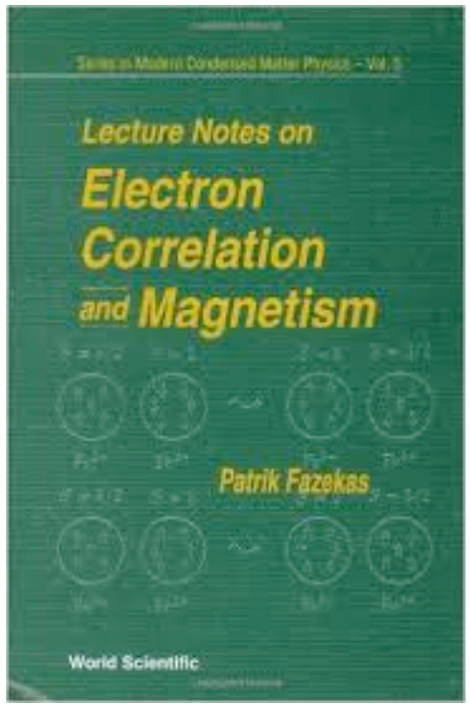
- Part 1: Basics of Mott insulators with orbital degrees of freedom

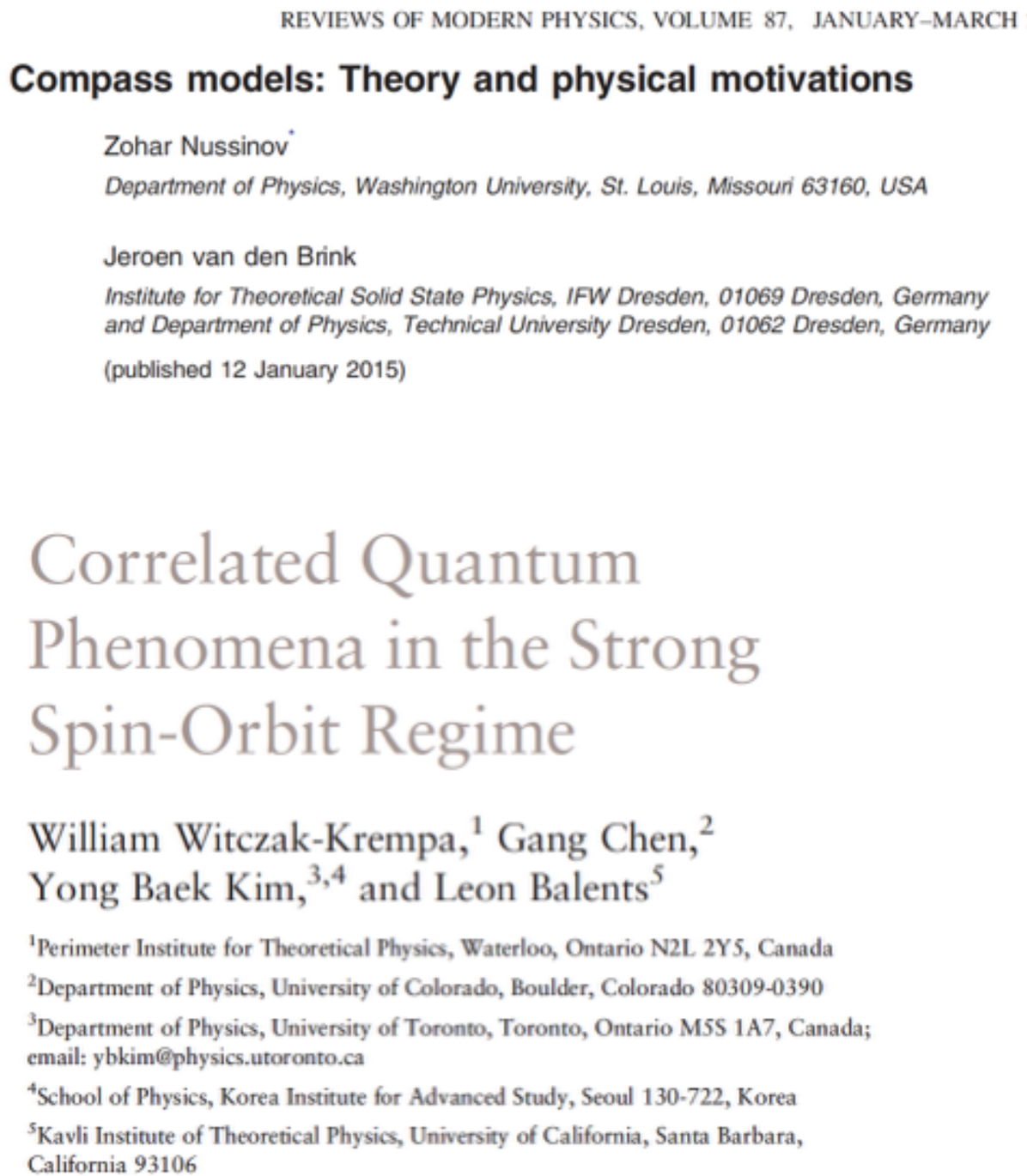
- Part 2: Magnetism in 3d transition metal oxides: weak spin-orbit coupling and strong electrostatic interactions

- Part 3: Magnetism in 4d and 5d transition metal oxides: strong spin-orbit coupling and weak electrostatic interaction

Books and reviews






REVIEWS OF MODERN PHYSICS, VOLUME 87, JANUARY–MARCH

Compass models: Theory and physical motivations

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(published 12 January 2015)

Correlated Quantum Phenomena in the Strong Spin-Orbit Regime

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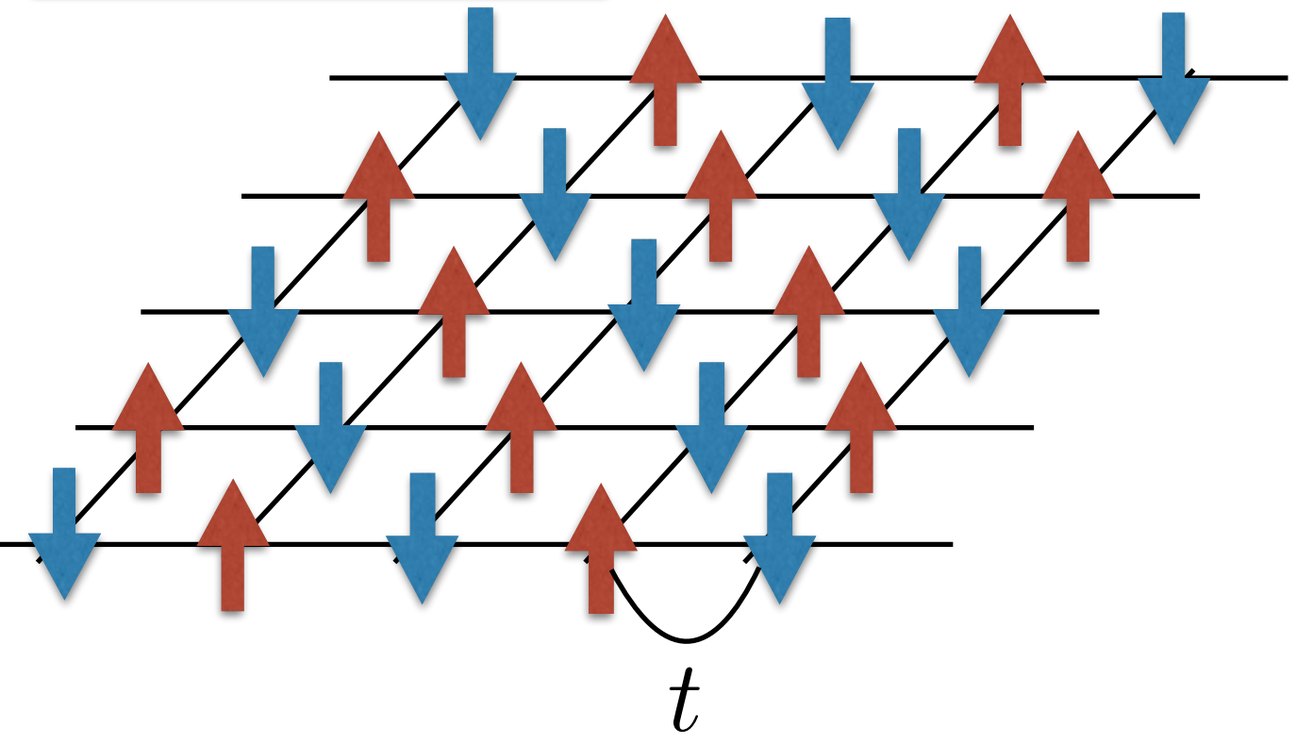
Part1: Basics

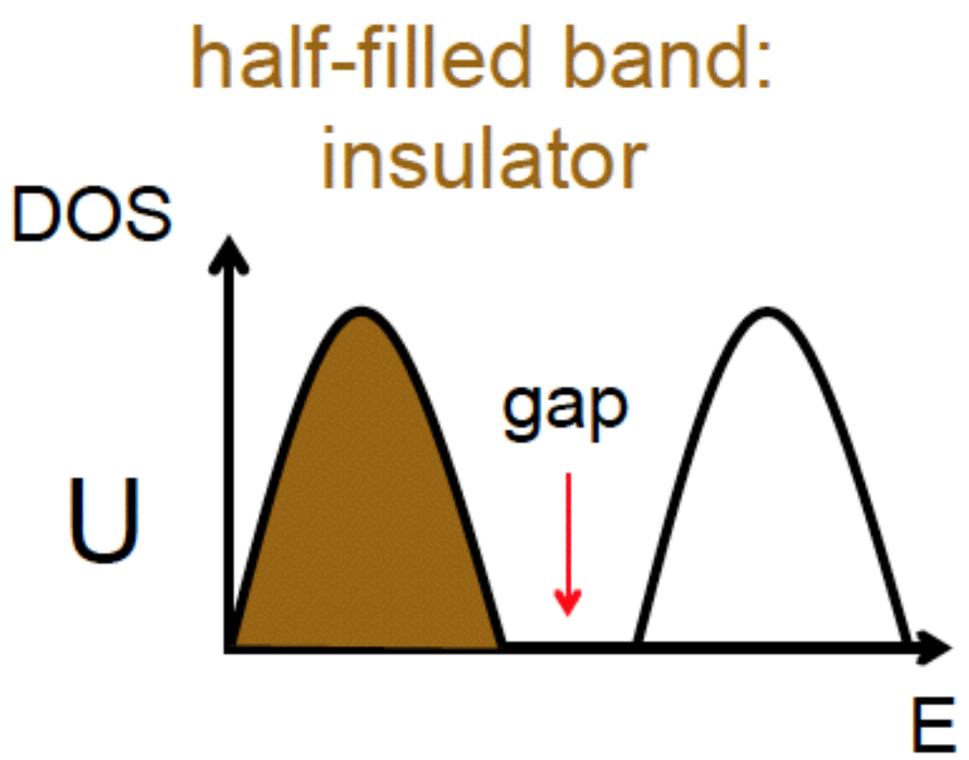
- Mott insulator
- Orbital degrees of freedom
- Multiorbital Hubbard Model
- Crystal field interactions
- Spin-orbit coupling

For details see lectures by Maurits Haverkort and Marco Grioni

Mott insulator

one electron per site



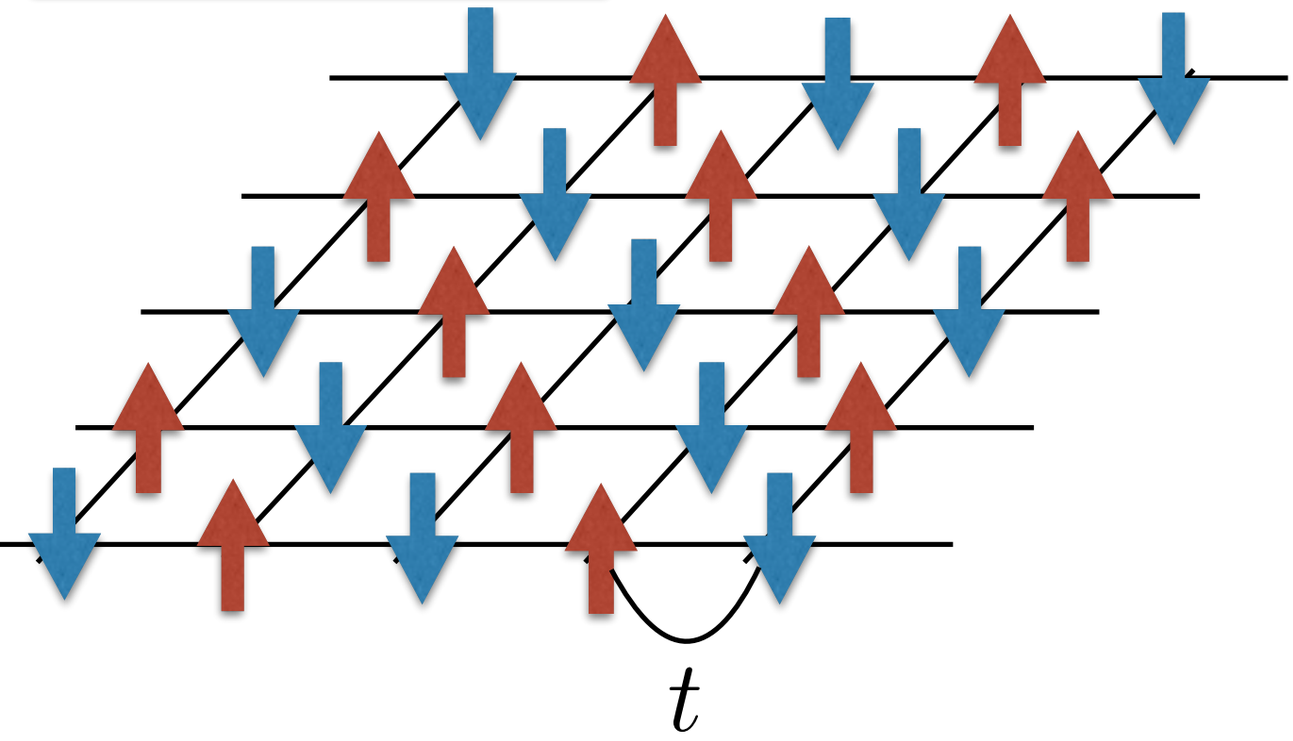


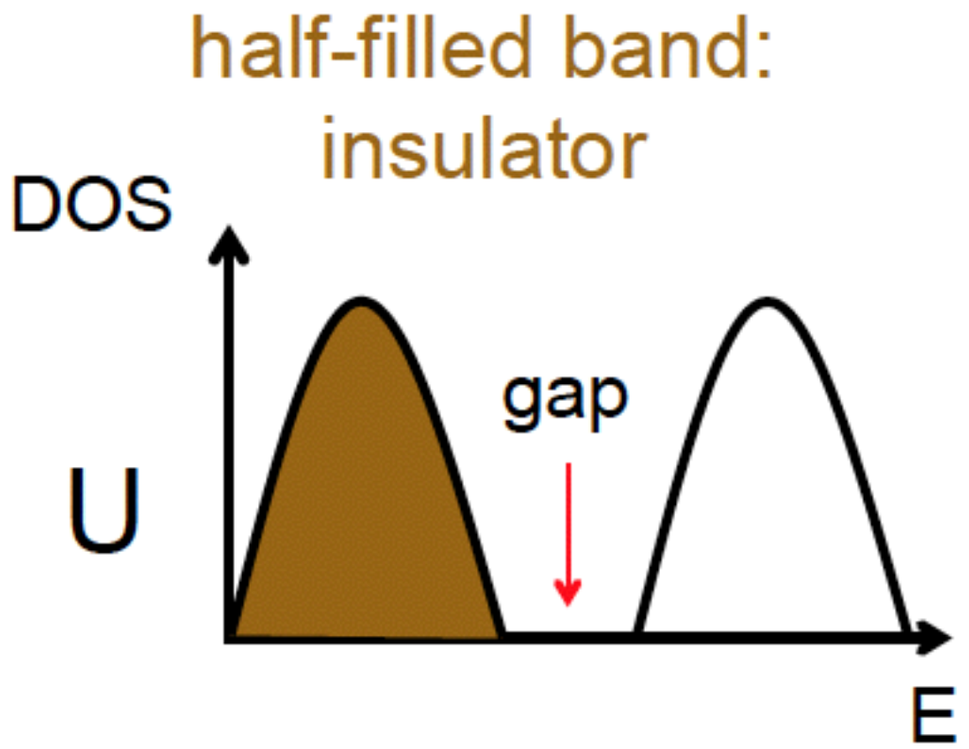
$$H_{\text{Hub}}^{\text{iso}} = \sum_{\langle ij\rangle,\alpha=\uparrow,\downarrow} t(c_{i\alpha}^{\dagger} c_{j\alpha} + \text{H.c.}) + U\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Coulomb repulsion U>>t Kinetic energy,
Charges become localized and gapped

Mott insulator

one electron per site



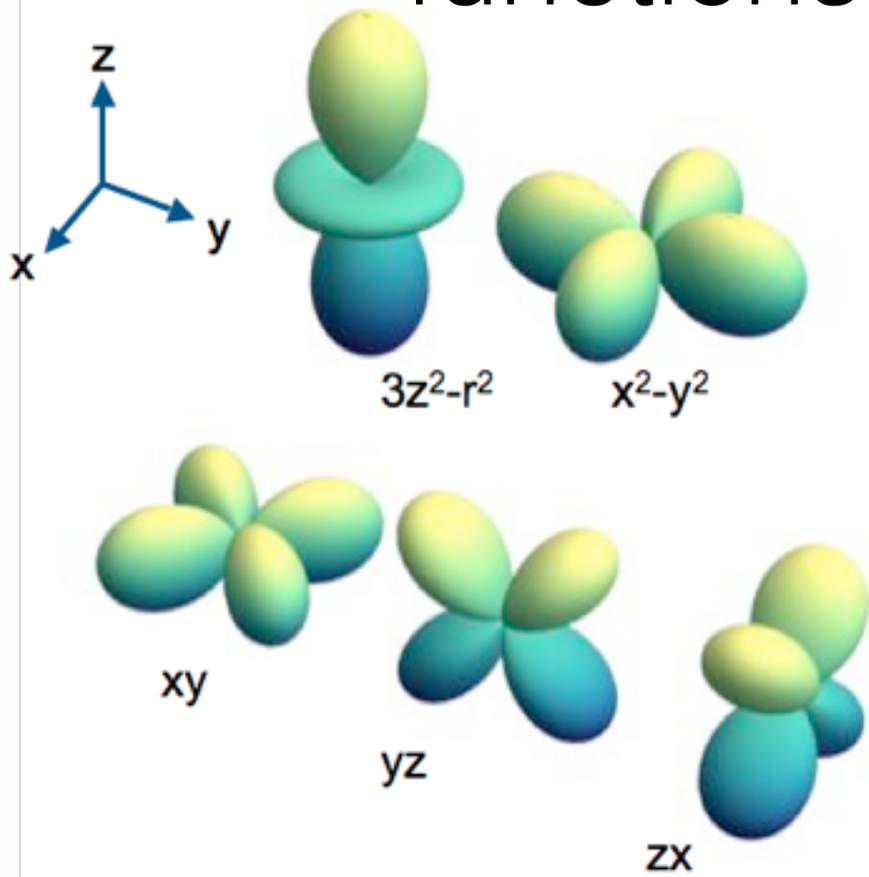


Even if in a Mott insulator, the electrons can hop between neighboring sites. This leads to the magnetic exchange between the spins of different electrons.

$$H = J \sum_{ij} \vec{S}_i \vec{S}_j \qquad J = \frac{4t^2}{U}$$

Orbital degrees of freedom

are already present in the electronic wave functions of the hydrogen atom



e_g

t_{2g}

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(2r/n)\cdot Y_l^m(\theta,\phi)$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1),$$

$$Y_2^1 = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi},$$

$$Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{i2\phi}.$$

e_g orbitals $\left\{ \begin{array}{c|c} Y_2^{-2} + Y_2^2 & x^2 - y^2, \\ \sqrt{2}Y_2^0 & (3z^2 - r^2)/\sqrt{3}, \end{array} \right.$

t_{2g} orbitals $\left\{ \begin{array}{c|c} Y_2^{-2} - Y_2^2 & xy, \\ Y_2^{-1} + Y_2^1 & yz, \\ Y_2^{-1} - Y_2^1 & zx, \end{array} \right.$

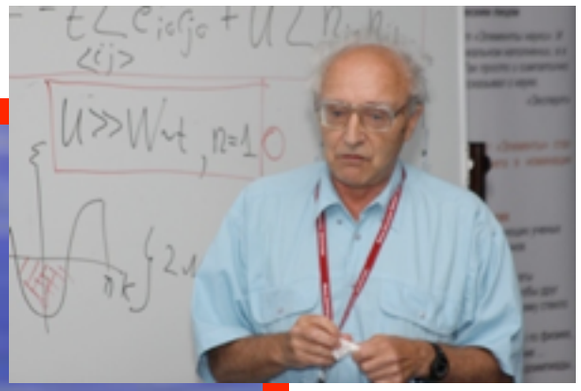
Multi-orbital Hubbard model

$$H_C = (U + 2J_H)\sum_{\boldsymbol{r},\alpha} n_{\boldsymbol{r},\alpha\uparrow} n_{\boldsymbol{r},\alpha\downarrow} - 2J_H \sum_{\boldsymbol{r},\alpha<\beta} \boldsymbol{S}_{\boldsymbol{r},\alpha} \cdot \boldsymbol{S}_{\boldsymbol{r},\beta}$$

$$+ (U - J_H/2) \sum_{\boldsymbol{r},\sigma,\sigma',\alpha<\beta} n_{\boldsymbol{r},\alpha\sigma} n_{\boldsymbol{r},\beta\sigma'}$$

$$+ J_H \sum_{\boldsymbol{r},\alpha,\beta} c^{\dagger}_{\boldsymbol{r},\alpha\uparrow} c^{\dagger}_{\boldsymbol{r},\alpha\downarrow} c_{\boldsymbol{r},\beta\downarrow} c_{\boldsymbol{r},\beta\uparrow}.$$

Note that U is strongly screened in a solid and depends on the polarizability of the ligands and the ligand coordination in a material. The magnetic interaction strength J_H instead is little screened.



Kugel-Khomskii model

Two degrees of freedom per site

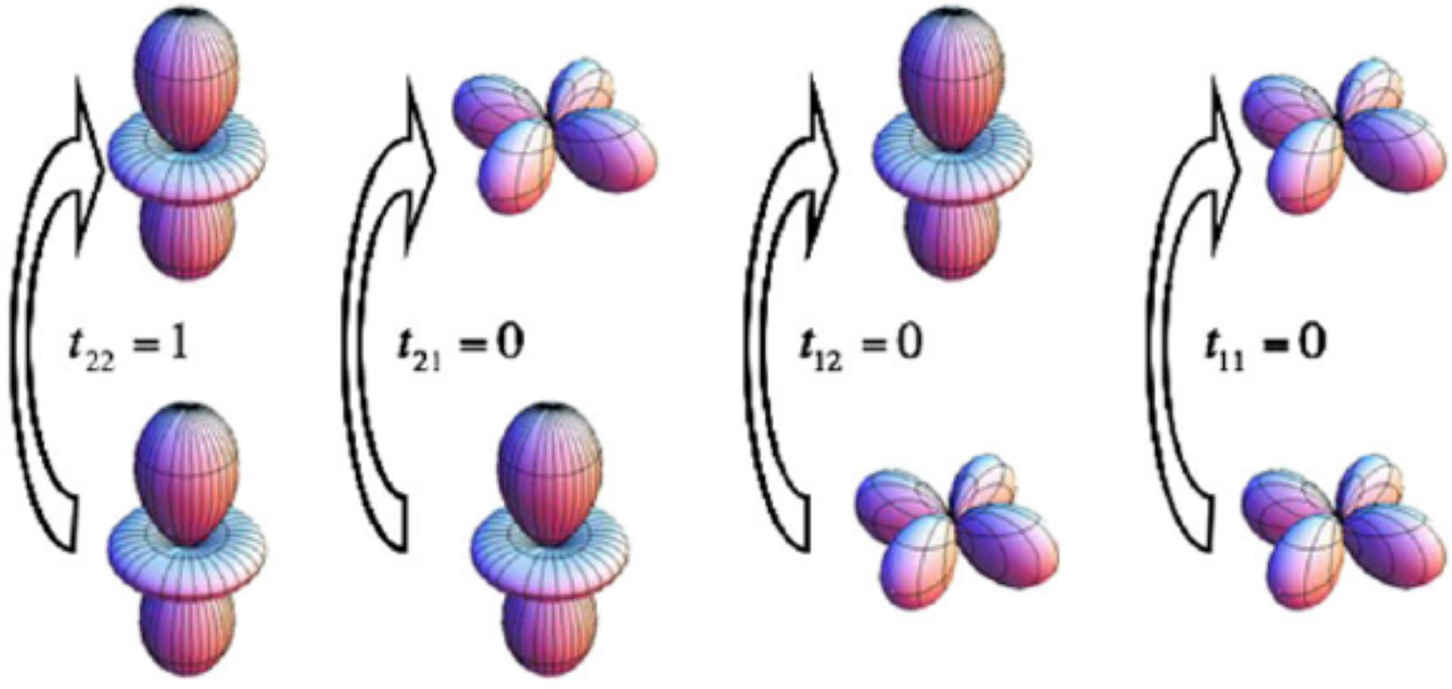
Spin

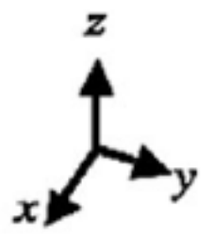
Pseudo-spin (orbital)

$$H = \sum_{i,j} J_{ij} \left(\vec{S}_i . \vec{S}_j \, K_1(\vec{\tau}_i, \vec{\tau}_j) + K_2(\vec{\tau}_i, \vec{\tau}_j) \right)$$

Anisotropic hopping

e_g-orbital hopping along z axis



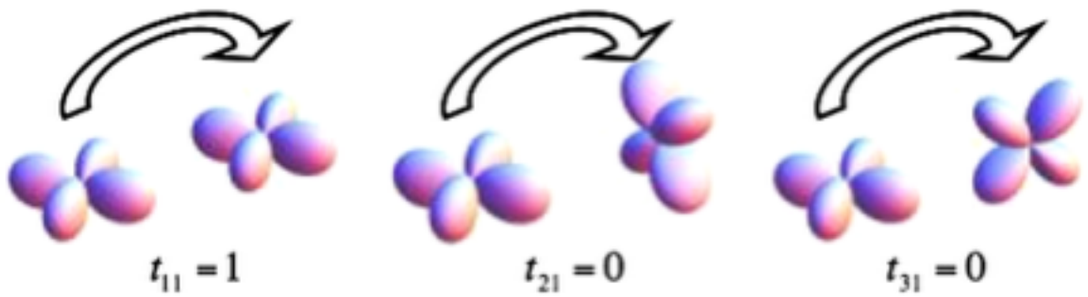


$$t^{\hat{z}}_{\alpha\beta} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Due to the symmetry, only hopping from one $3z^2 - r^2$ orbital to another $3z^2 - r^2$ one is allowed along the z direction. This fully specifies the hopping between orbitals on a cubic lattice.

Anisotropic hopping

t_{2g}-orbital hopping along



$$t^{\hat{x}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

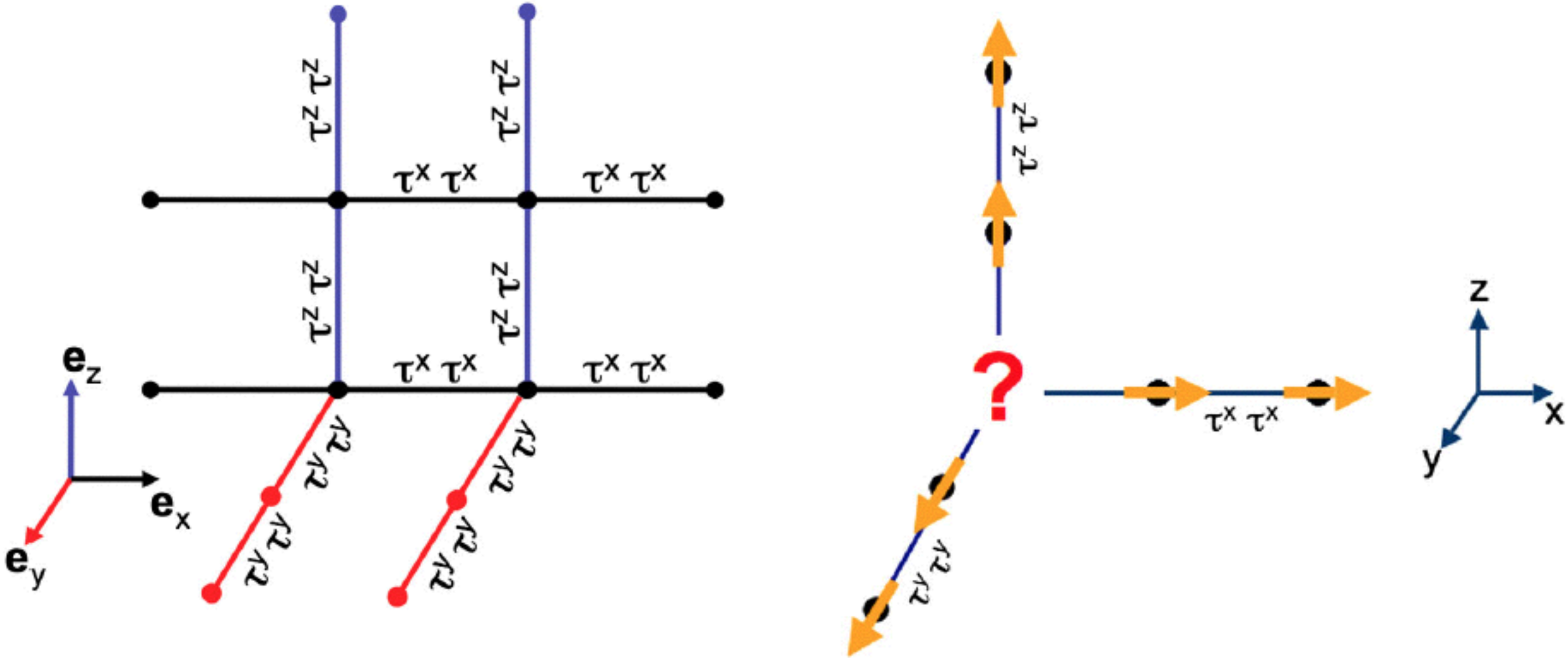
$$t^{\hat{y}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$t^{\hat{z}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The hopping matrix is diagonal: orbital flavor is conserved in the hopping process. Moreover, along the x axis the hopping between yz orbitals vanishes.

Compass orbital models

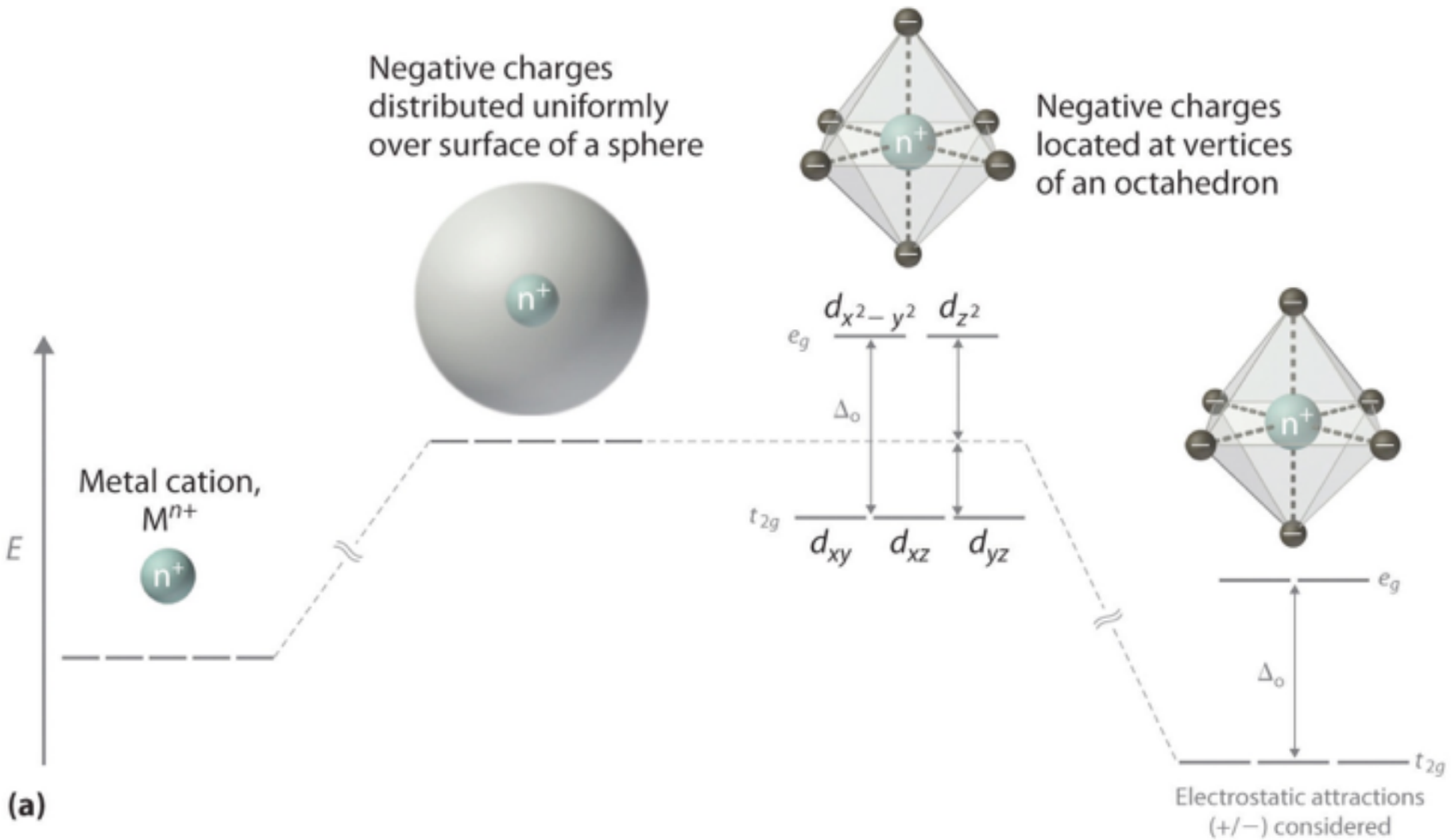
$$H_{3\square}^{90^\circ} = -J \sum_{\boldsymbol{r}} \left(\tau_{\boldsymbol{r}}^x \tau_{\boldsymbol{r}+\boldsymbol{e}_x}^x + \tau_{\boldsymbol{r}}^y \tau_{\boldsymbol{r}+\boldsymbol{e}_y}^y + \tau_{\boldsymbol{r}}^z \tau_{\boldsymbol{r}+\boldsymbol{e}_z}^z \right)$$



Z. Nussinov, J. van der Brink, RMP 2015

Crystal field interactions

Crystal field is purely electrostatic metal–ligand interaction between negative point charge distribution around the positive cation of metal ion.

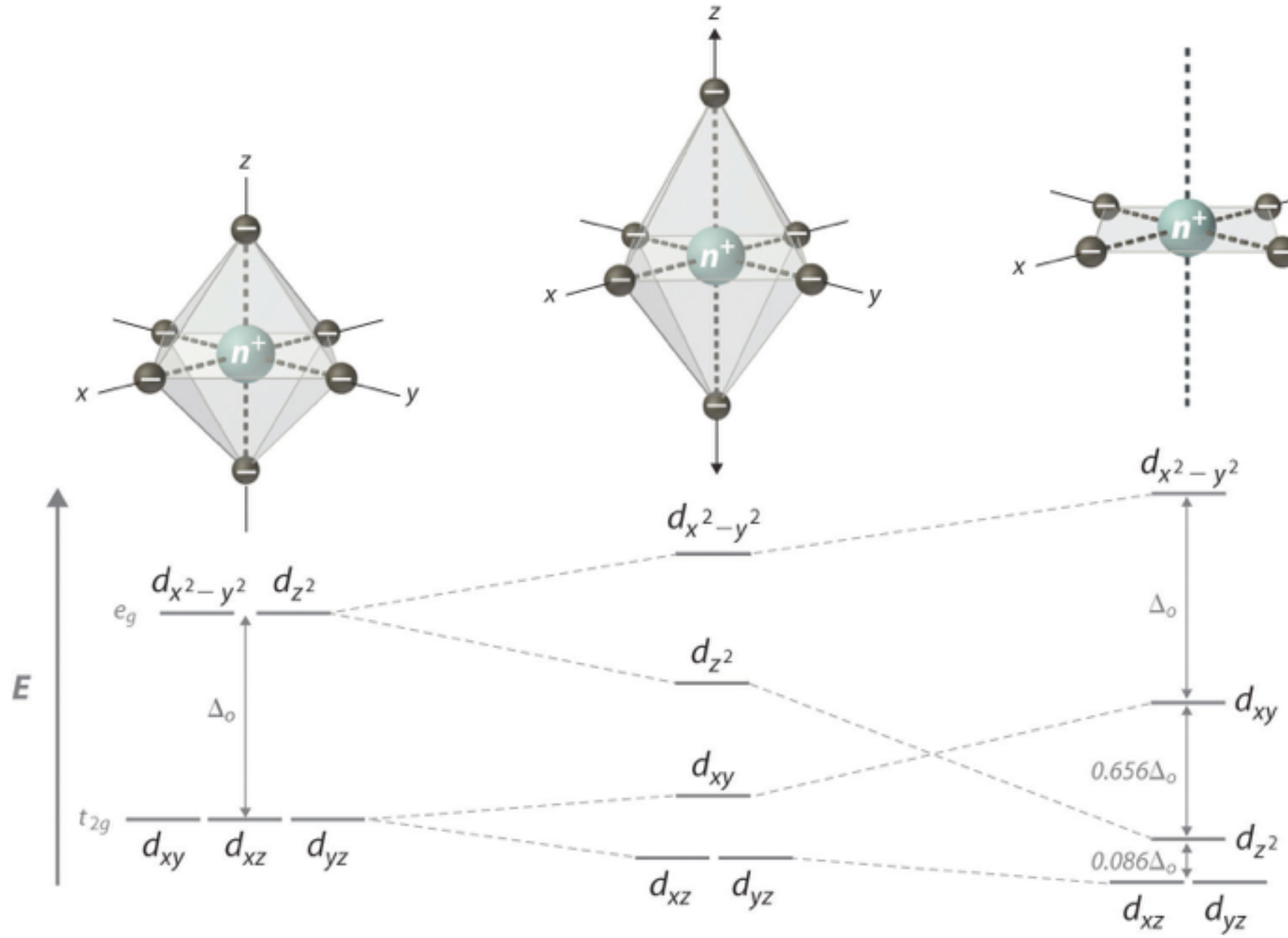


Bethe(1929) and VanVleck (1932)

Crystal field breaks orbital degeneracy in transition metal complexes due to the presence of ligands.

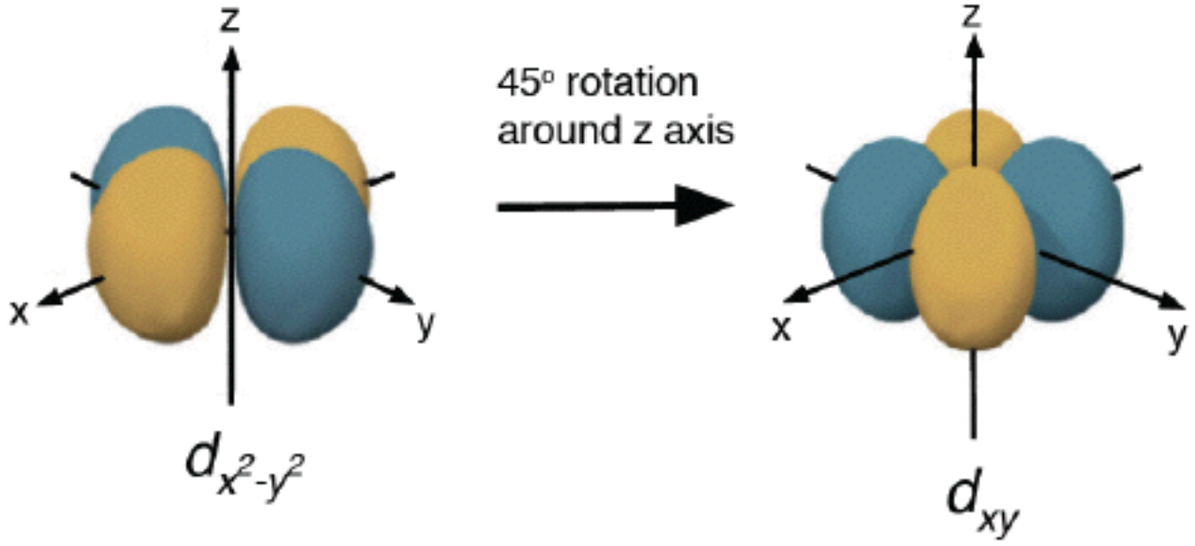
Further splitting…

Moving the two axial ligands away from the metal ion along the z axis initially generates an elongated octahedral complex and eventually produces a square planar complex.



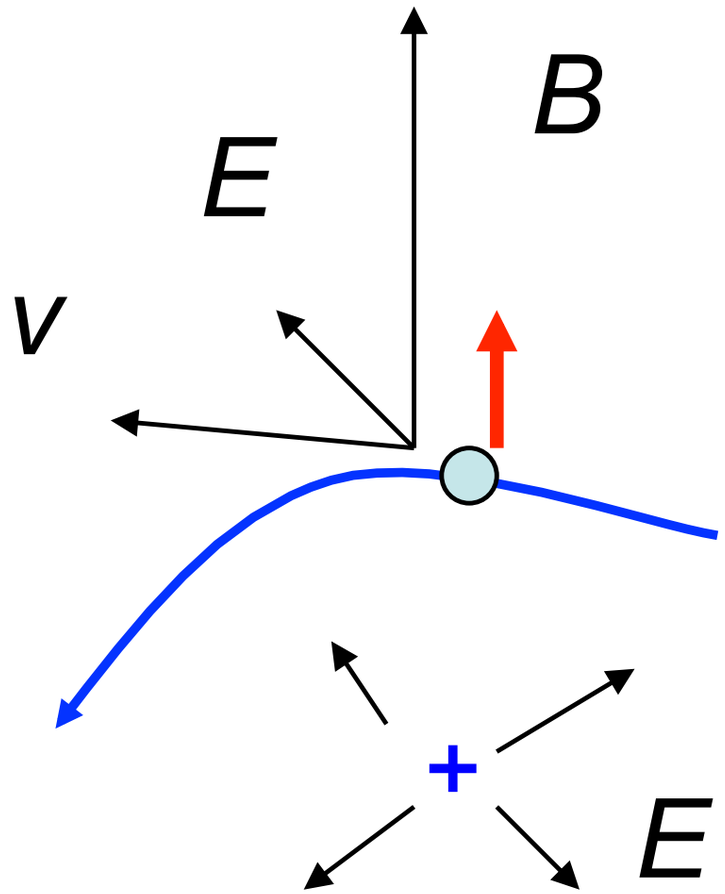
Quenching of orbital angular momentum

If an orbital can be transformed into another degenerate orbital (same energy) by a rotation, it is considered to contribute to the electronic angular momentum.
For example, an electron moving from x^2-y^2 orbital to xy orbital corresponds to orbital motion about the z axis.



If, however, there is an energy cost associated with this transformation, we say that the orbital angular momentum L has been **quenched** and will not contribute to the total magnetic moment. The time average is <L>=0.

Origin of the relativistic spin-orbit coupling



In a frame associated with the electron:

$$\mathbf{B} = \frac{1}{c}\mathbf{E} \times \mathbf{v} = \frac{1}{mc}\mathbf{E} \times \mathbf{p}$$

Zeeman energy in the orbital field:

$$\hat{H} = \frac{\mu_B}{mc}\vec{\sigma}\bullet(\mathbf{E} \times \hat{\mathbf{p}}) = -\frac{i\hbar^2}{2m^2c^2}\vec{\sigma}\bullet(\vec{\nabla}V \times \nabla)$$

Full relativistic treatment: 1/c expansion of the Dirac equation

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + eV}_{\text{non-relativistic}} + \underbrace{\frac{\hat{p}^4}{8m^2c^2}}_{\text{K.E. correction}} + \underbrace{\frac{\hbar^2}{8m^2c^2}\nabla^2 V}_{\text{Darwin term}} + \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma}\bullet(\vec{\nabla}V \times \hat{\mathbf{p}})}_{\text{SOI}}$$

Smaller by a factor of 2
("Thomas' factor of two", 1926)
Reason: non-inertial frame

All three correction terms are of the same order

Lecture by Maurits Haverkort

How big is spin-orbit coupling constant? SOC ~ Z^?

QUANTUM MECHANICS

NON-RELATIVISTIC THEORY

by

L. D. LANDAU AND E. M. LIFSHITZ

calculate the energy, average it with respect to the unperturbed state. The main contribution to the energy is given by distances close to the nucleus, of the order of the Bohr radius ($\sim \hbar^2/Zme^2$) for a nucleus with charge Ze. In this region the field of the nucleus is almost unscreened and the potential energy is

$$|U(r)| \sim Ze^2/r \sim Z^2me^4/\hbar^2,$$

so that

$$\alpha \sim \hbar^2 U/m^2c^2r^2$$

$$\sim Z^4(e^2/\hbar c)^2me^4/\hbar^2.$$

The mean value of α is obtained by multiplying by the probability w of finding the electron near the nucleus. According to (71.3), $w \sim Z^{-2}$, so that we have finally that the energy of the spin–orbit interaction of the electron is given by

$$\bar{\alpha} \sim \left(\frac{Ze^2}{\hbar c}\right)^2 \frac{me^4}{\hbar^2},$$

i.e. differs from the fundamental energy of the outer electrons in the atom ($\sim me^4/\hbar^2$) only by the factor $(Ze^2/\hbar c)^2$. This factor increases rapidly with the atomic number, and reaches values of the order of unity in heavy atoms.

order of magnitude estimate

$$\mathcal{E}_{so} \sim \frac{\hbar}{m^2c^2} p \frac{V}{r} \sim \frac{\hbar^2}{m^2c^2} \frac{V}{r^2}$$

$$V \sim \frac{Ze^2}{r}, \quad r \sim \frac{a_B}{Z} = \frac{\hbar^2}{Zme^2}$$

$$\mathcal{E}_{so} \sim \frac{\hbar^2}{m^2c^2} \frac{Ze^2}{r^3} = Z^4 \left(\frac{e^2}{\hbar c}\right)^2 \frac{me^4}{\hbar^2}.$$

This needs to be multiplied by the probability to find an electron at distance r from the nucleus $= |\Psi(r)|^2 r^3$.

WKB wavefunction in atomic units ($a_B = 1$, $me^4/\hbar^2 = 1$)

$r \sim 1/Z$; $v \sim Z/r$, $V|_{r \sim 1/Z} \sim Z^2$.

$$|\Psi| \sim \frac{1}{r\sqrt{p}} \sim \frac{1}{r|V|^{1/4}} \sim \frac{Z}{(Z^2)^{1/4}} \sim \sqrt{Z}$$

$$|\Psi|^2 r^3 \sim Z \frac{1}{Z^3} \sim \frac{1}{Z^2}.$$

Typical energy of SO interaction

$$\mathcal{E}_{so} \cdot \frac{1}{Z^2} \sim \left(\frac{Ze^2}{\hbar c}\right)^2 \left(\frac{me^4}{\hbar^2}\right)$$

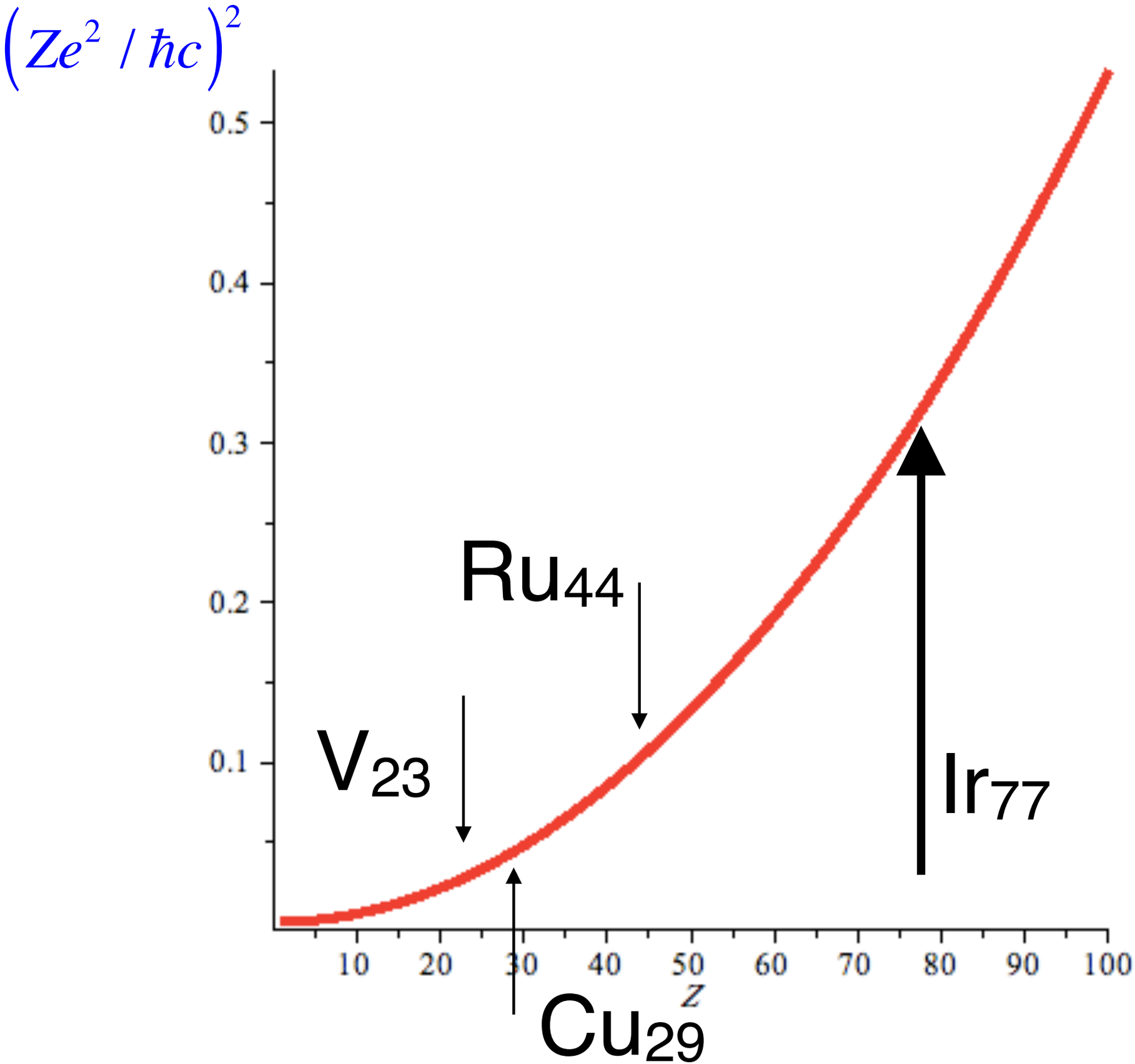
~ 10 eV

$$\frac{Ze^2}{\hbar c} = \frac{Z}{137}$$

^{92}U : $\left(\frac{Z}{137}\right)^2 = 0.45$

Acknowledge D.Maslov & D.Khomskii

Spin-orbit coupling constant



Light atoms: Russel-Saunders coupling

The spin-orbit coupling is a weak perturbation with respect to electrostatic interaction between spins and orbital moments.

First the total spin and the total orbital momentum are combined separately, the the weak spin orbit coupling split each term in a fine structure labeled by J.

$$\vec{L} = \sum_{i=1}^{Z} \vec{l}_i \qquad \vec{S} = \sum_{i=1}^{Z} \vec{s}_i$$

$$\vec{J} = \vec{L} + \vec{S}$$

Heavy atoms: j-j coupling

The spin-orbit coupling is strong with respect to electrostatic interaction between spins and orbital moments.

For each electron, its spin and orbital moments are coupled separately, and then the weaker electrostatic interaction couples the individual total magnetic moments.

$$\vec{j}_i = \vec{l}_i + \vec{s}_i \qquad \vec{J} = \sum_{i=1}^{Z} \vec{j}_i$$