From Models to Materials: Simulation of Strongly Correlated Electron Systems

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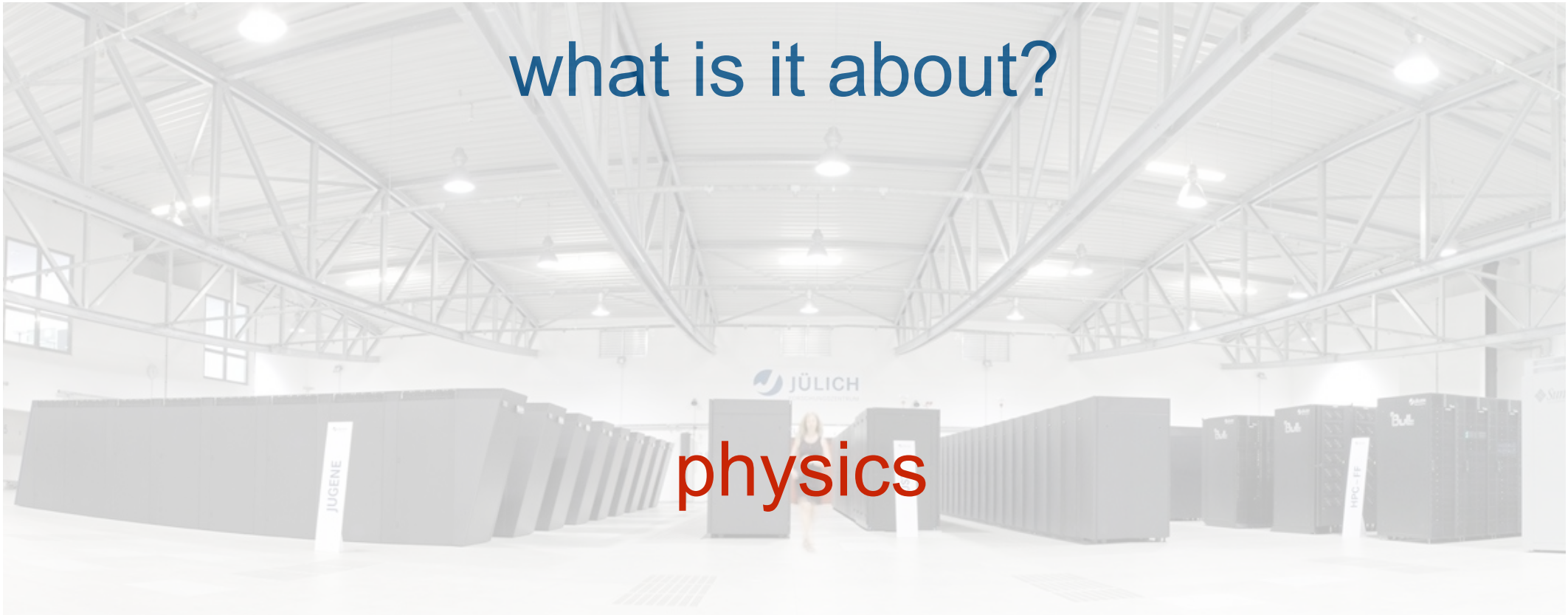
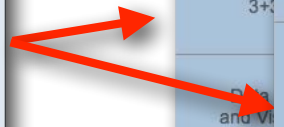

what is it about?
physics

simulation science master

+ alternative focus area

1st Semester (Winter) 30 CP	2nd Semester (Summer) 30 CP	3rd Semester (Winter) 30 CP	4th Semester (Summer) 30 CP
Numerical Methods for Partial Differential Equations 4+2, 8 CP	Fast Iterative Solvers 2+1, 4CP	SiSc Laboratory 0+3, 6 CP	Master's Thesis 27 CP
	Parallel Computing in Simulation Sciences 3+2, 6 CP	Elective Courses 24 CP	
From Molecular to Continuum Physics I 3+2, 6 CP	From Molecular to Continuum Physics II 3+2, 5 CP		
Applied Quantum Mechanics 3+3, 6 CP	Model Based Estimation Methods 2+2, 5 CP		
Data Analysis and Visualization 2+1, 4 CP	Elective Courses 10 CP		
Parallel Programming I 3+2, 6 CP			Master's Colloquium 3 CP



Simulations in Engineering

Numerical Methods for Partial Differential Equations 4+2

Fast Iterative Solvers 2+1, 4CP

SiSc Laboratory 0+3, 6 CP

Simulations in Physics

Numerical Methods for Partial Differential Equations 4+2, 8 CP	Fast Iterative Solvers 2+1, 4CP	SiSc Laboratory 0+3, 6 CP	Master's Thesis 27 CP
	Parallel Computing in Simulation Sciences 3+2, 6 CP	Elective Courses 24 CP	
From Molecular to Continuum Physics I 3+2, 6 CP	materials		
Applied Quantum Mechanics 3+3, 6 CP	many-body		
Data Analysis and Visualization 2+1, 4 CP	Elective Courses 10 CP		
Parallel Programming I 3+2, 6 CP			Master's Colloquium 3 CP

SiSc Seminar

simulation science master

focus area: physics

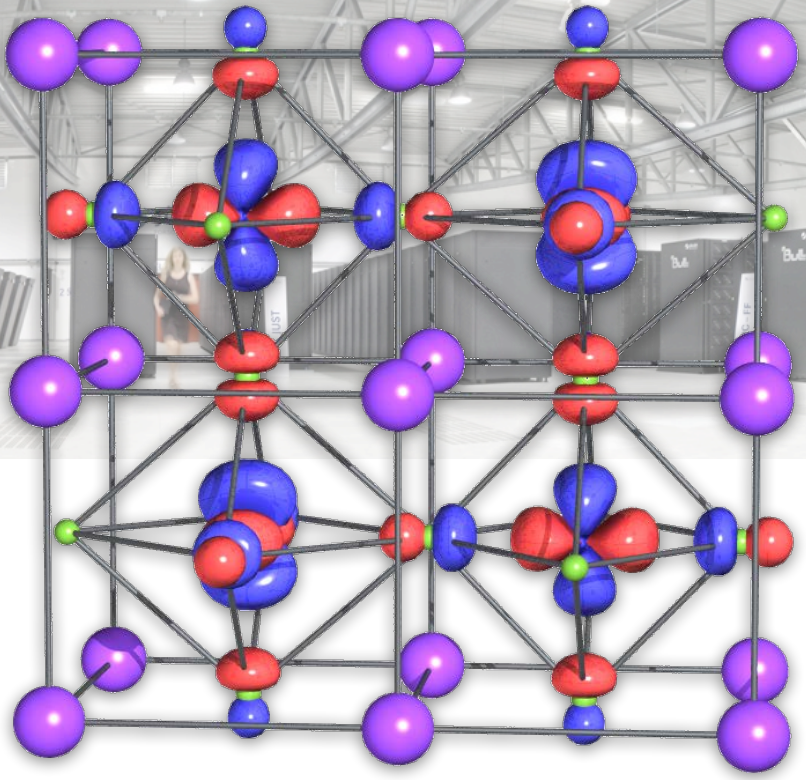
lectures

WS	quantum mechanics
SS	computational many-body theory
	correlated systems
WS	symmetries in many-body problem

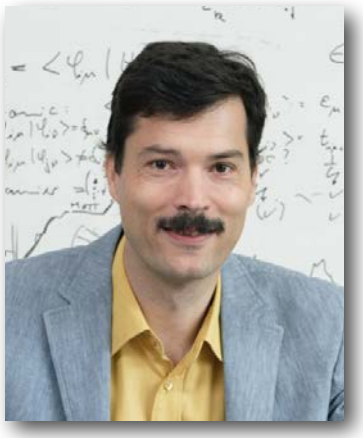
physics of strongly-correlated systems

http://iffwww.iff.kfa-juelich.de/~pavarini/group.html

http://www.grs-sim.de/research/computational-materials-science/team/koch.html



Erik Koch



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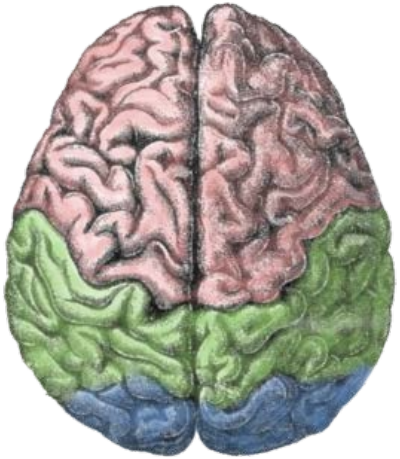
what it the aim?

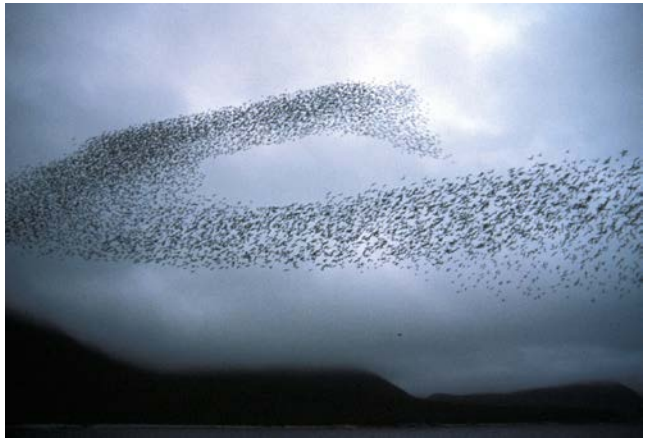
understand emergent phenomena
in electronic systems

emergence around you

human brain



flocking



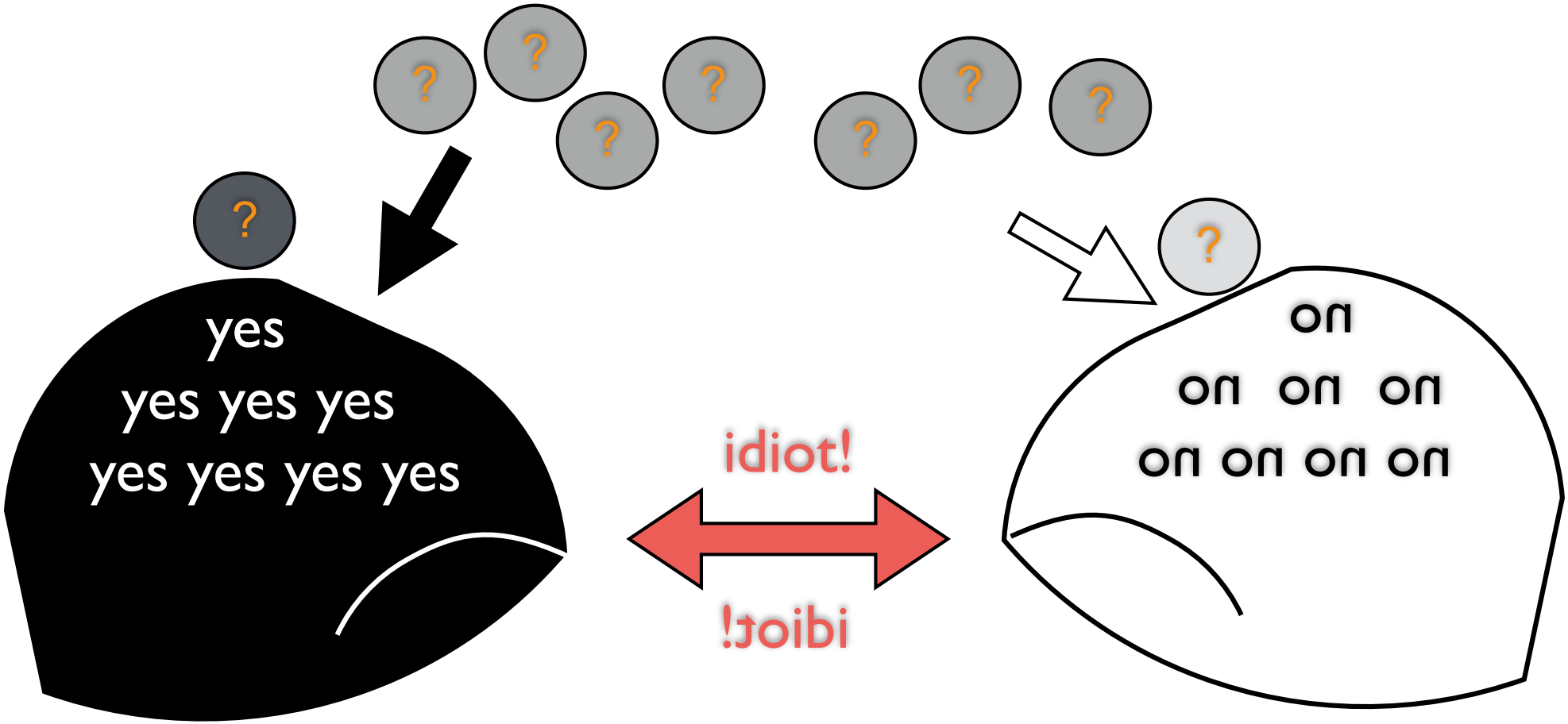
sand dunes

traffic jam

(photos from wikipedia)

emergence in social media

formation of polarized opinion-bubbles



opinions vs information

the earth is flat! alternative *facts*

emergence in physics

phase transitions

ferromagnetism

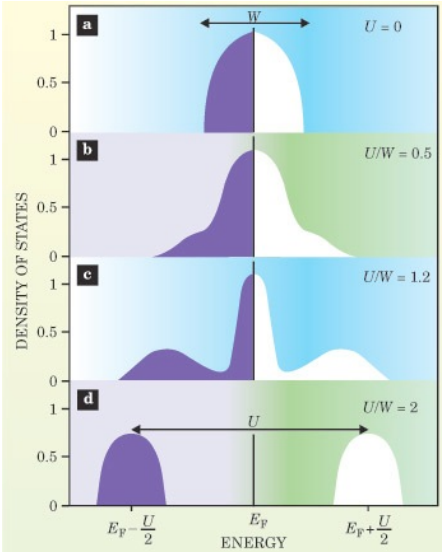
Fe_3O_4 **Magnetite**

T_C=858 K

1000 BC ?

photo from wikipedia

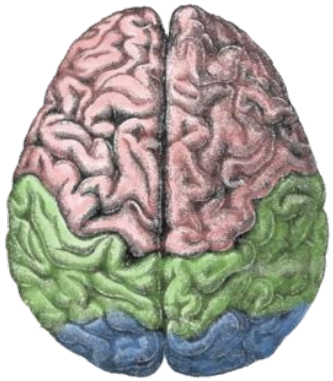
Mott metal-insulator transition



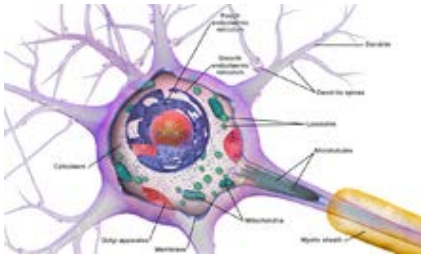
G. Kotliar and D. Vollhardt,
Physics Today **57,** 53 (2004)

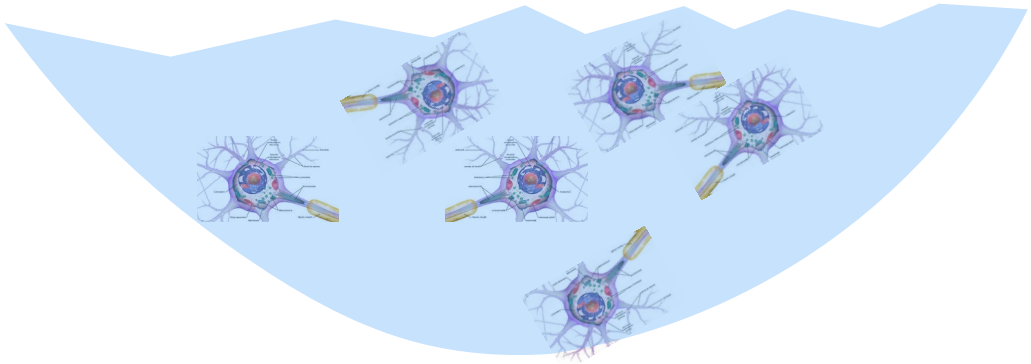
cannot be described in *independent component* picture

human brain



is different from N non-interacting neurons swimming in an average see of information





(photos from wikipedia)

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emergent phenomena arise from strong correlations

what are strong correlations?

when simple interactions among many particles lead to co-operative behavior

more is different

The main fallacy in this kind of thinking is that the reductionist hypothesis does not by any means imply a "constructionist" one: The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe. In fact, the more the ele-

Philip Warren Anderson

Nobel Prize in Physics 1977

4 August 1972, Volume 177, Number 4047 **SCIENCE** **(1972)**

the classical N body problem

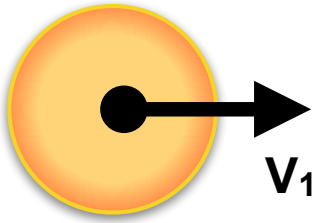
(physics/engineering bachelor)

the classical case

1-body, no interaction

$$E = \frac{1}{2} m_1 \dot{\mathbf{r}}_1^2$$

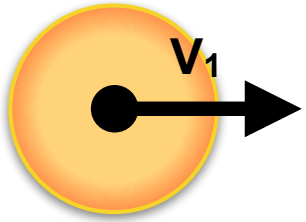
$$m_1 \ddot{\mathbf{r}}_1 = 0$$



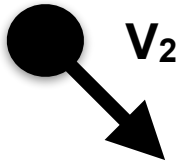
2-bodies, no interaction

$$E = \frac{1}{2} m_1 \dot{\mathbf{r}}_1^2 + \frac{1}{2} m_2 \dot{\mathbf{r}}_2^2$$

$$m_1 \ddot{\mathbf{r}}_1 = 0$$

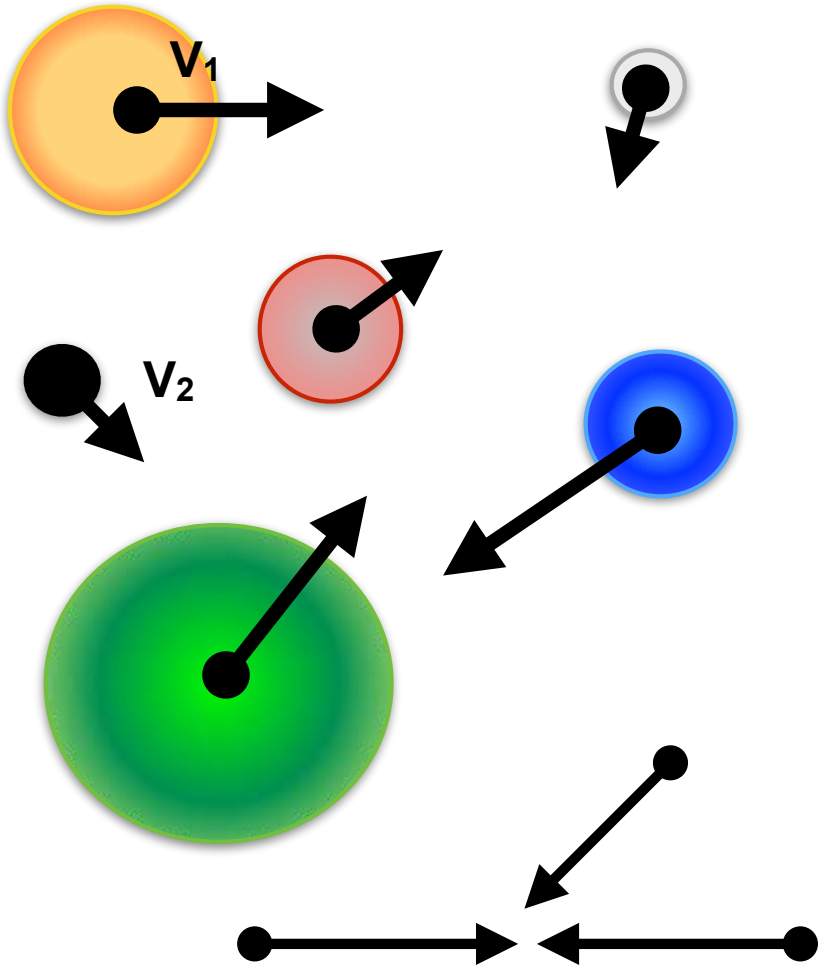


$$m_2 \ddot{\mathbf{r}}_2 = 0$$

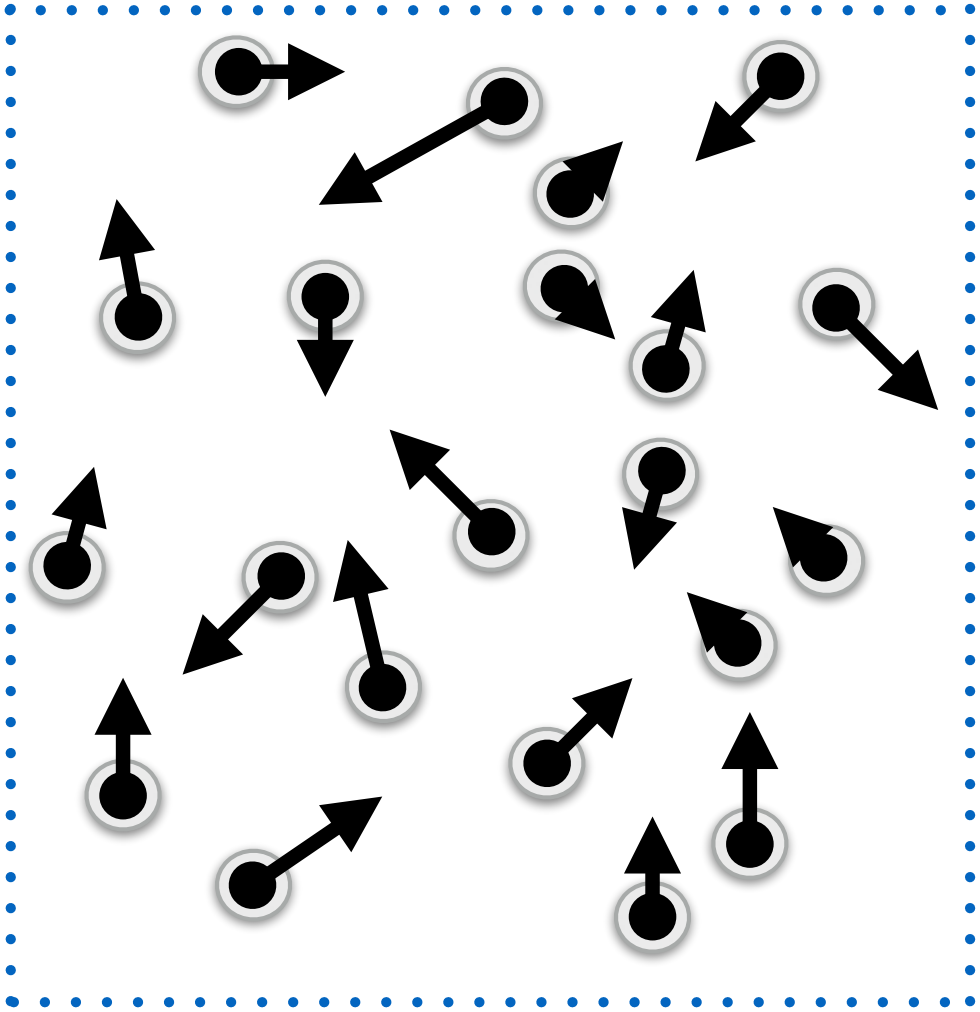


N-bodies, no interaction

$$E = \sum_i \frac{1}{2} m_i \dot{\mathbf{r}}_i^2$$

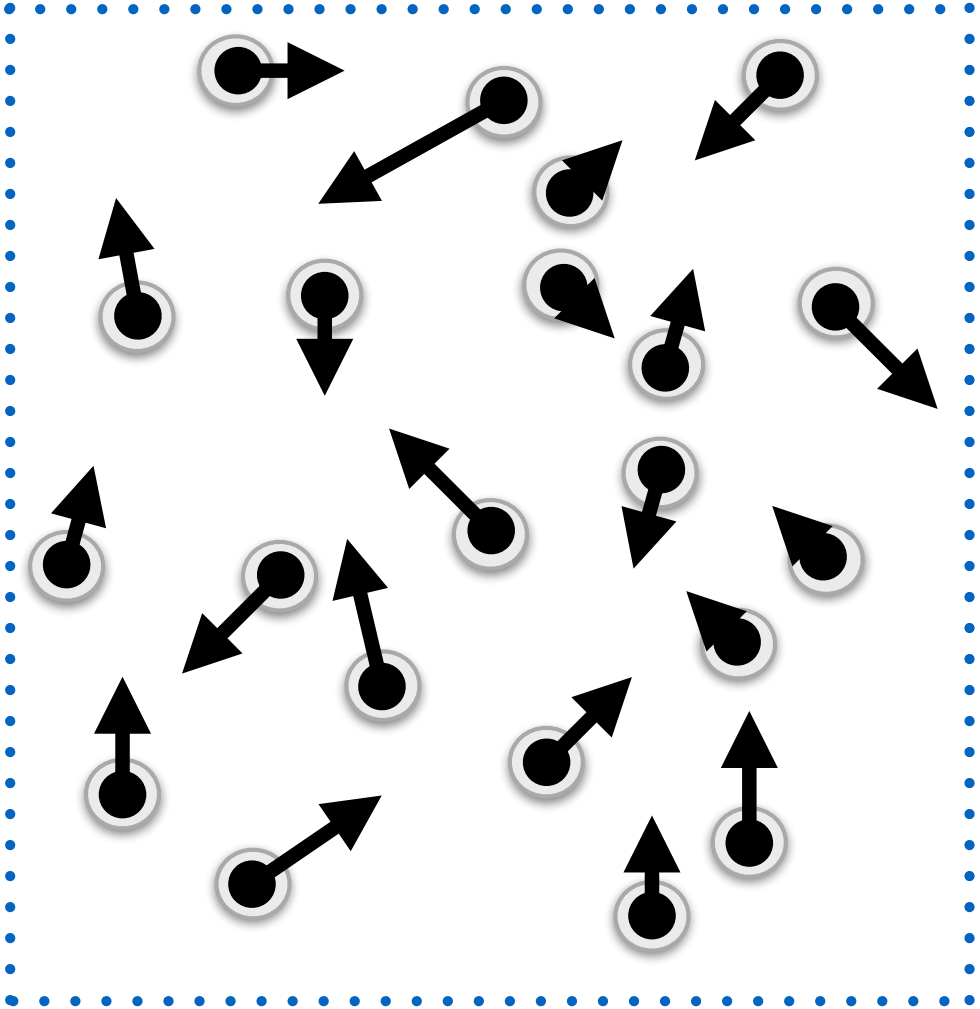


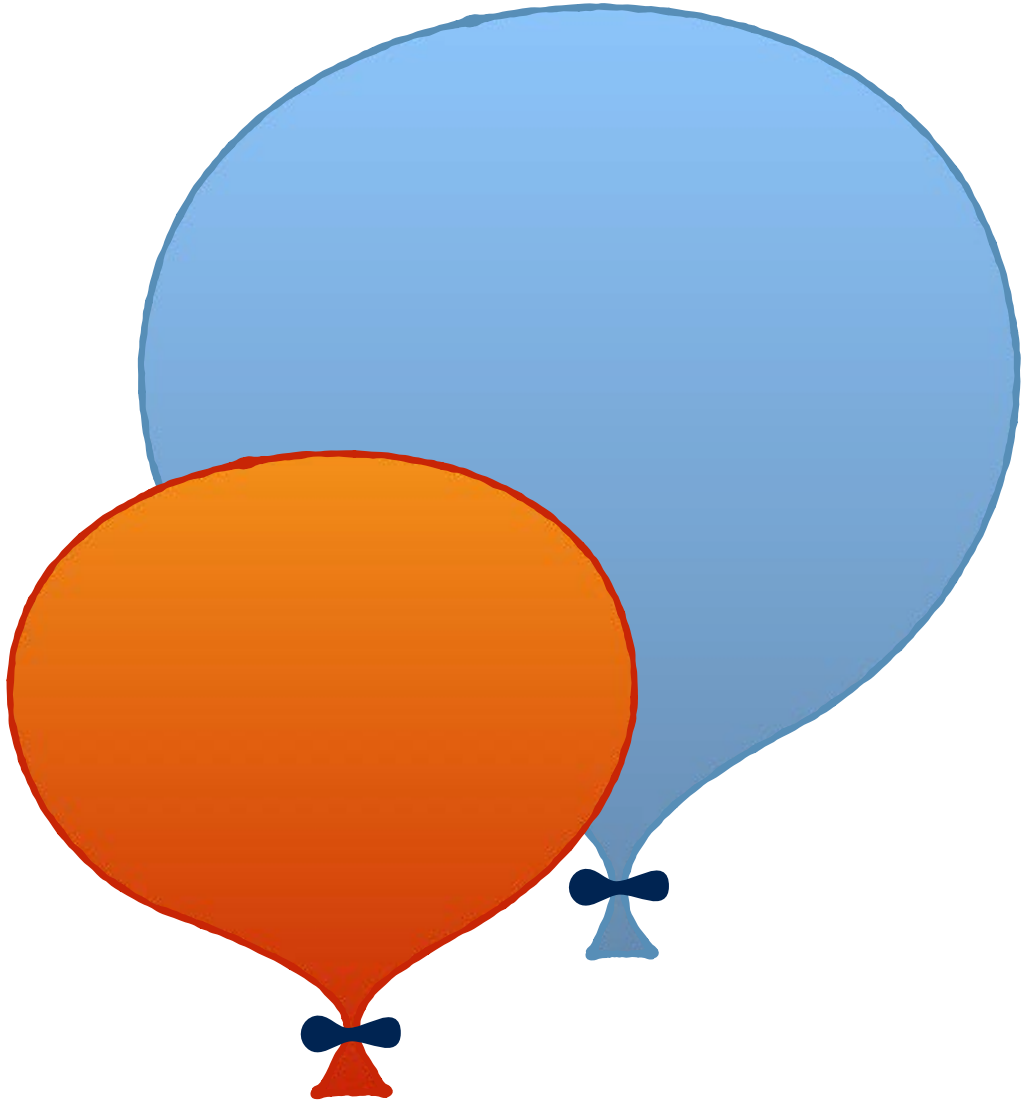
$PV=Nk_BT$



ideal gas

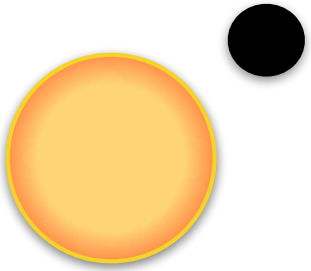
$PV=Nk_BT$



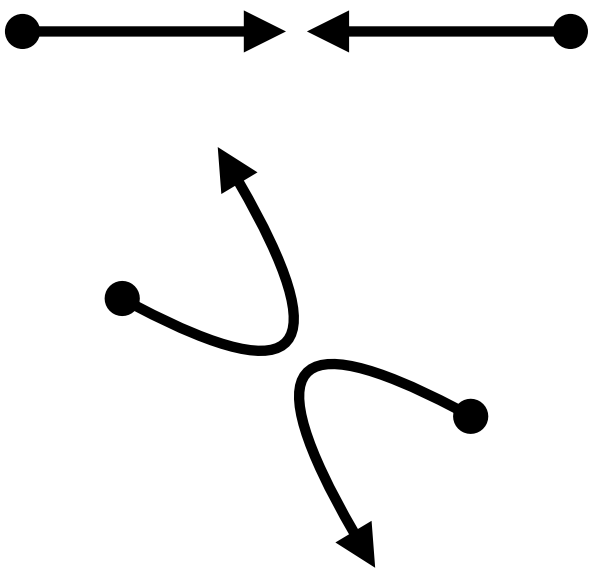


interacting classical 2-body problem

two bodies: analytically solvable problem



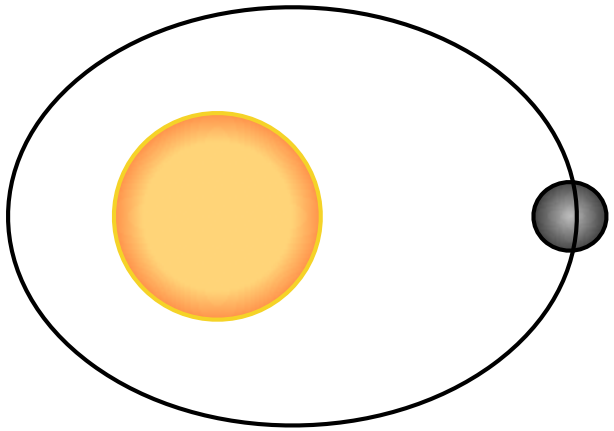
$$\begin{cases} m_1 \ddot{\mathbf{r}}_1 = \mathbf{F}_{12} \\ m_2 \ddot{\mathbf{r}}_2 = \mathbf{F}_{21} \end{cases}$$



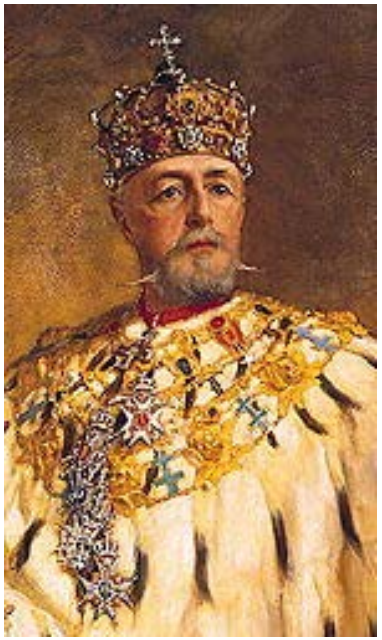
center of mass and relative coordinates

$$\mathbf{R} = \frac{\mathbf{r}_1 m_1 + \mathbf{r}_2 m_2}{m_1 + m_2} \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$M = m_1 + m_2 \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$



classical 3-body problem



Oscar II's Prize Competition and the Error in Poincaré's Memoir on the Three Body Problem

JUNE BARROW-GREEN

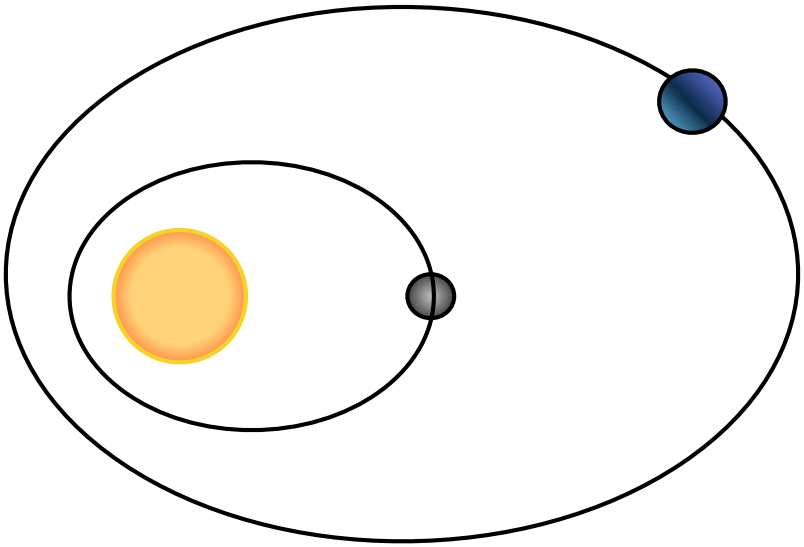
Communicated by JESPER LÜTZEN

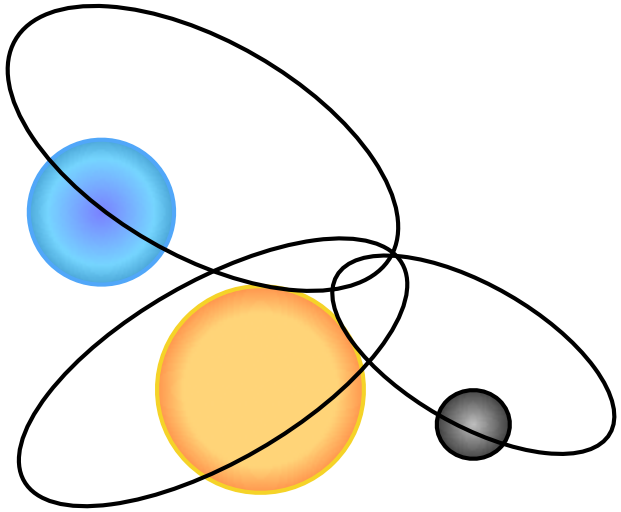
Introduction

In the autumn of 1890 HENRI POINCARÉ's memoir on the three body problem [1] was published in the journal *Acta Mathematica* as the winning entry in the international prize competition sponsored by OSCAR II, King of Sweden and Norway, to mark his 60th birthday on January 21, 1889. Today POINCARÉ's published memoir is renowned both for providing the foundations for his celebrated three-volume *Méthodes Nouvelles de la Mécanique Céleste* [2] and for containing the first mathematical description of chaotic behavior in a dynamical system.

interacting classical 3-body problem

chaotic behavior is possible





butterfly effect: behavior highly sensitive to initial conditions

the present determines the future,
but the approximate present does not approximately determine the future
(Edward Lorenz)

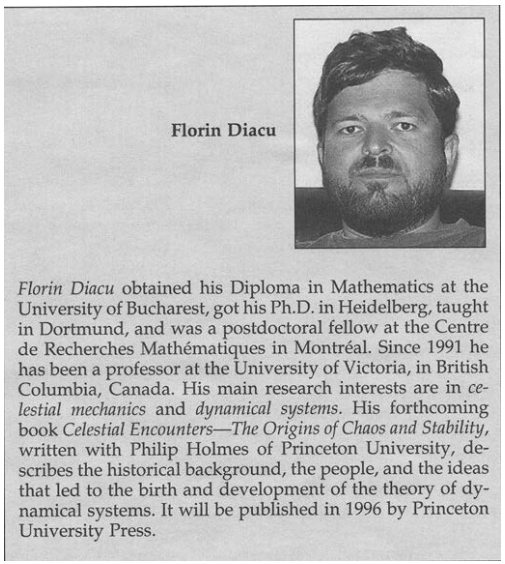
Sundmann series solution (1907-1912)

For the 3-body problem there is series solution in powers of $t^{1/3}$ which converges for any $t^{(*)}$

(*) with exception of some initial conditions

Karl Frithiof Sundman

Finnish



Florin Diacu

Florin Diacu obtained his Diploma in Mathematics at the University of Bucharest, got his Ph.D. in Heidelberg, taught in Dortmund, and was a postdoctoral fellow at the Centre de Recherches Mathématiques in Montréal. Since 1991 he has been a professor at the University of Victoria, in British Columbia, Canada. His main research interests are in *celestial mechanics* and *dynamical systems*. His forthcoming book *Celestial Encounters—The Origins of Chaos and Stability*, written with Philip Holmes of Princeton University, describes the historical background, the people, and the ideas that led to the birth and development of the theory of dynamical systems. It will be published in 1996 by Princeton University Press.

The Solution of the *n*-body Problem*

Florin Diacu

what about N > 3 ?

The Solution of the *n*-body Problem*

Florin Diacu

[...] It took about 7 decades until the general case was solved. In 1991, a Chinese student, Quidong (Don) Wang, published a beautiful paper [Wa], [D1], in which he provided a convergent power series solution of the *n*-body problem.

Did this mean the end of the *n*-body problem? Was this old question—unsuccessfully attacked by the greatest mathematicians of the last 3 centuries—merely solved by a student in a moment of rare inspiration?

[...] Paradoxically [...] not; in fact we know nothing more than before having this solution.

exact solution does not help

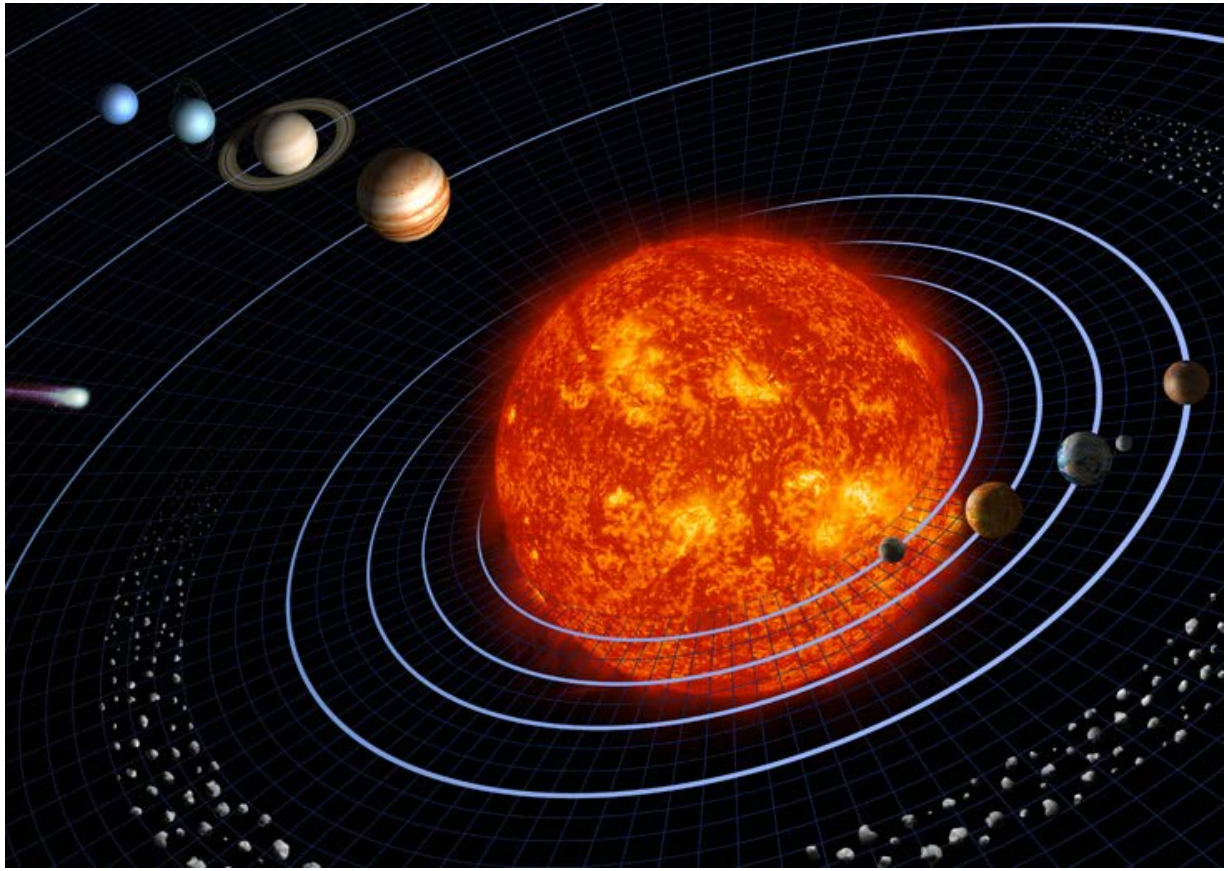
The Solution of the *n*-body Problem*

Florin Diacu

The Foundations of Mathematics

What Sundman and Wang did is in accord with the way solutions of initial value problems are defined; everything is apparently all right; but there is a problem, a big one: these series solutions, though convergent on the whole real axis, have very slow convergence. One would have to sum up millions of terms to determine the motion of the particles for insignificantly short intervals of time. The round-off errors make these series unusable in numerical work. From the theoretical point of view, these solutions add nothing to what was previously known about the *n*-body problem.

emergent behavior: novel approaches



(from NASA website)

Kolmogorov–Arnold–Moser theorem

If masses, eccentricities, and inclinations of planets are small enough, many initial conditions lead to quasiperiodic planetary trajectories

and in quantum mechanics?

the quantum N-body problem

already 1 body is difficult

- uncertainty principle $\Delta x \Delta v \geq \frac{1}{2}\frac{\hbar}{m}$
- described via wavefunction $\Psi(\mathbf{r}) \quad |\Psi(\mathbf{r})|^2$
- eigenvalue problem & discrete energies $\hat{H}_0 \Psi(\mathbf{r}) = \varepsilon \Psi(\mathbf{r})$

2-bodies non interacting

- particles are identical **and** indistinguishable

- fermions $\psi(r_1)\psi(r_2) - \psi(r_2)\psi(r_1)$

Slater determinant

$$\hat{H}_0 = \sum_i \hat{H}_i^0$$

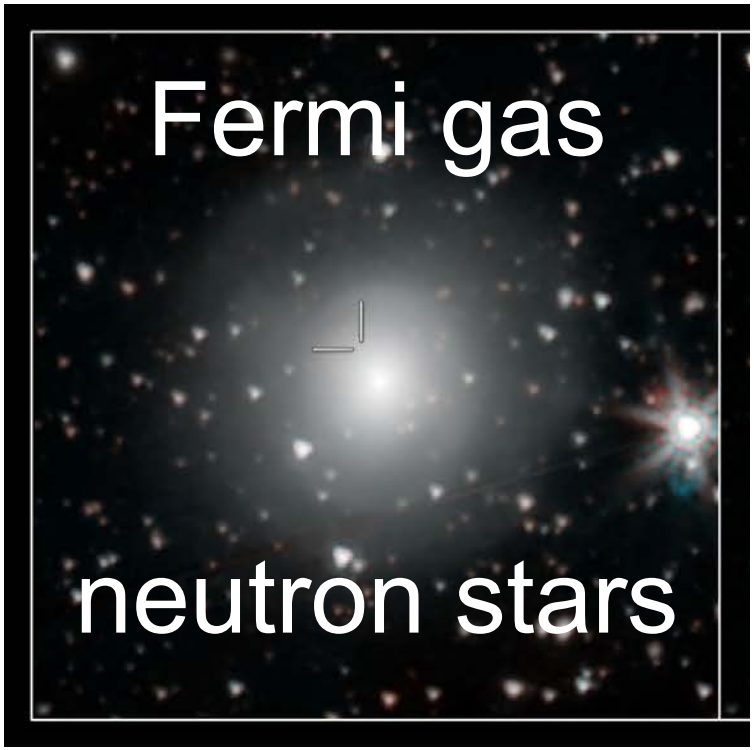
quantum N-body problem, no interaction

$$\hat{H}_0 = \sum_i \hat{H}_i^0 \qquad \hat{H}_i^0 \Psi(r_i) = \varepsilon_i \Psi(r_i) \qquad E = \sum_i \varepsilon_i$$

$$\Psi = \Psi(r_1)\Psi(r_2)...\Psi(r_N)$$

(classical/mean field)

+ antisymmetrization
(Slater determinant)



the Schrödinger equation

Erwin Rudolf Josef Alexander Schrödinger

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

$$\hat{H} = \sum_i \hat{H}_i^0 + \sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} + \hat{H}_n$$

$$\hat{H}_i^0 = -\frac{1}{2}\nabla_i^2 - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}$$

the interacting quantum N-body problem

the theory of almost everything

$$\hat{H} = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} + \hat{H}_n$$

kinetic+potential energy electron-electron interaction

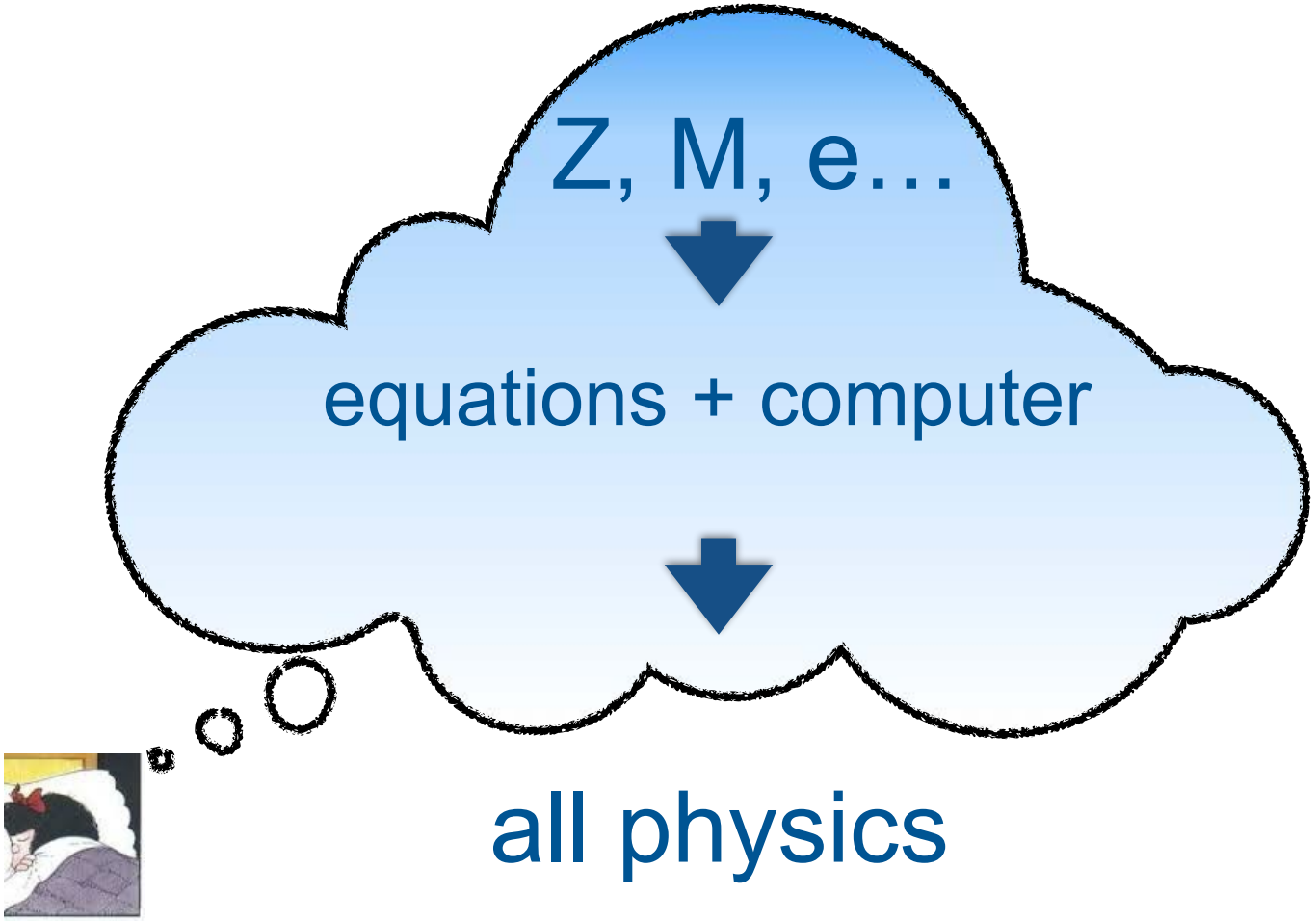
$$\hat{H}_i^0 = -\frac{1}{2}\nabla_i^2 - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}$$

can we solve this problem?

In so far as quantum mechanics is correct, chemical questions are problems in ***applied mathematics***

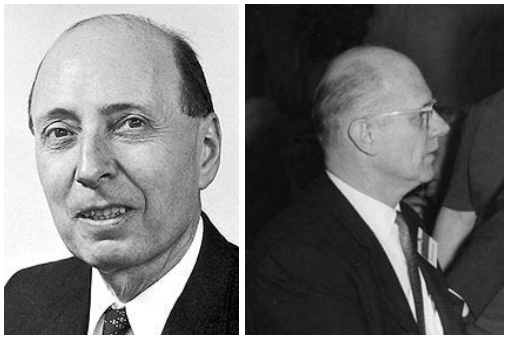
H. Eyring, J.E. Walter and E. Kimball, *Quantum Chemistry*, 1949

if yes, can we make a Great Dream Machine?



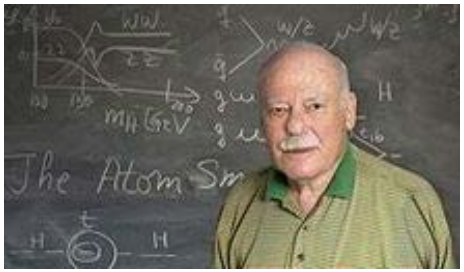
however, *quantum* N-body problem: no exact solution

… and the exact solution would be useless



E. Wigner and F. Seitz

If one had a great calculating machine, one might apply it to the problem of solving the Schrödinger equation for each metal […] It is not clear, however, that a great deal would be gained by this. Presumably the results would agree with the experimentally determined quantities and nothing vastly new would be learned from the calculation. [. . .].



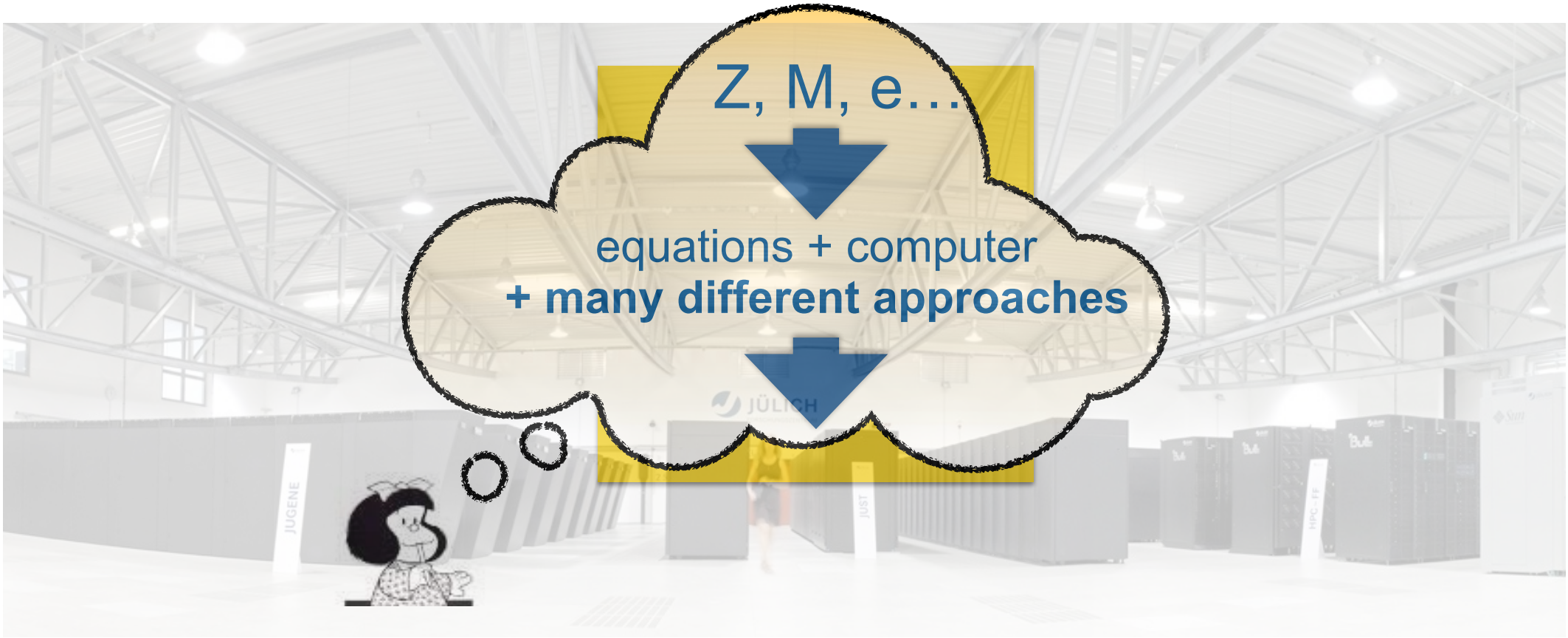
H.J. Lipkin

On the other hand, the exact solution of a many-body problem is really irrelevant since it includes a large mass of information about the system which although measurable in principle is never measured in practice.

[..] An incomplete description of the system is considered to be sufficient if these measurable quantities and their behavior are described correctly.

E. Pavarini and E. Koch, Autumn School on Correlated Electron 2013, Introduction

the Practical Great Dream Machine



answer to relevant questions

the Practical Great Dream Machine

why do atom exist? how can we explain the periodic table?

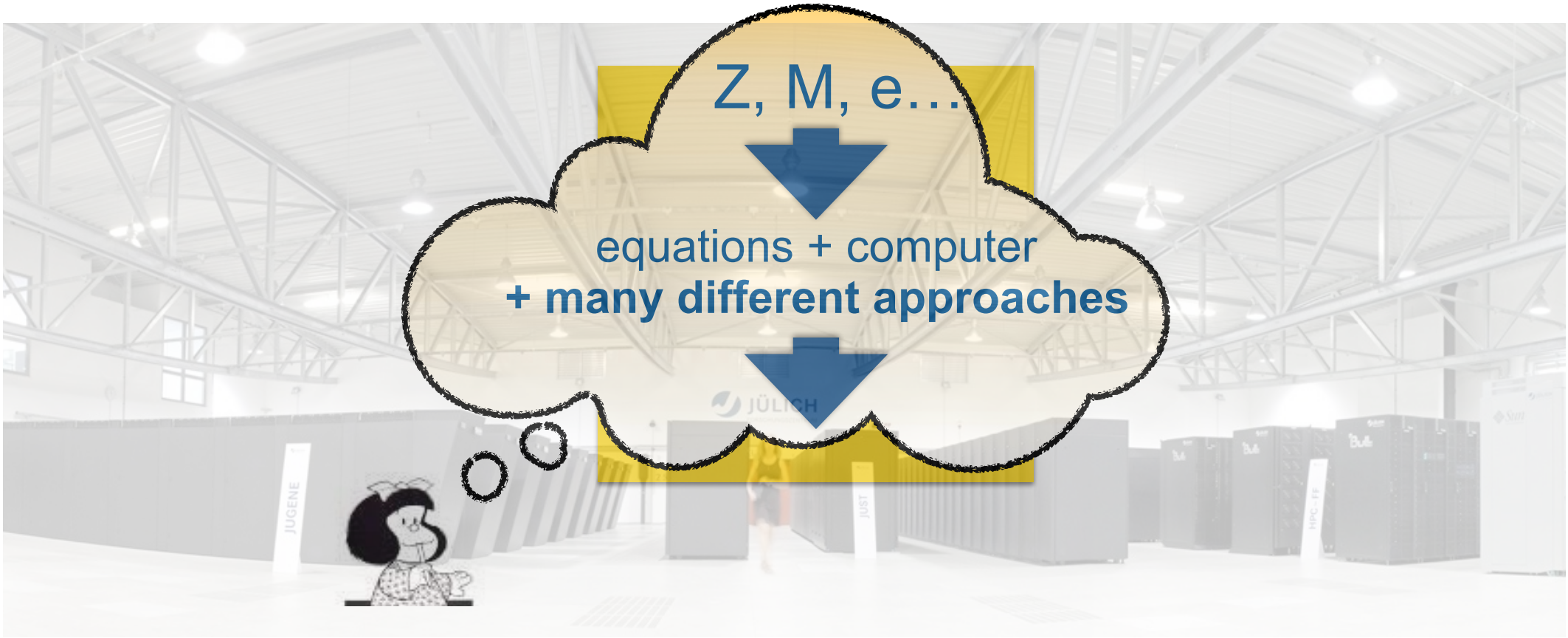
what is the mechanism of high-Tc superconductivity?

why are some systems metals and other insulators?

what is the mechanism of orbital ordering?

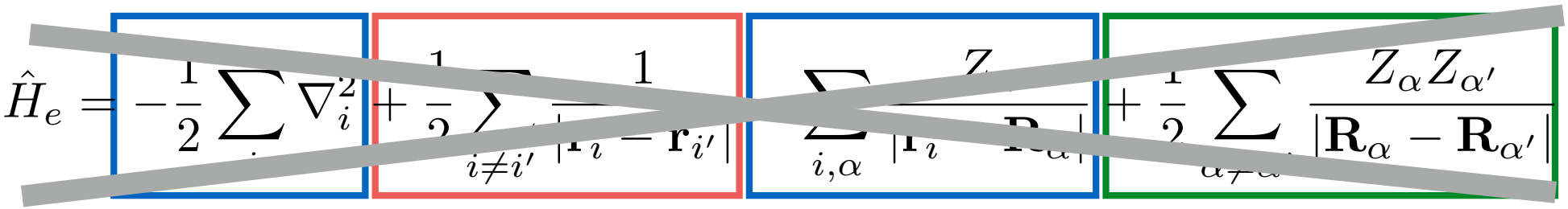
no two samples are identical: **generic** features only

the Practical Great Dream Machine



answer to relevant questions

give up exact solutions

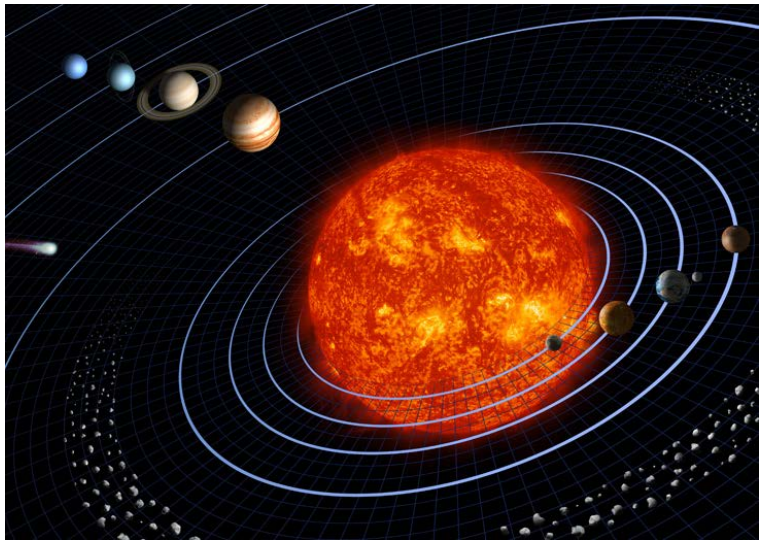


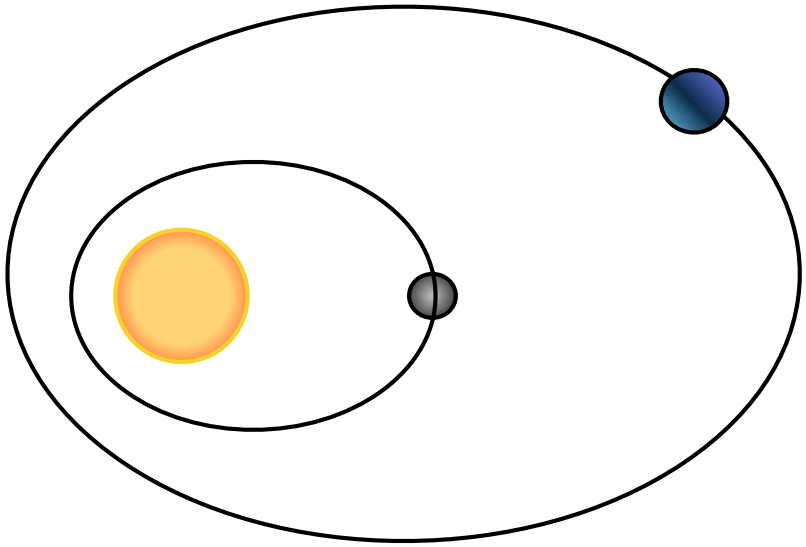
minimal model for a given class of phenomena

as system-specific as possible

& find approximate methods that work

minimal models that capture the phenomenon



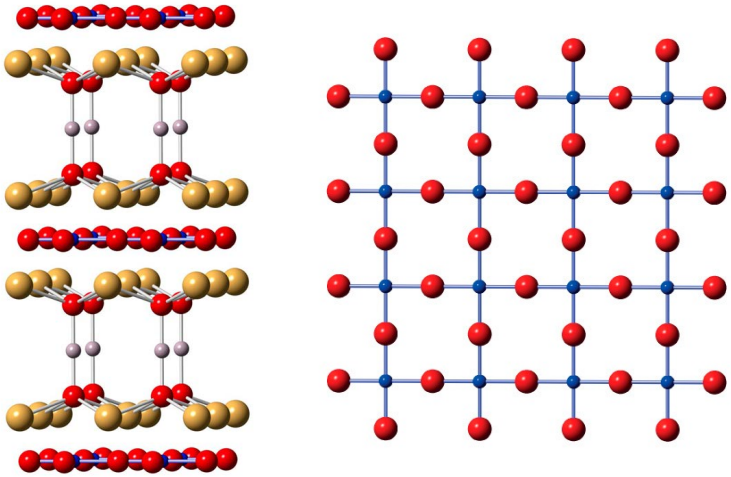


which phenomena?

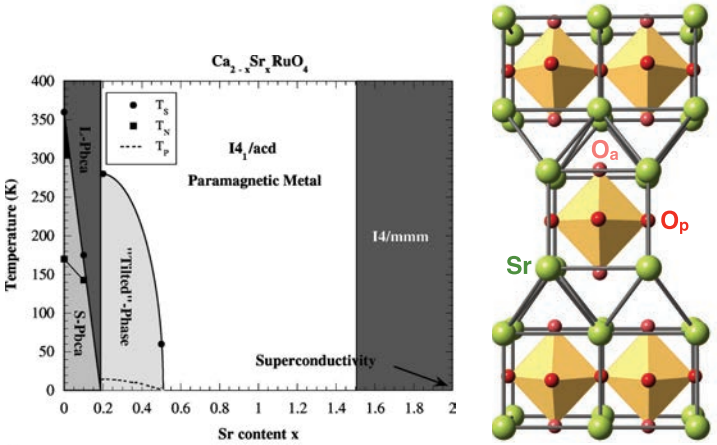
open challenges

high-temperature superconductivity

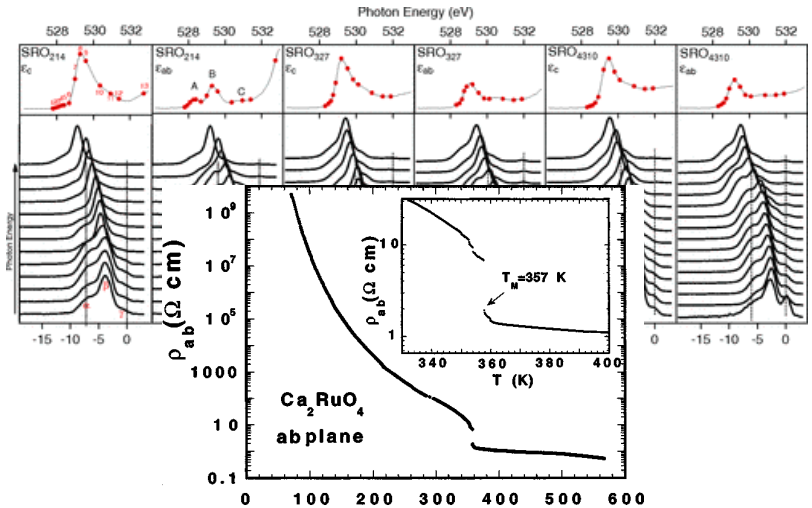
$HgBa_2CuO_4$



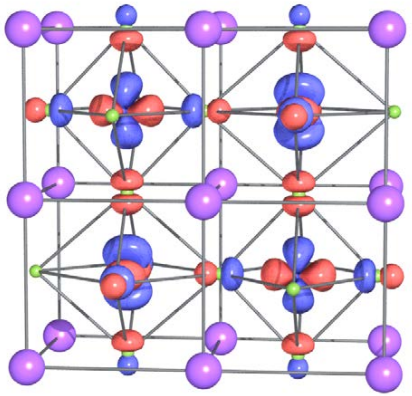
unconventional superconductivity



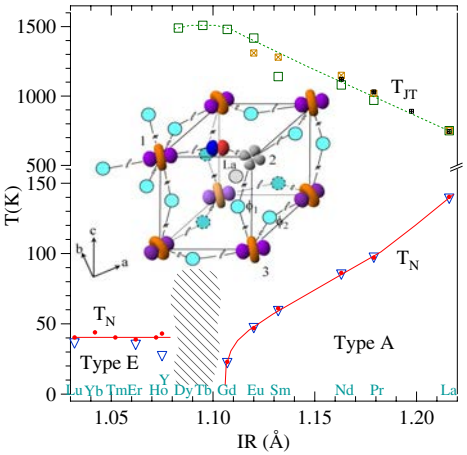
the metal-insulator transition



orbital order



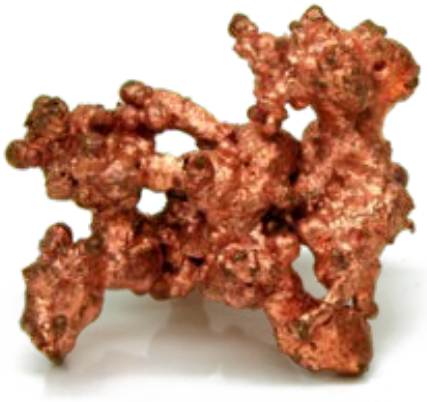
order-to-disorder



a key problem: metal or insulator?

diamond

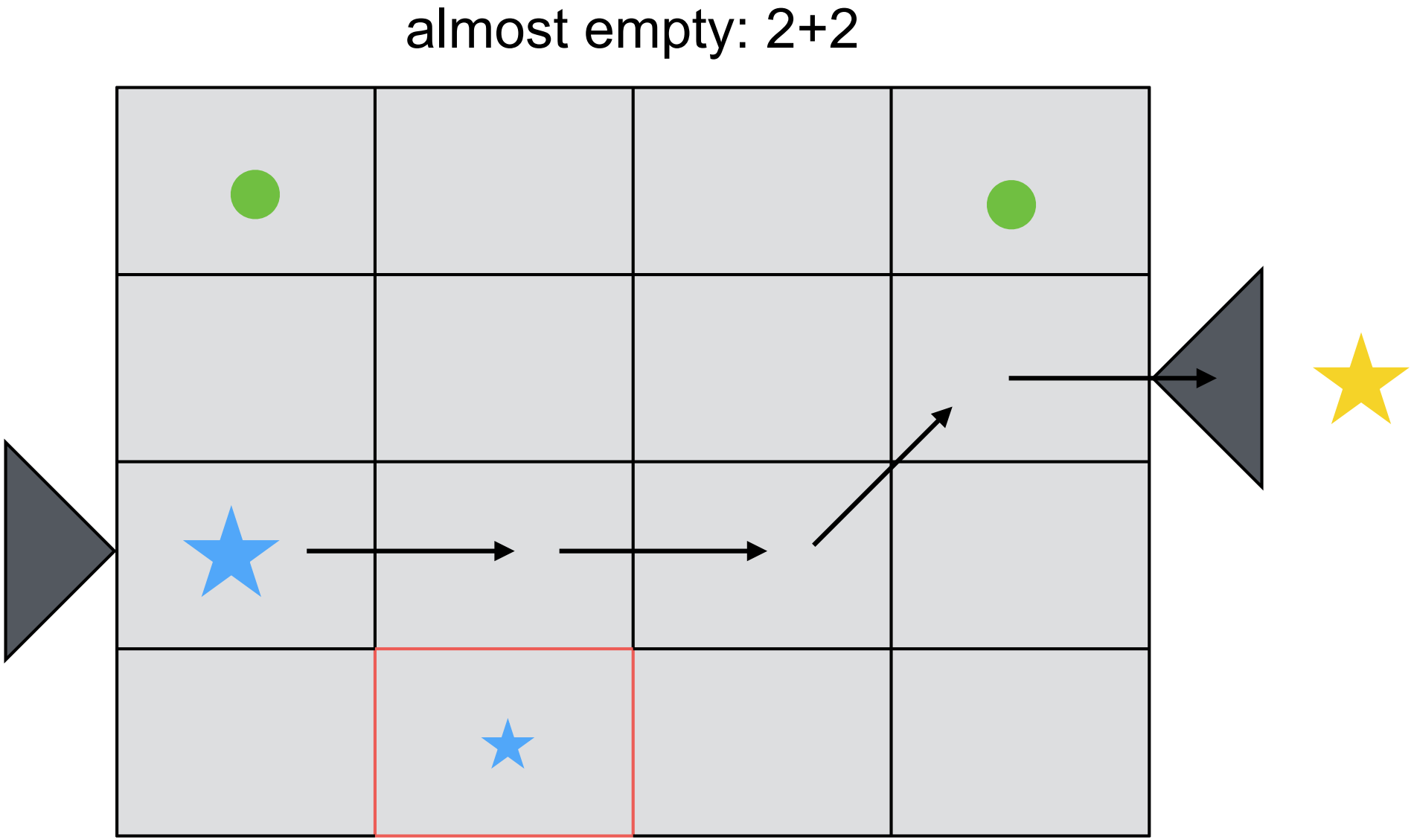
silicon



copper

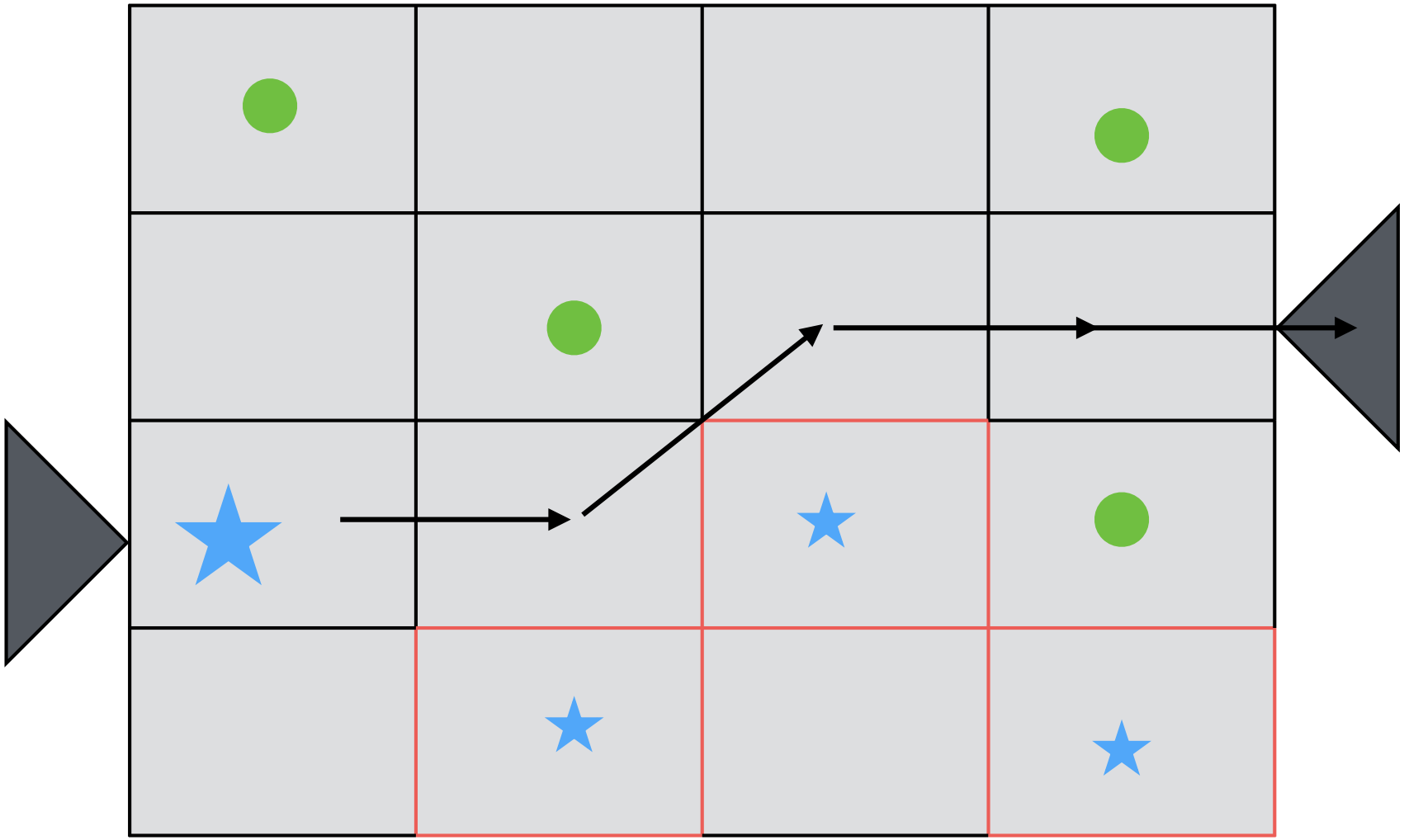
photos from wikipedia

independent particle picture



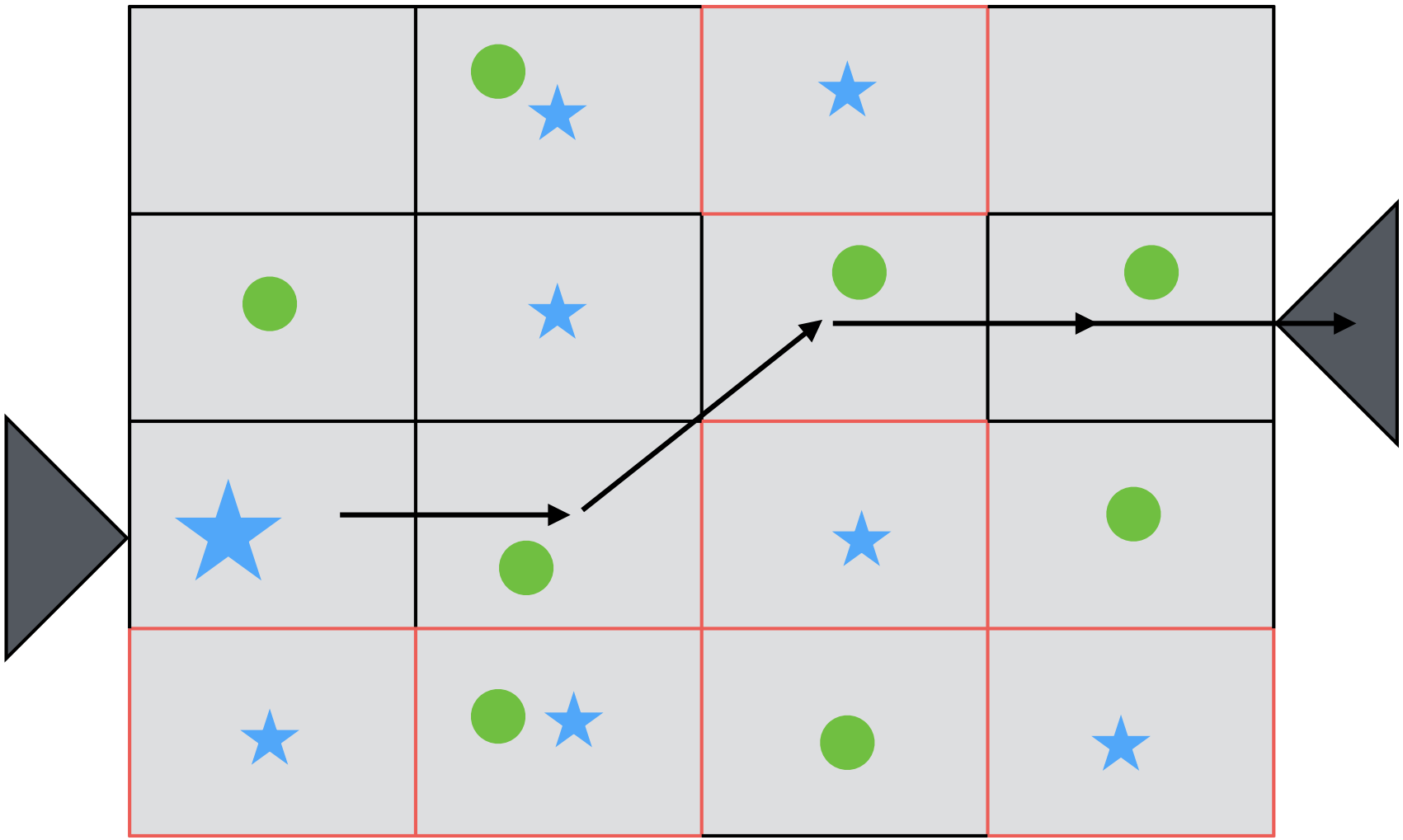
independent particle picture

low filling: 4+4

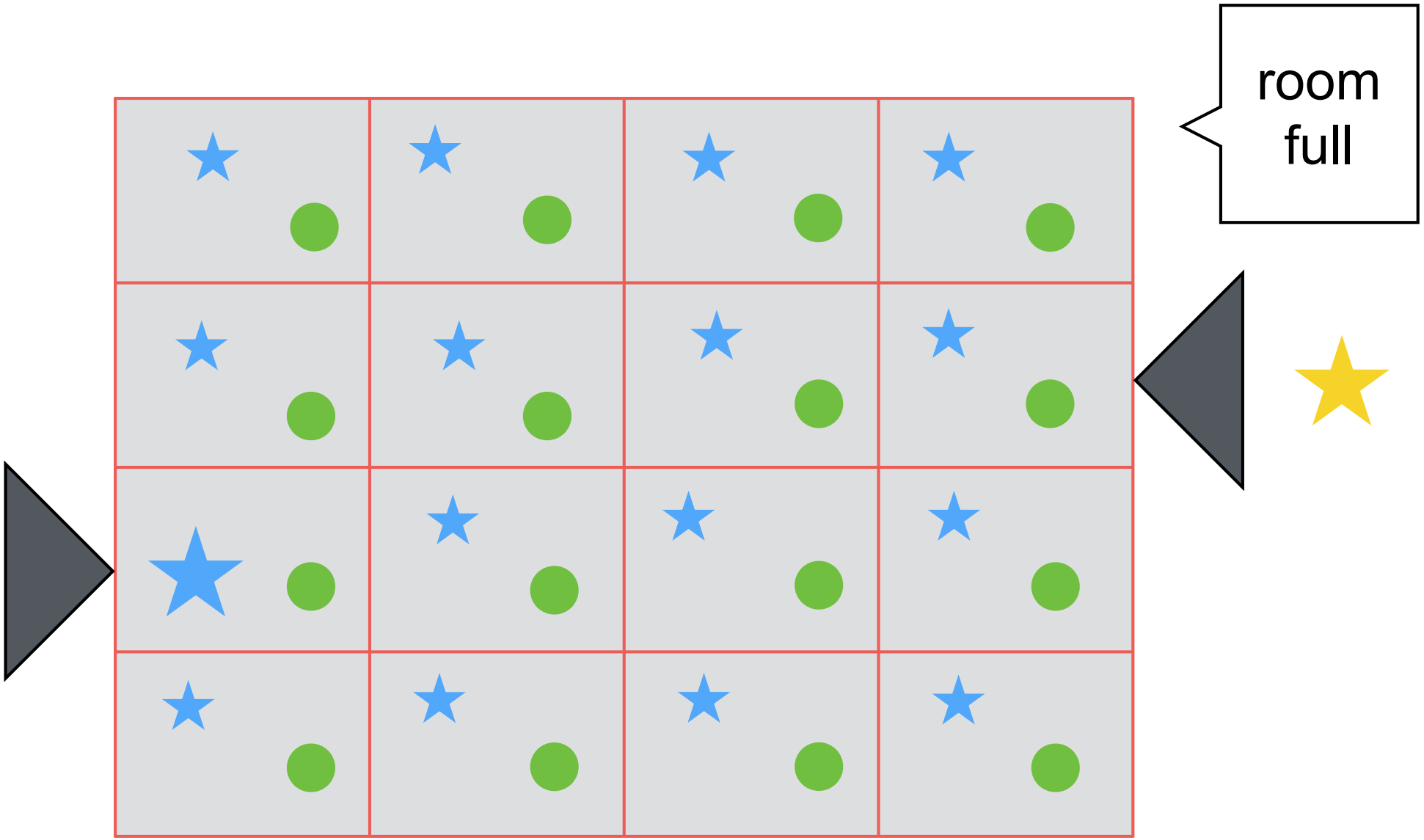


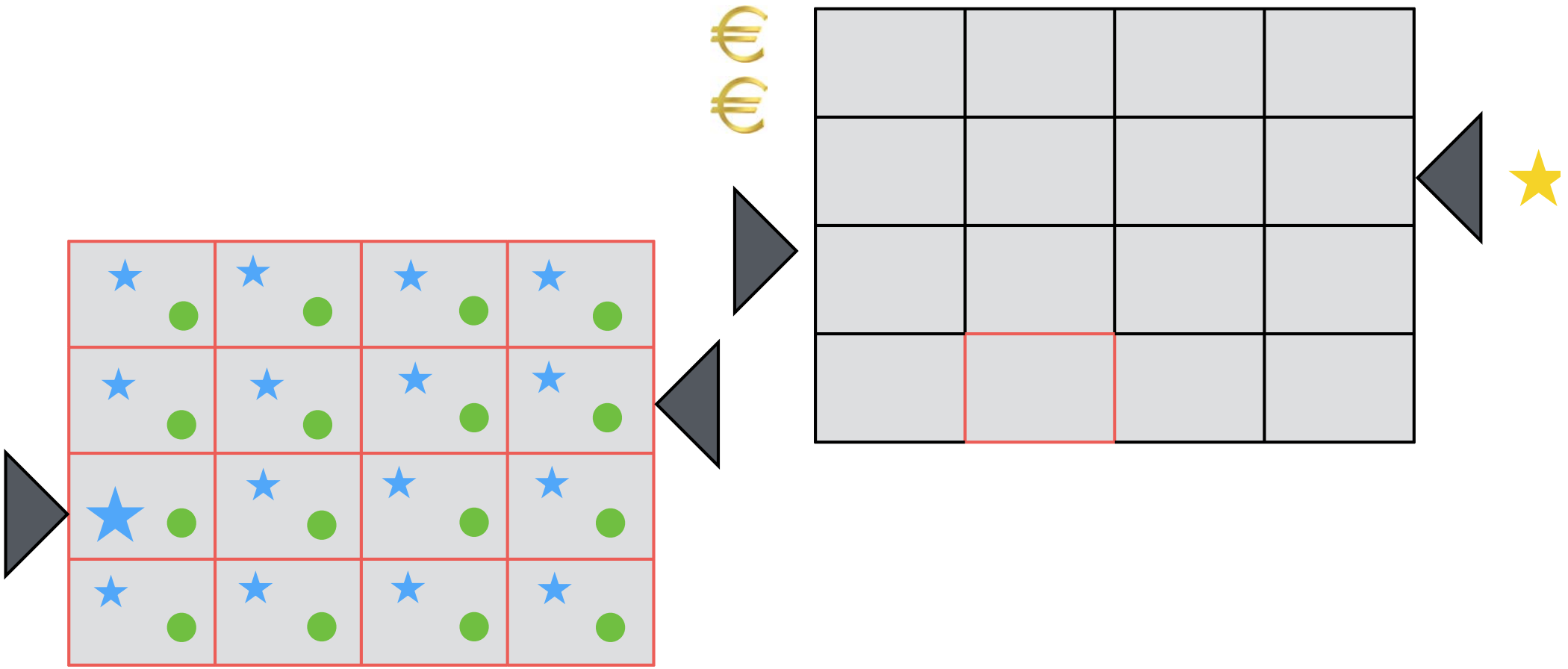
independent particle picture

half filling: 8+8



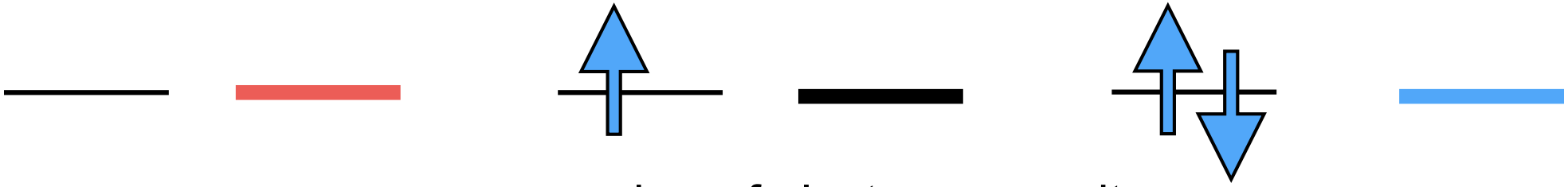
independent particle picture





independent-electron picture

Pauli principle: each level is filled with max two electrons

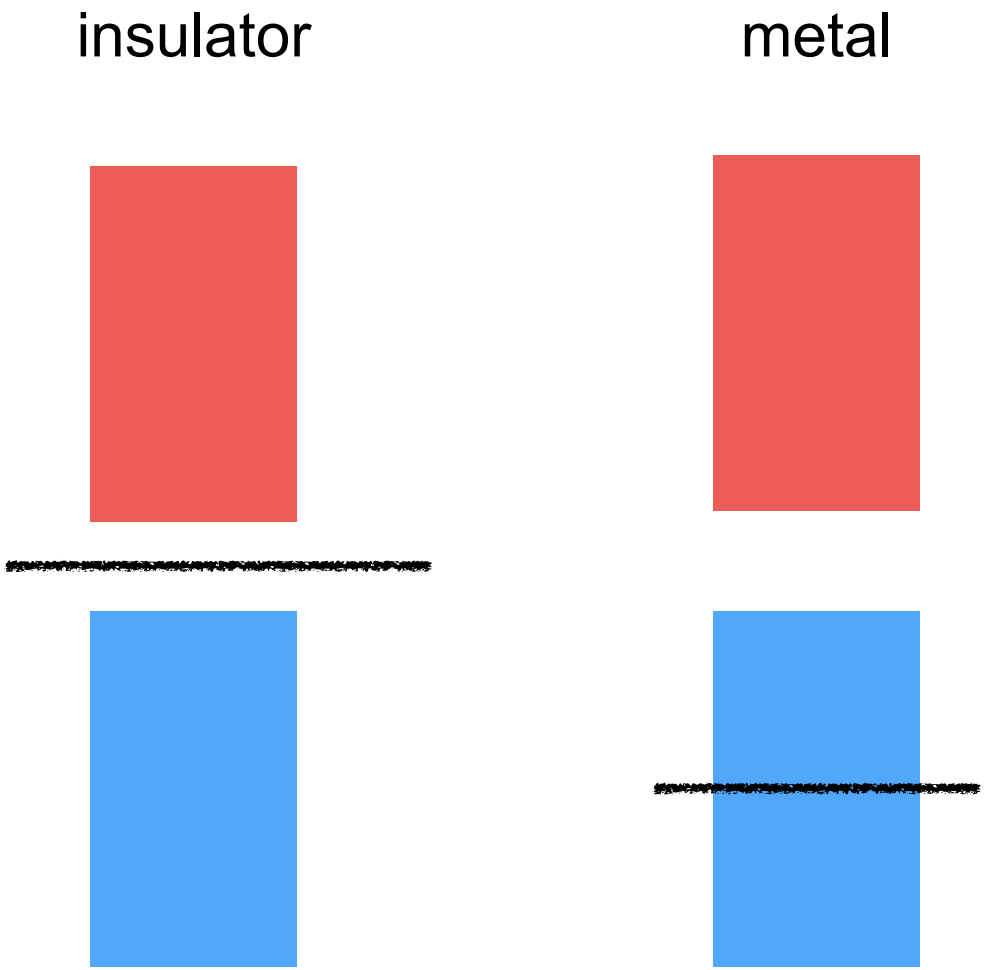


even number of electrons per site
might result in a gapped system (insulator)

independent-electron picture

odd number of electrons per site yield a system with no gap

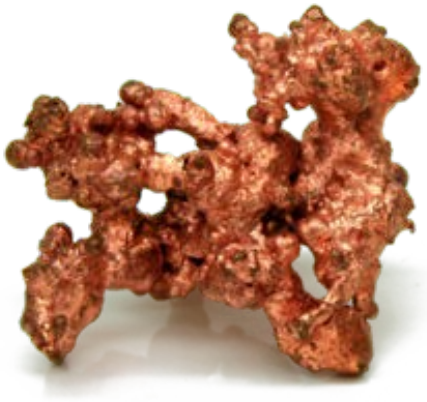
independent-electron picture



within this picture

diamond

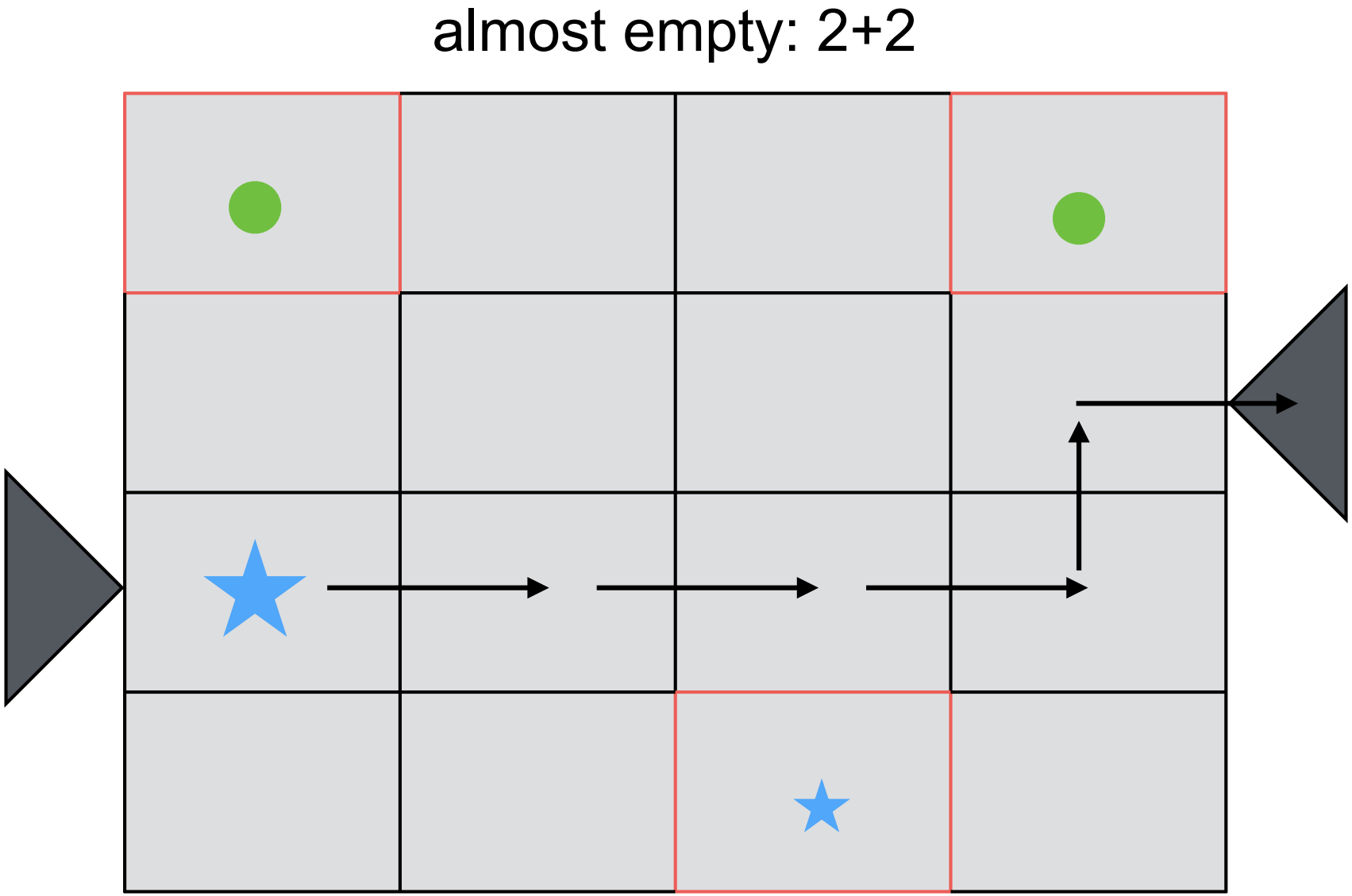
silicon



copper

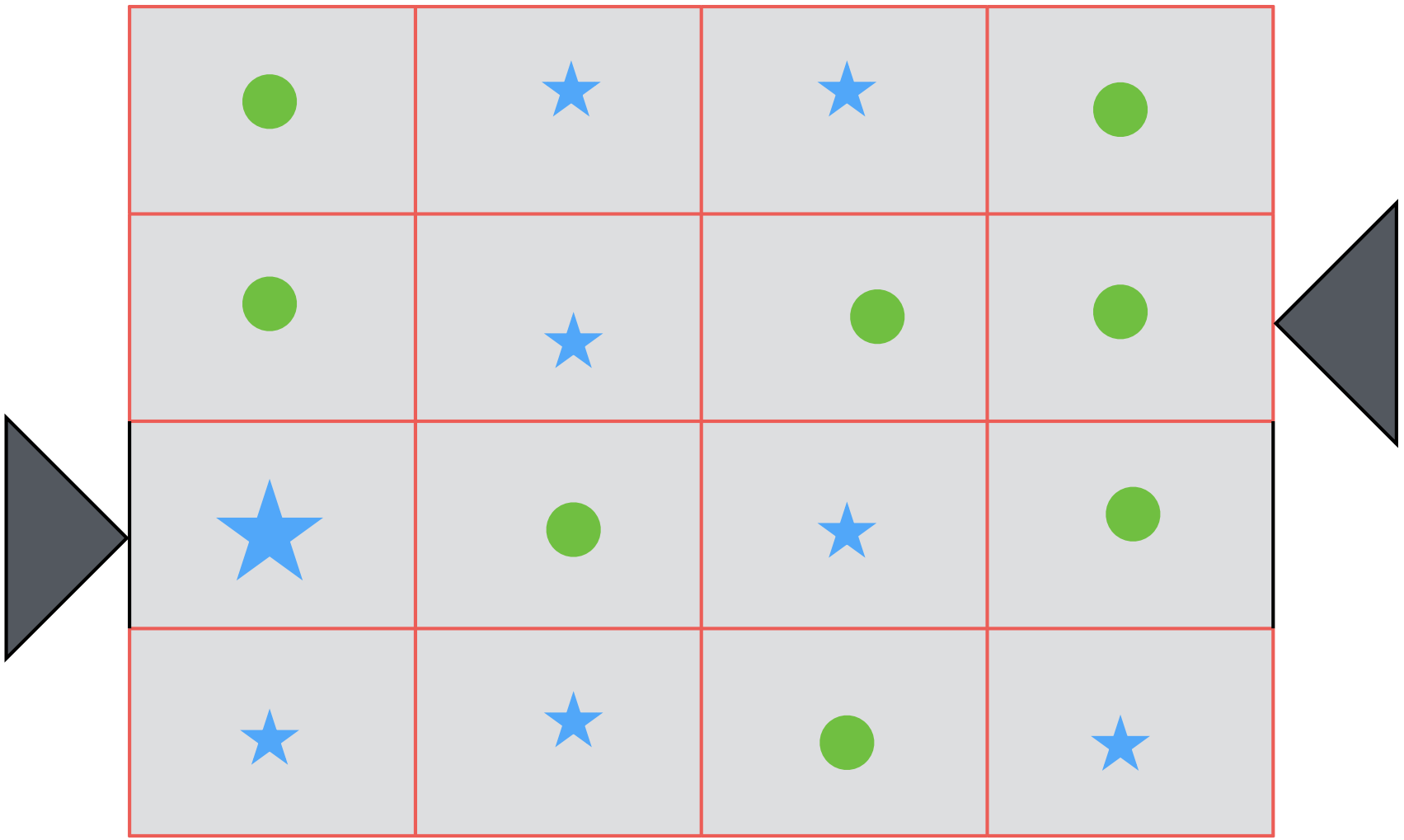
photos from wikipedia

interacting particle picture



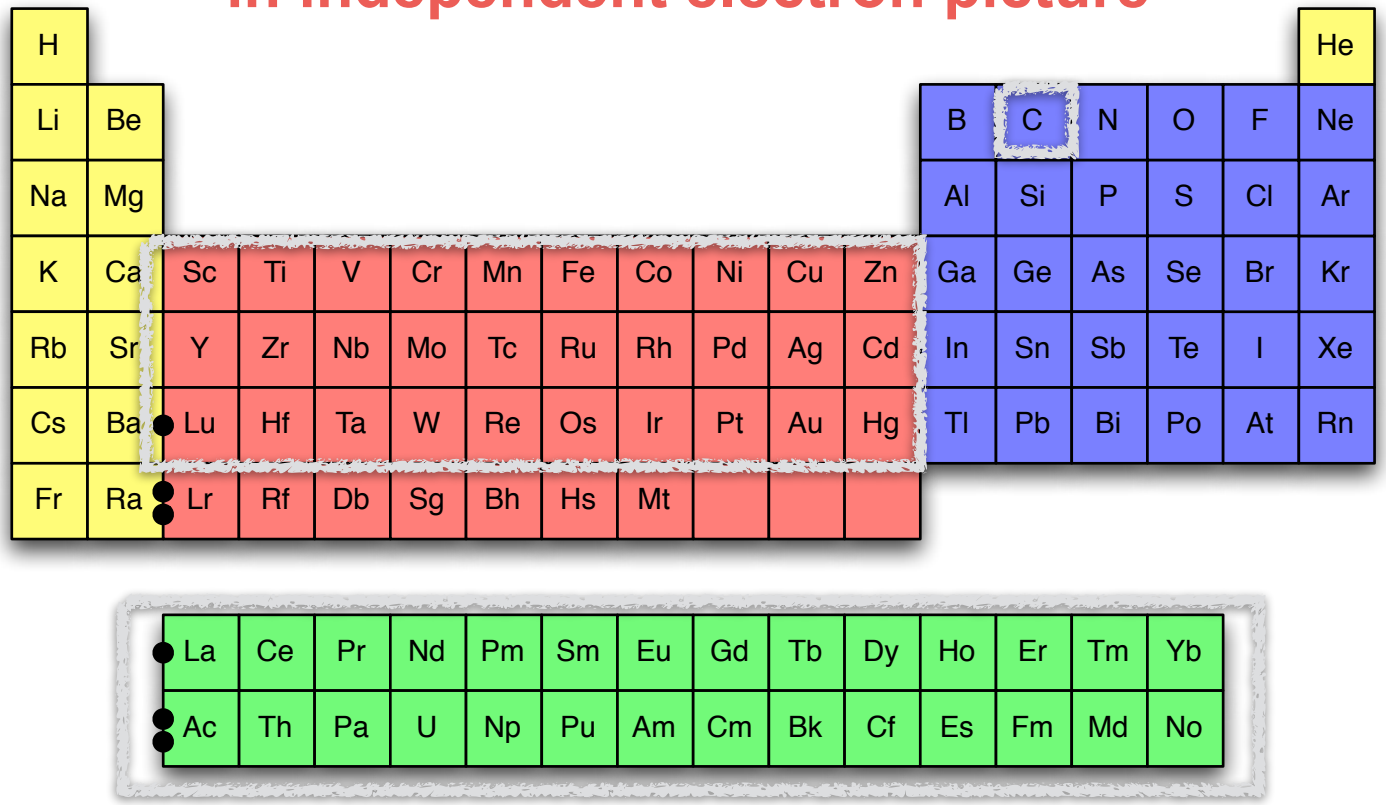
independent particle picture

half filling (1 particle per site): 8+8



strongly correlated systems

paramagnetic Mott insulators are either metals or magnetically ordered insulators
in independent electron picture

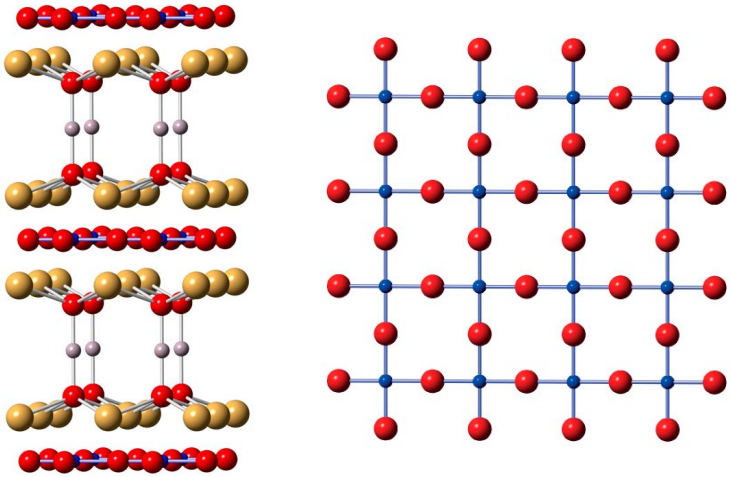


Coulomb-induced metal-insulator transition
heavy-Fermions
unconventional superconductivity
spin-charge separation

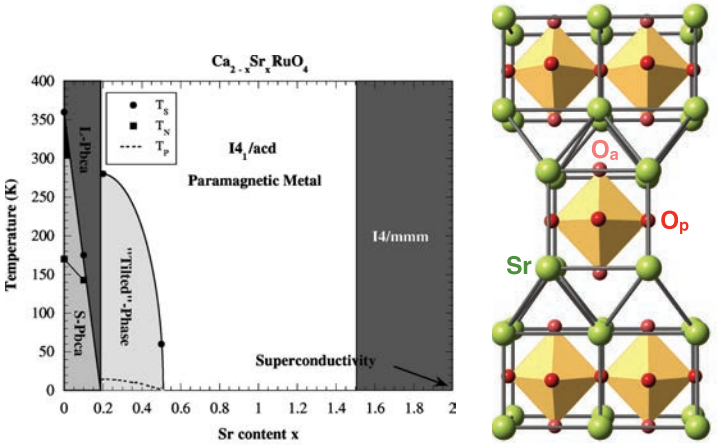
open challenges

high-temperature superconductivity

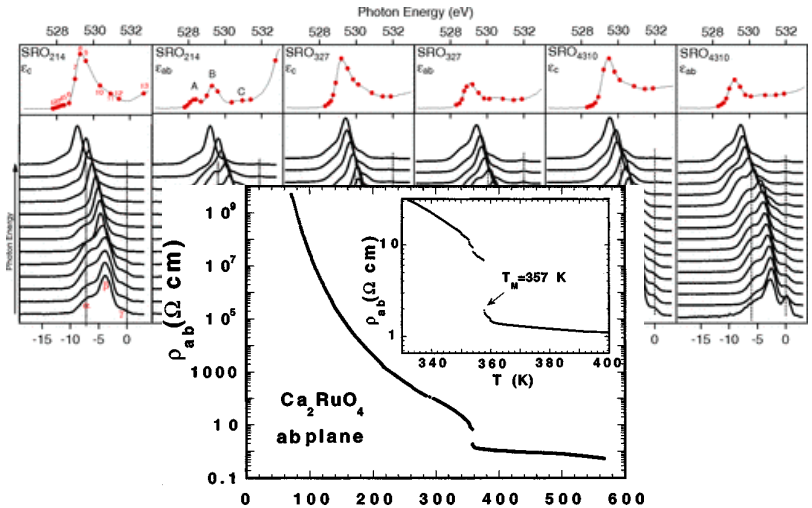
$HgBa_2CuO_4$



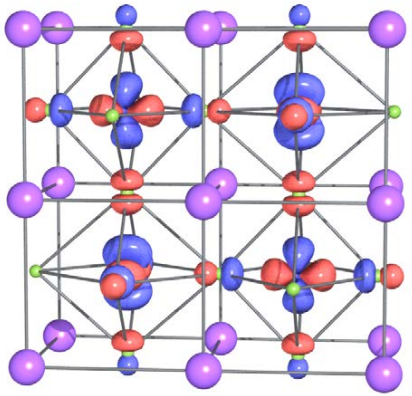
unconventional superconductivity



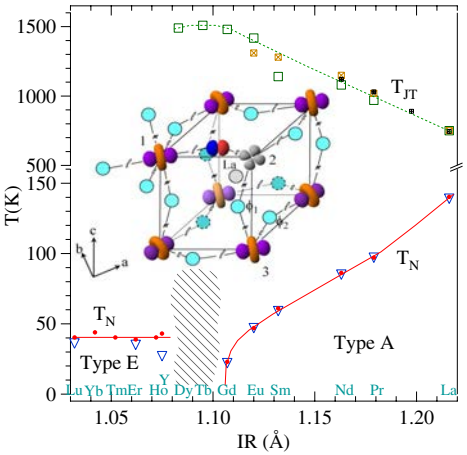
the metal-insulator transition



orbital order



order-to-disorder



how do we describe these phenomena?

0. electronic Hamiltonian in 2nd quantization

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2}\sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$

complete one-electron basis set!

where to learn this: lectures SS

1. build minimal models

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$

$$\hat{\tilde{H}}_e = \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b$$

DFT Kohn-Sham *ab-initio* Hamiltonian

very good approach for weakly correlated systems

where to learn this: lectures SS

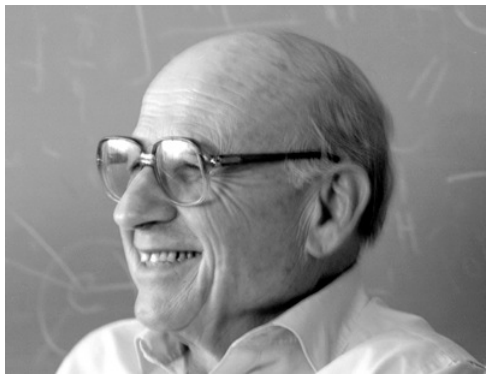
density-functional theory

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

Kohn-Sham auxiliary Hamiltonian

$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i)\right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$

$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$



Walter Kohn

Nobel Prize in Chemistry (1998)

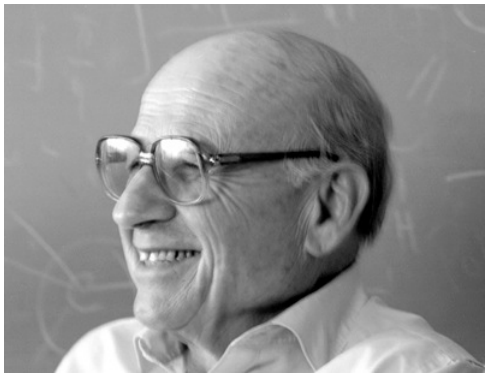
Kohn-Sham equations

(in practice: LDA,GGA,…)

understand and predict properties of solids, molecules, biological systems, geological systems...

where to learn this: lectures SS

density functional theory



Walter Kohn

$$E_{xc}[n] = \int d\mathbf{r} \epsilon_{xc}^{\mathrm{LDA}}(n(\mathbf{r}))n(\mathbf{r})$$

homogeneous electron gas

understand and predict properties of solids, molecules, biological systems, geological systems...

Nobel Prize in Chemistry (1998)

The practical DFT-based Great Dream Machine

weakly correlated systems

what do the parameters contain?

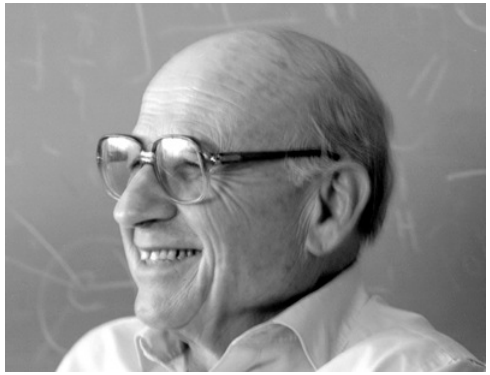
$$t_{a,b} = -\int d\mathbf{r}\, \overline{\psi_a}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_b(\boldsymbol{r}),$$

Hartree

$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$

potential

exchange-correlation



Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

understand and predict properties of solids, molecules, biological systems, geological systems...

a big success, new challenges

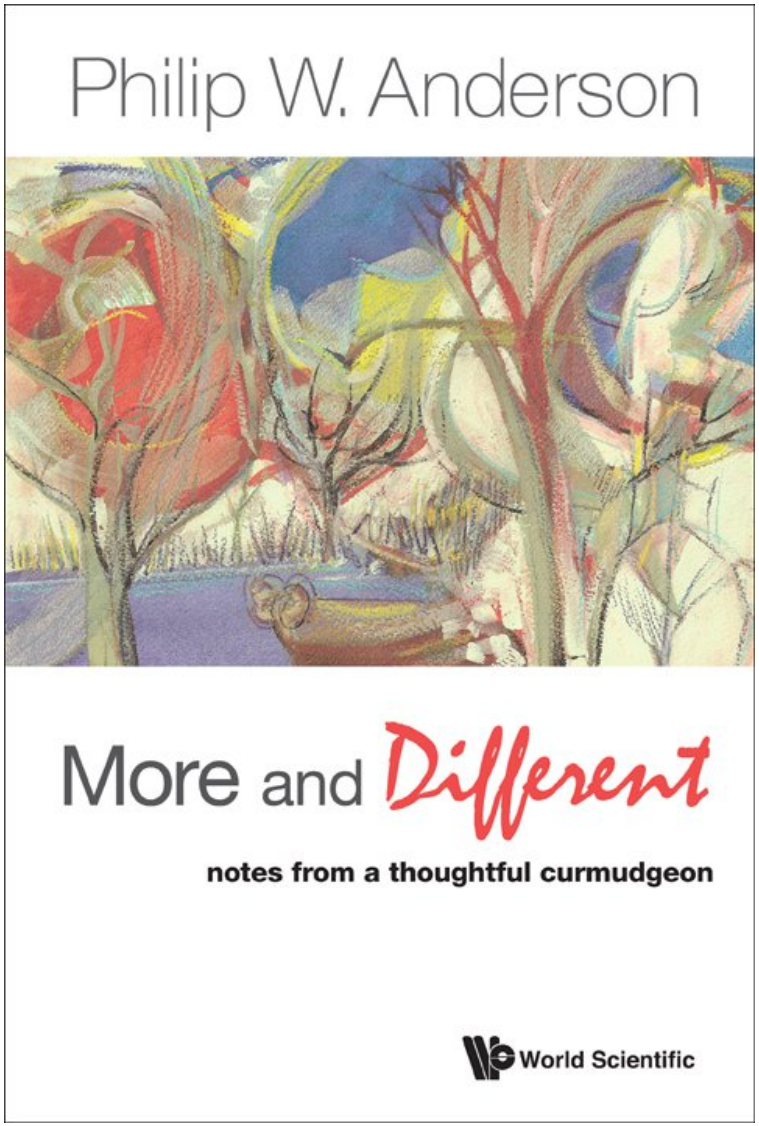
"the labours and controversies . . . in understanding the chemical binding in materials had finally come to a resolution in favour of 'LDA' and the modern computer" **(1998)**

but "**very deep problems**" remain **(1998)**

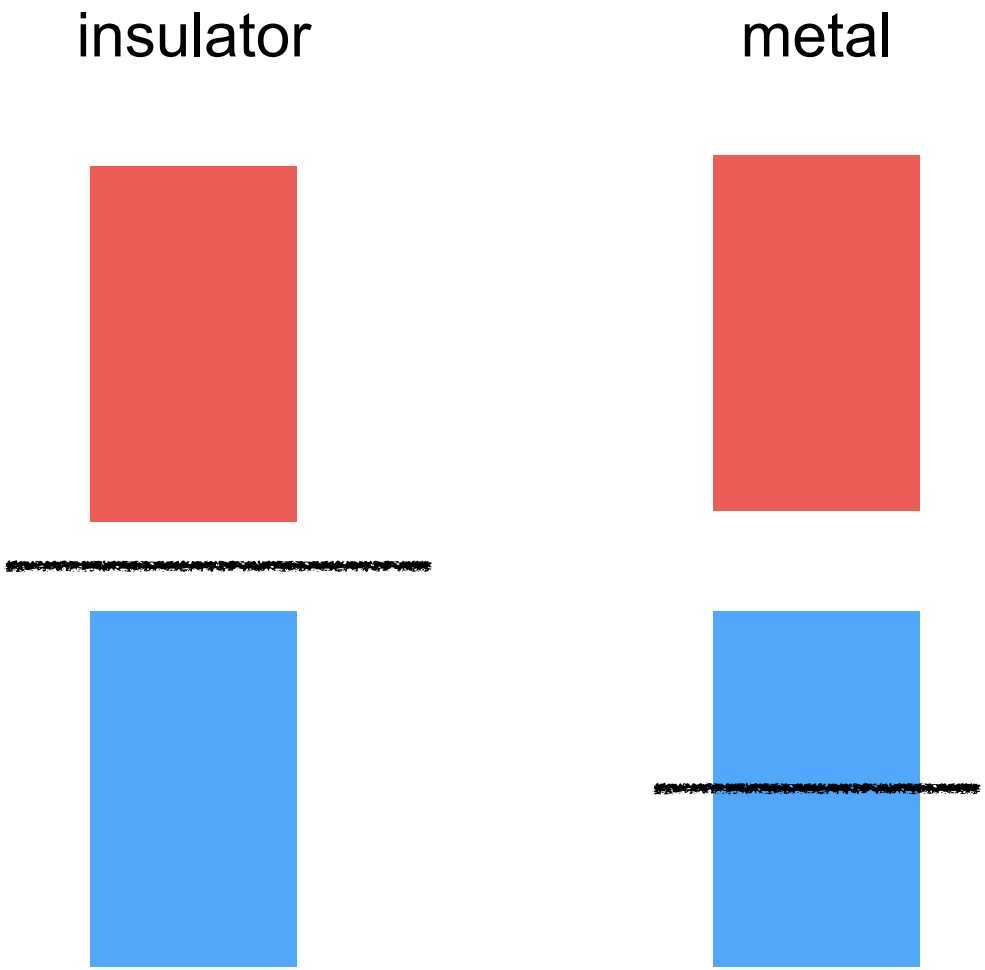
origin of failures: one-electron picture

(RO Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

more and different



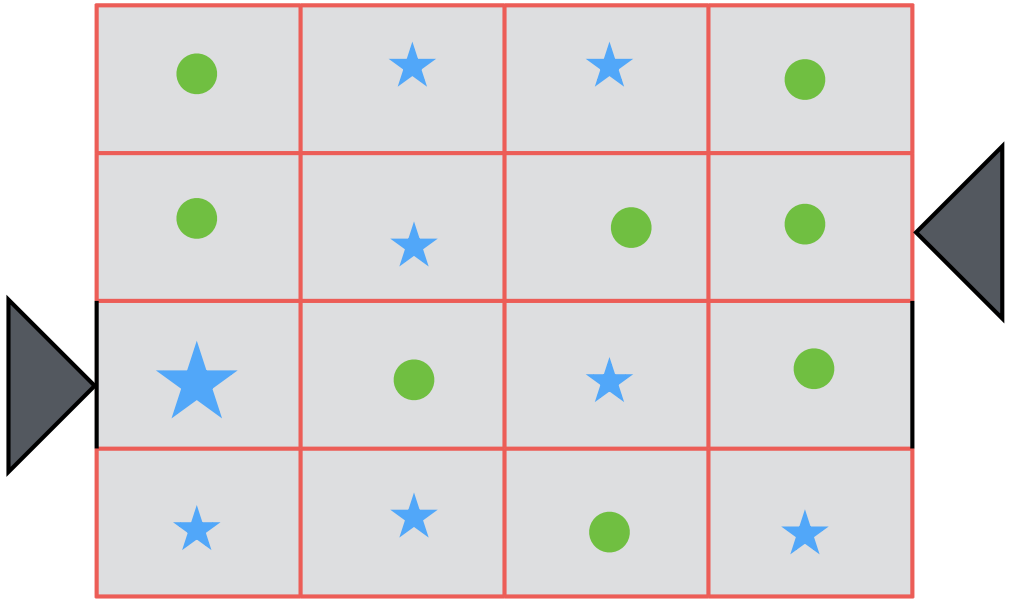
origin of failures: one-electron picture

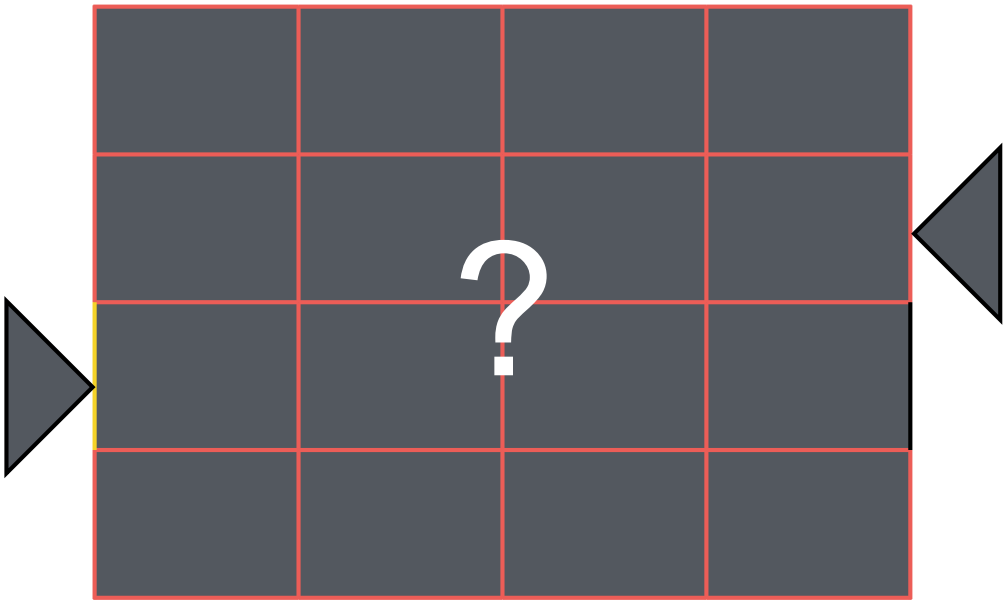


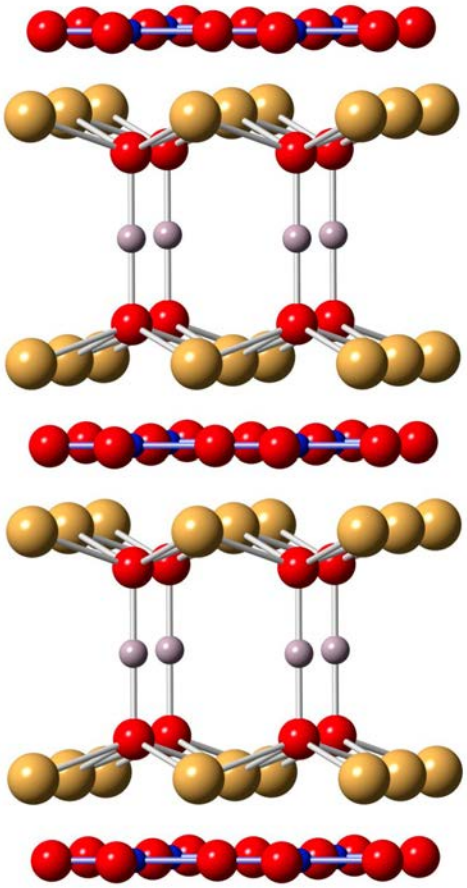
can I *cure* this ? No!

find alternative one-electron pictures?

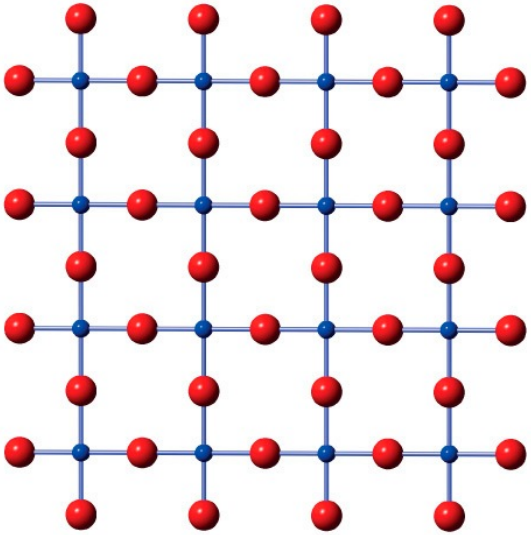
half filling (1 particle per site): 8+8



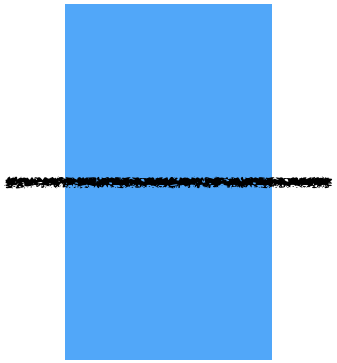




$HgBa_2CuO_4$

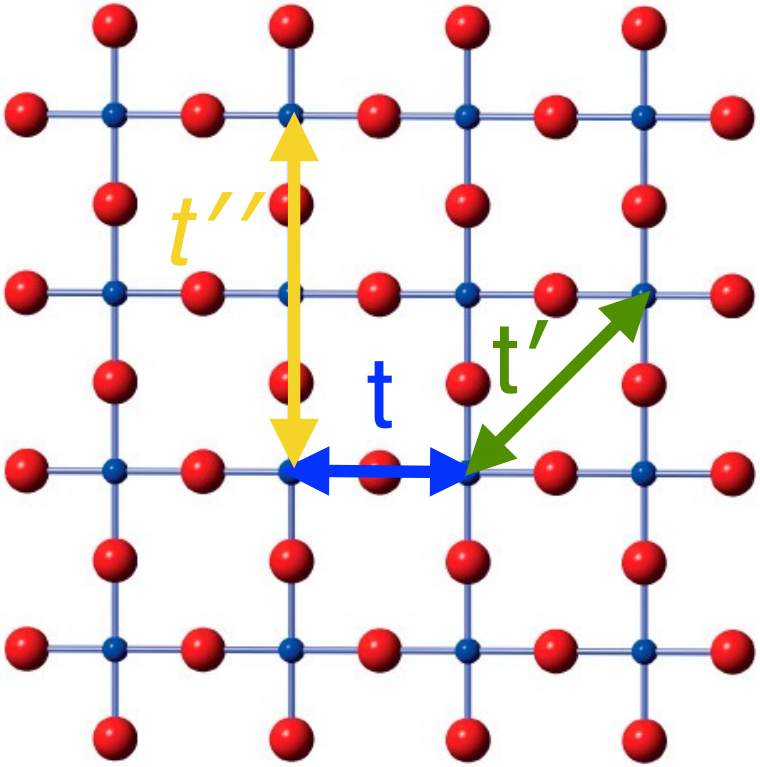


metal

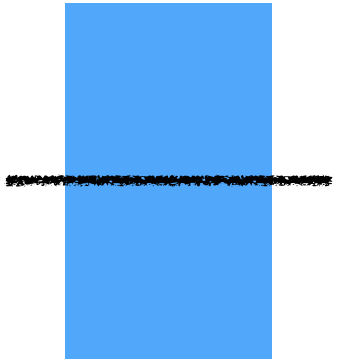


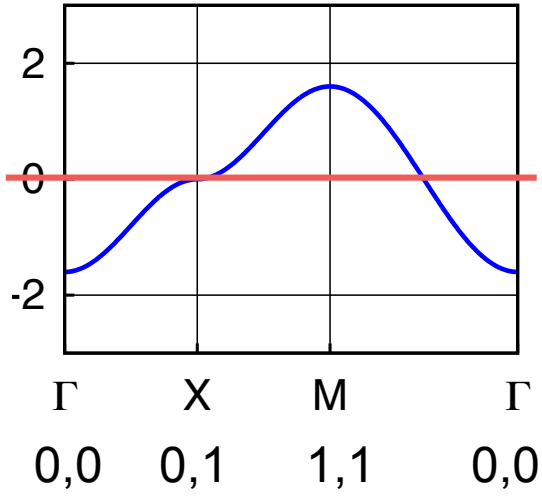
electron counting argument

one electron per site



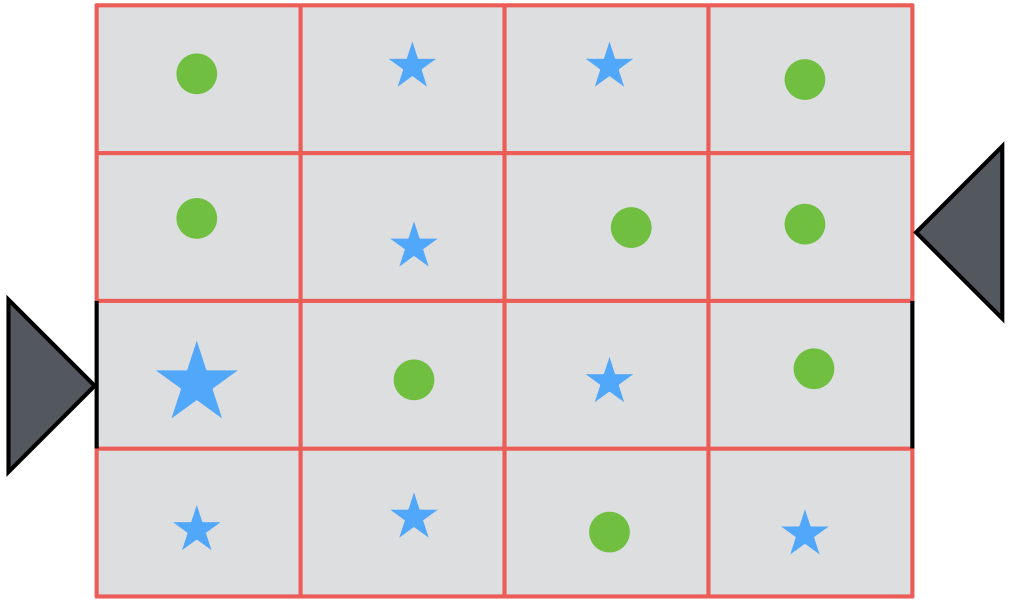
$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$



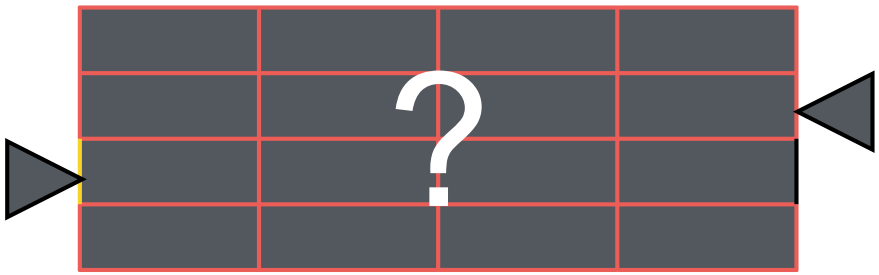


find alternative one-electron pictures?

half filling (1 particle per site): 8+8

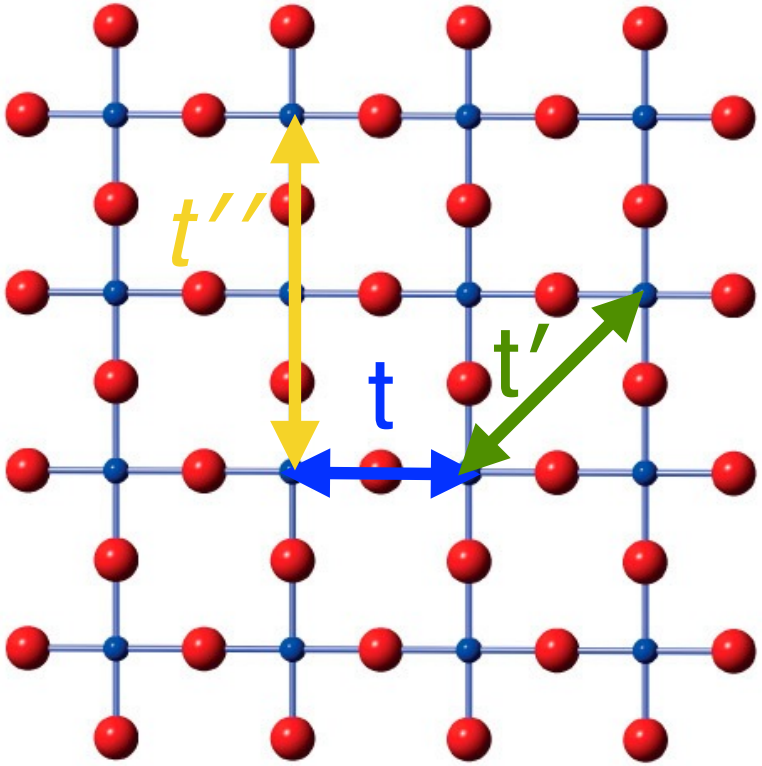


modify shape?



electron counting argument

one electron per site



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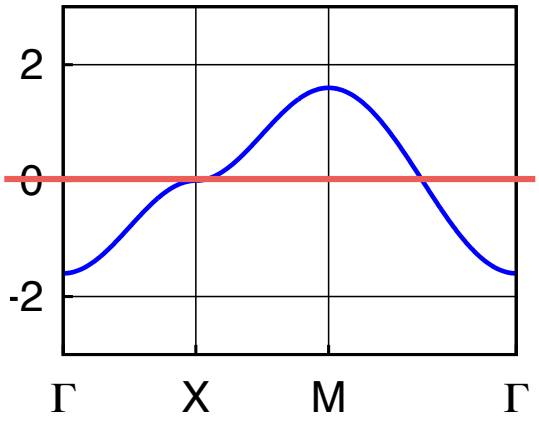
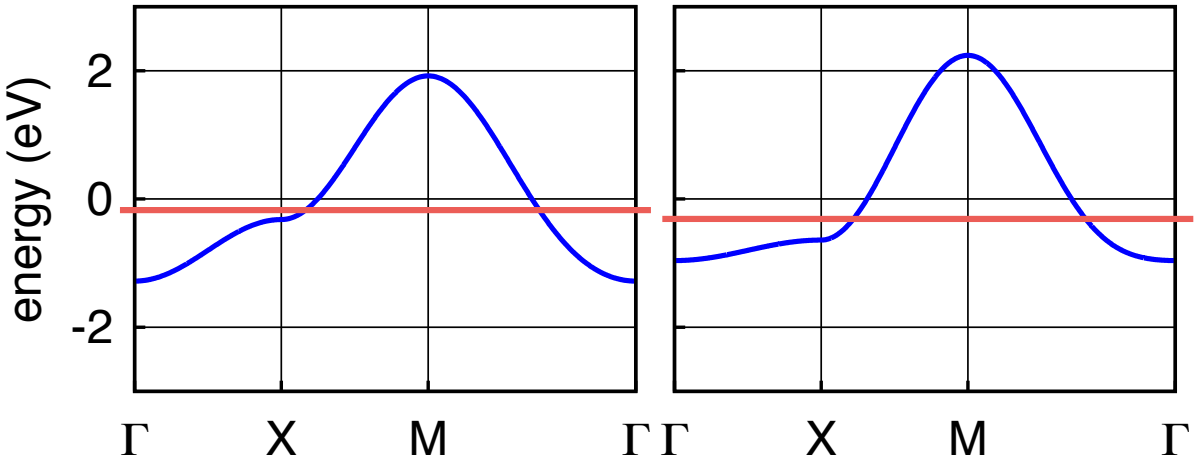
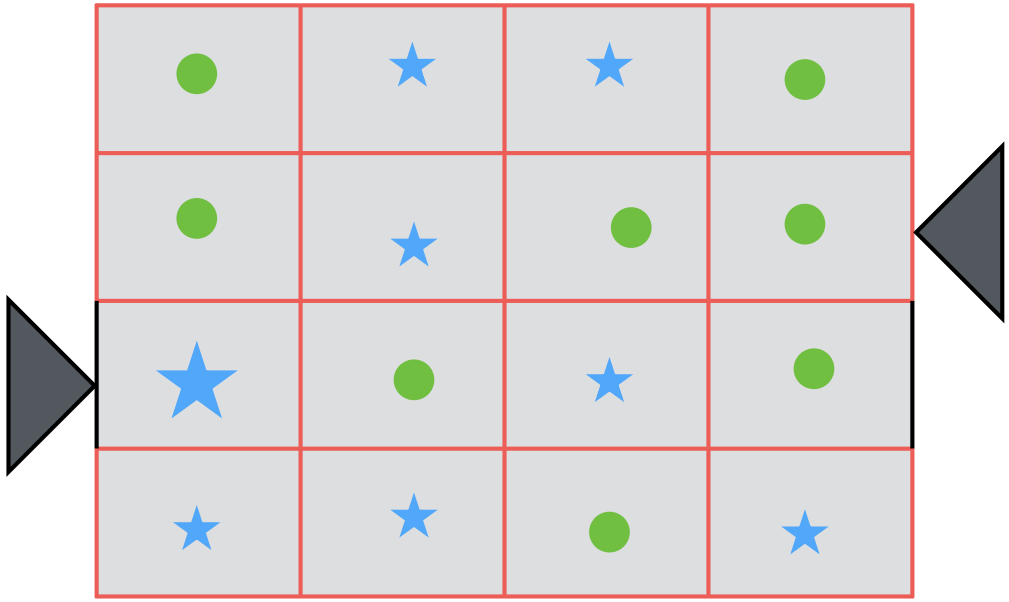


t′/t= =0.2

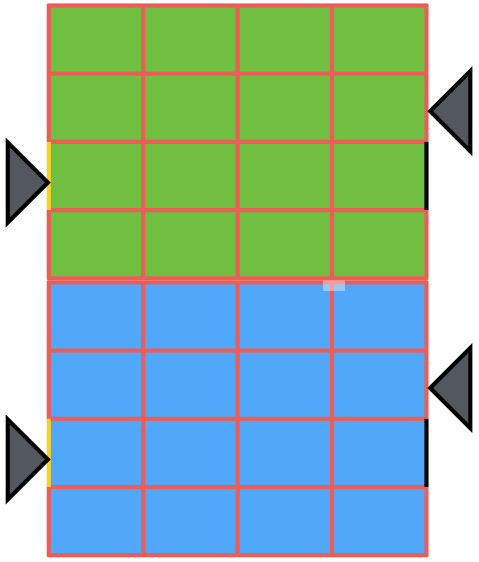
t′/t= =0.4



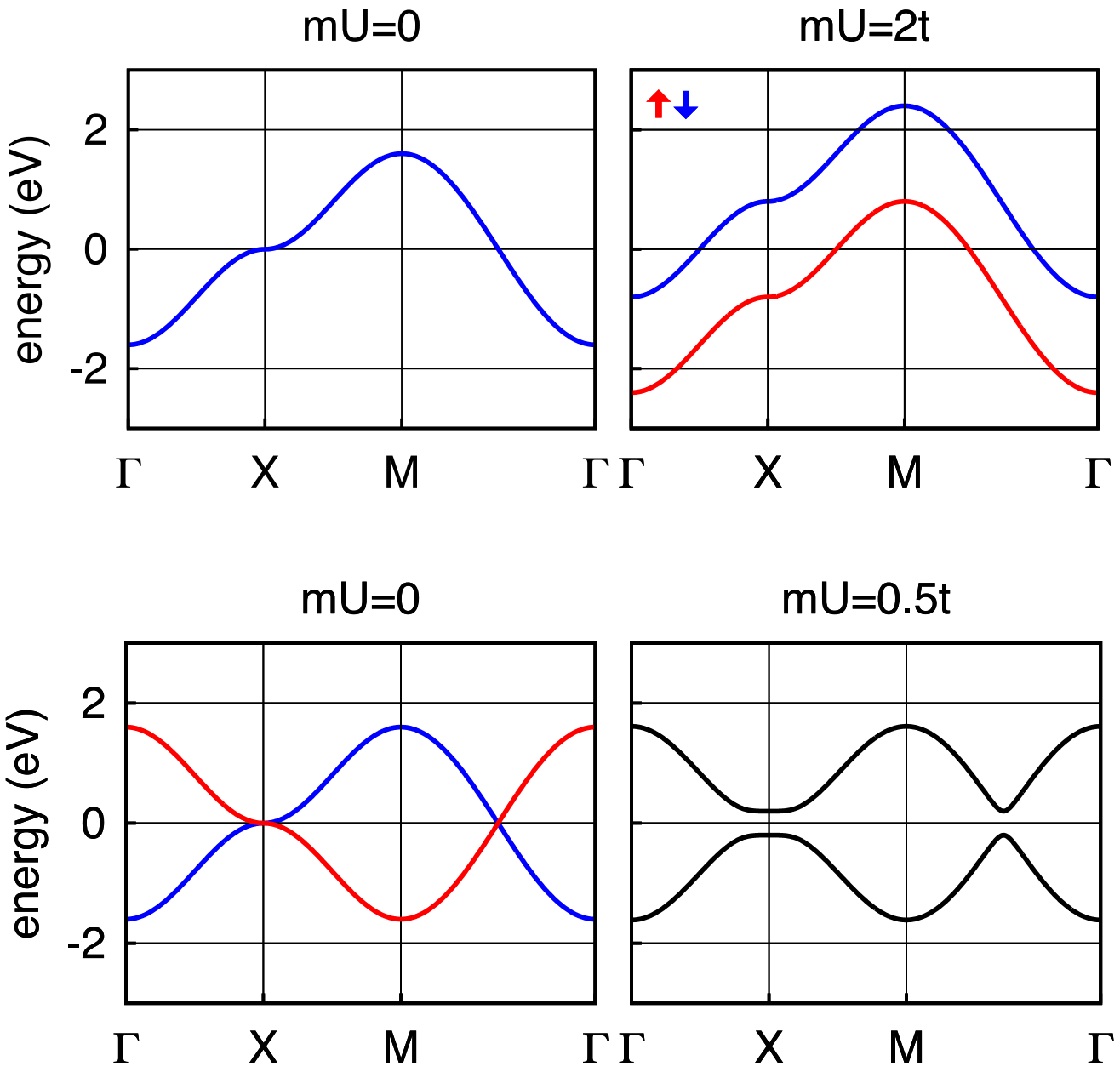
half filling (1 particle per site): 8+8



one box for star,
one for circles?

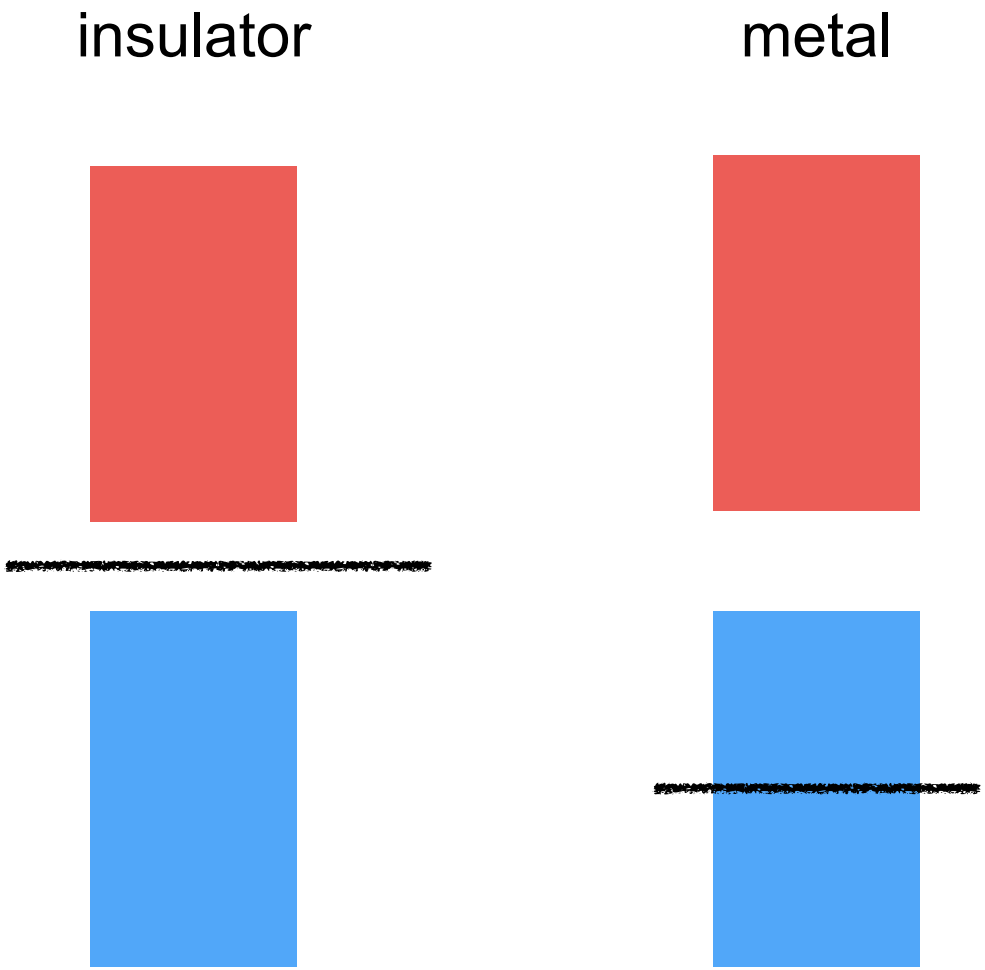


how could I open a gap?



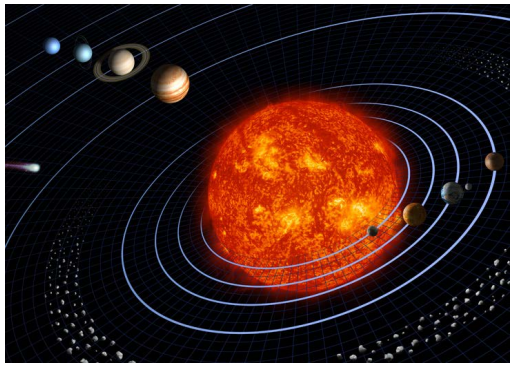
works but magnetic…

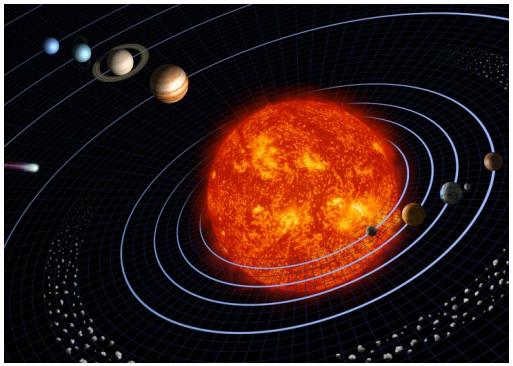
origin of failures: one-electron picture

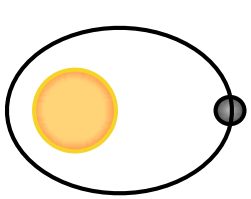


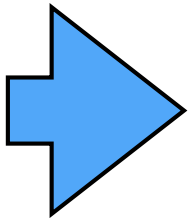
can I *cure* this ? No!

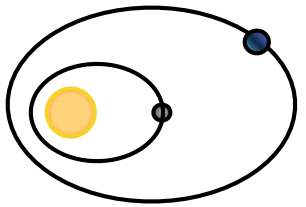
we need a new method





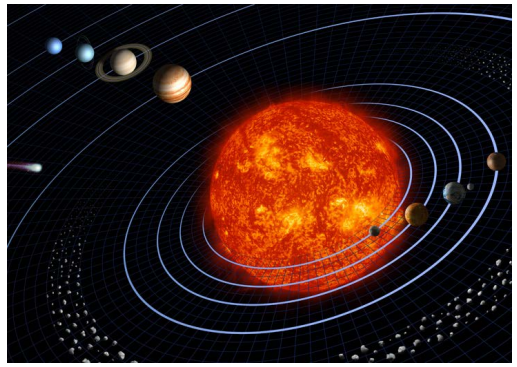






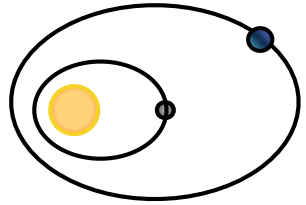
1. minimal models that capture the phenomenon

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$



minimal model for metal-insulator transition

$$H = -t \sum_{\sigma} \sum_{\langle ii' \rangle} c_{i\sigma}^\dagger c_{i'\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$



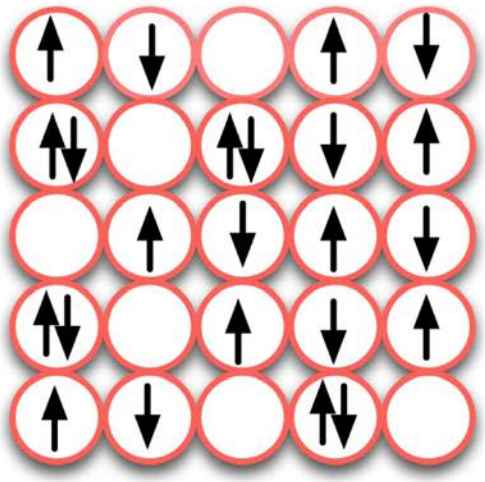
Hubbard model at half filling

local Coulomb produce strong correlation effects

Hubbard model at half-filling

atomic hoppings atomic

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U$$



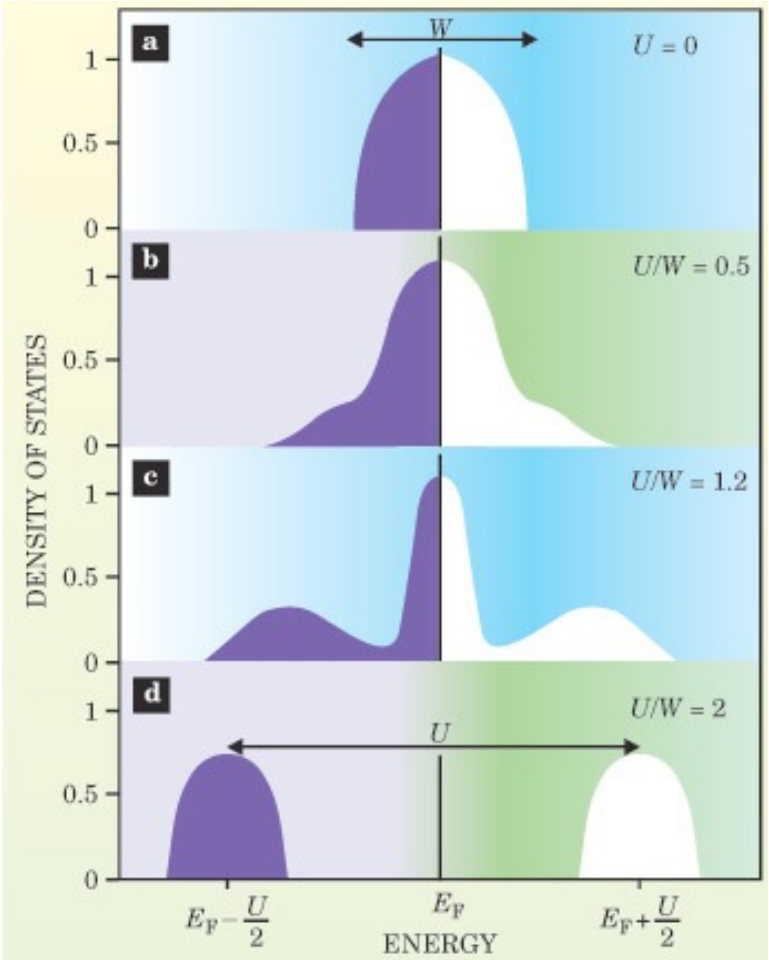
1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

2. find approximate methods that work

dynamical mean-field theory

metallic phase

transition



insulating phase

G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)

Dynamical Mean-Field Theory (DMFT)

Korrelierte Gitter-Fermionen
in hohen Dimensionen

Von der Mathematisch-Naturwissenschaftlichen Fakultät
- Fachbereich 1 -
der Rheinisch-Westfälischen Technischen Hochschule Aachen
zur Erlangung des akademischen Grades
eines Doktors der Naturwissenschaften
genehmigte Dissertation

vorgelegt von

Diplom-Physiker

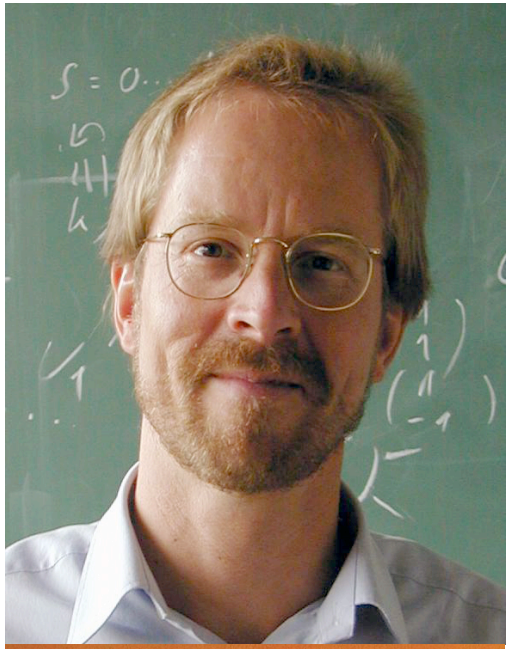
Walter Metzner

aus

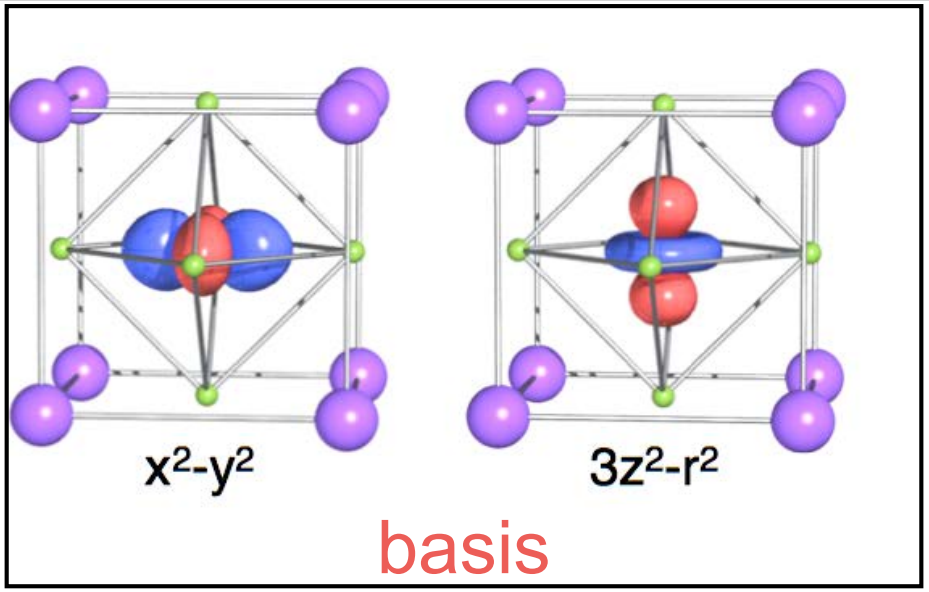
München

Referent: Universitätsprofessor Dr. D. Vollhardt
Korreferent: Universitätsprofessor Dr. G. Czycholl

Tag der mündlichen Prüfung: 19. Dezember 1989



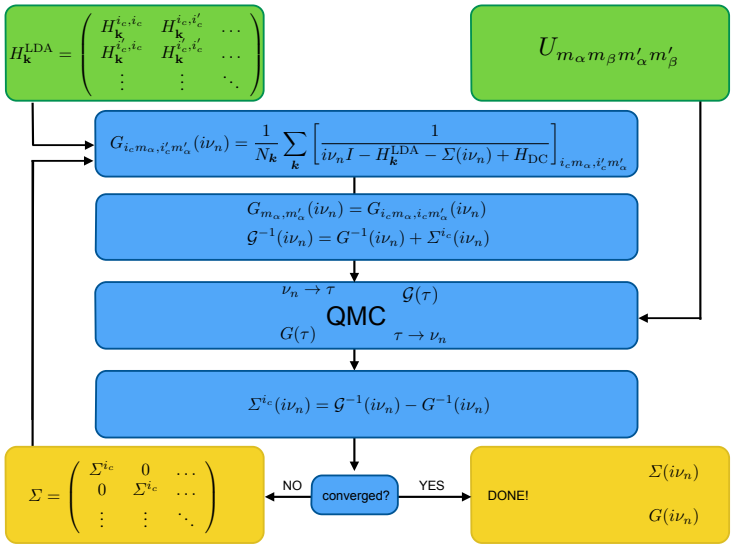
3. make it more realistic: LDA+DMFT



basis

$$
\begin{aligned}
H = & - \sum_{ii'} \sum_{mm'} \sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} \\
& + U \sum_{im} n_{im\uparrow} n_{im\downarrow} \\
& + \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} \\
& - J \sum_{m \neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})
\end{aligned}
$$

models

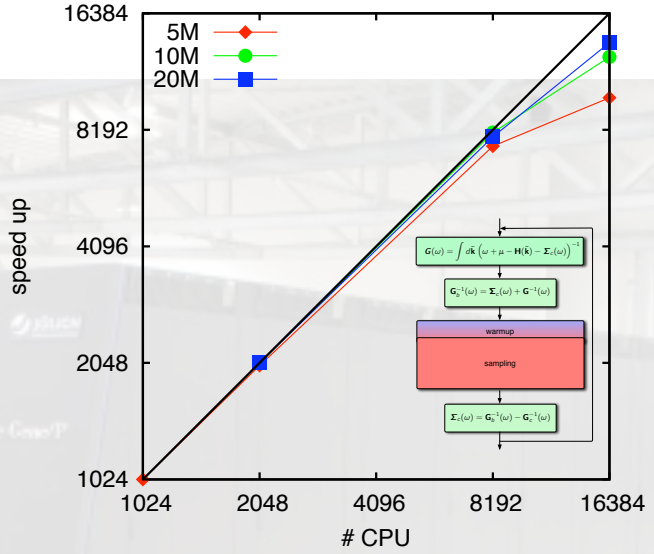


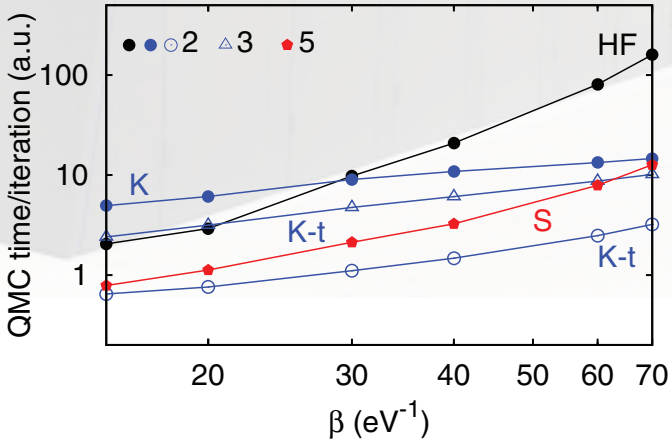
method extensions

where to learn this: lectures SS+ autumn school

we need supercomputers!

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma}$$
$$+ U \sum_{im} n_{im\uparrow} n_{im\downarrow}$$
$$+ \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'}$$
$$- J \sum_{m \neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$





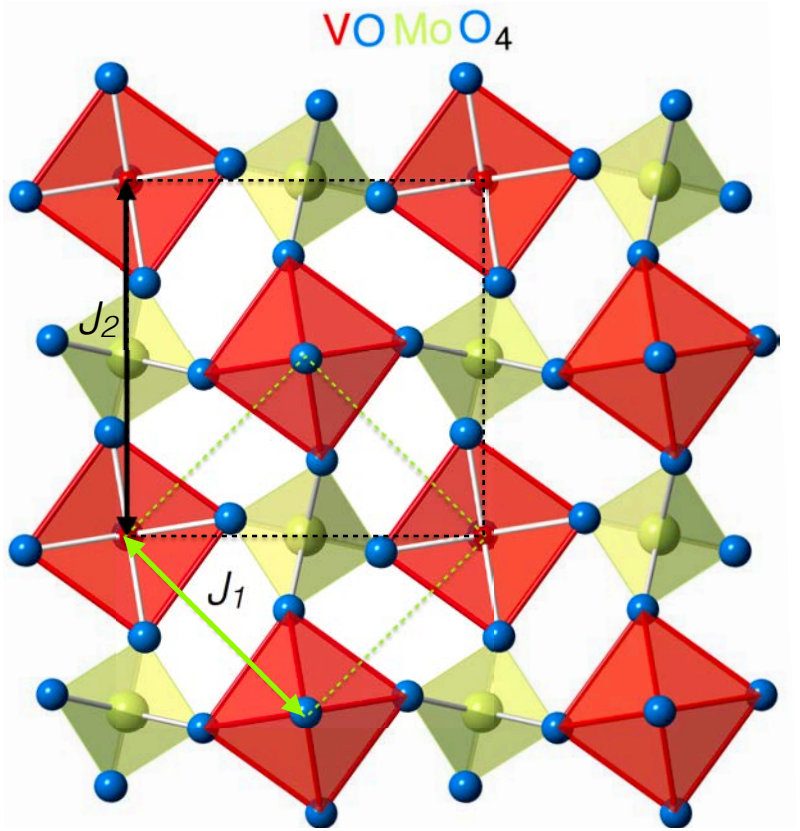
DMFT and cDMFT

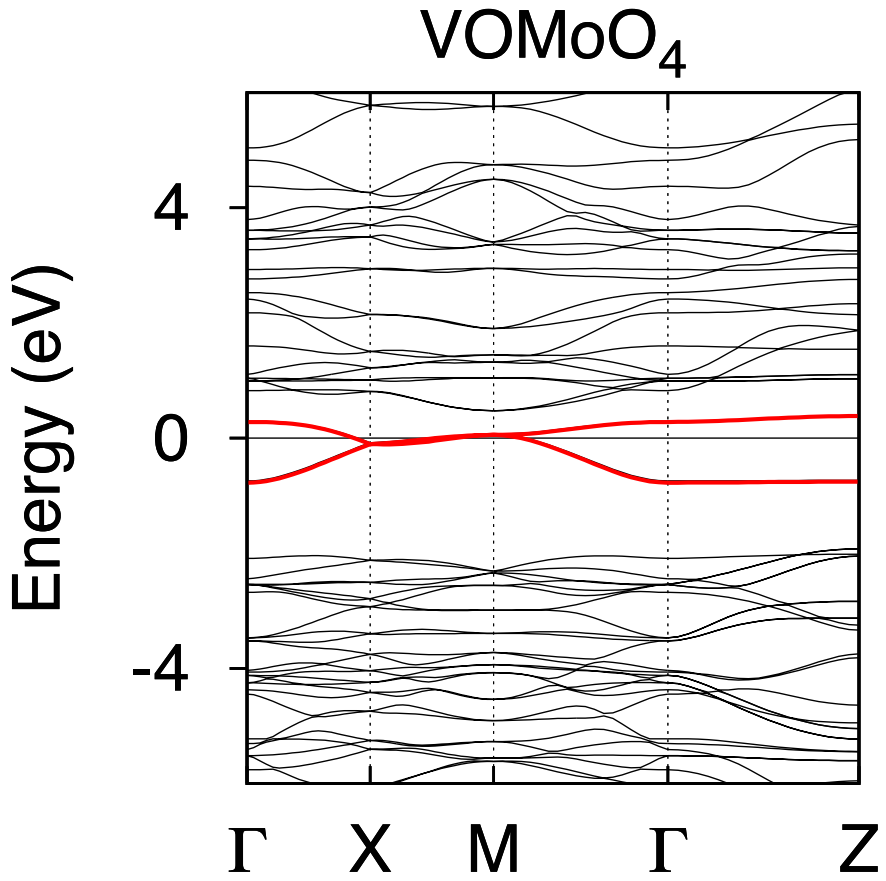
quantum impurity solvers:

general HF QMC
general CT-INT QMC
general CT-HYB QMC

JÜLICH
FORSCHUNGSZENTRUM

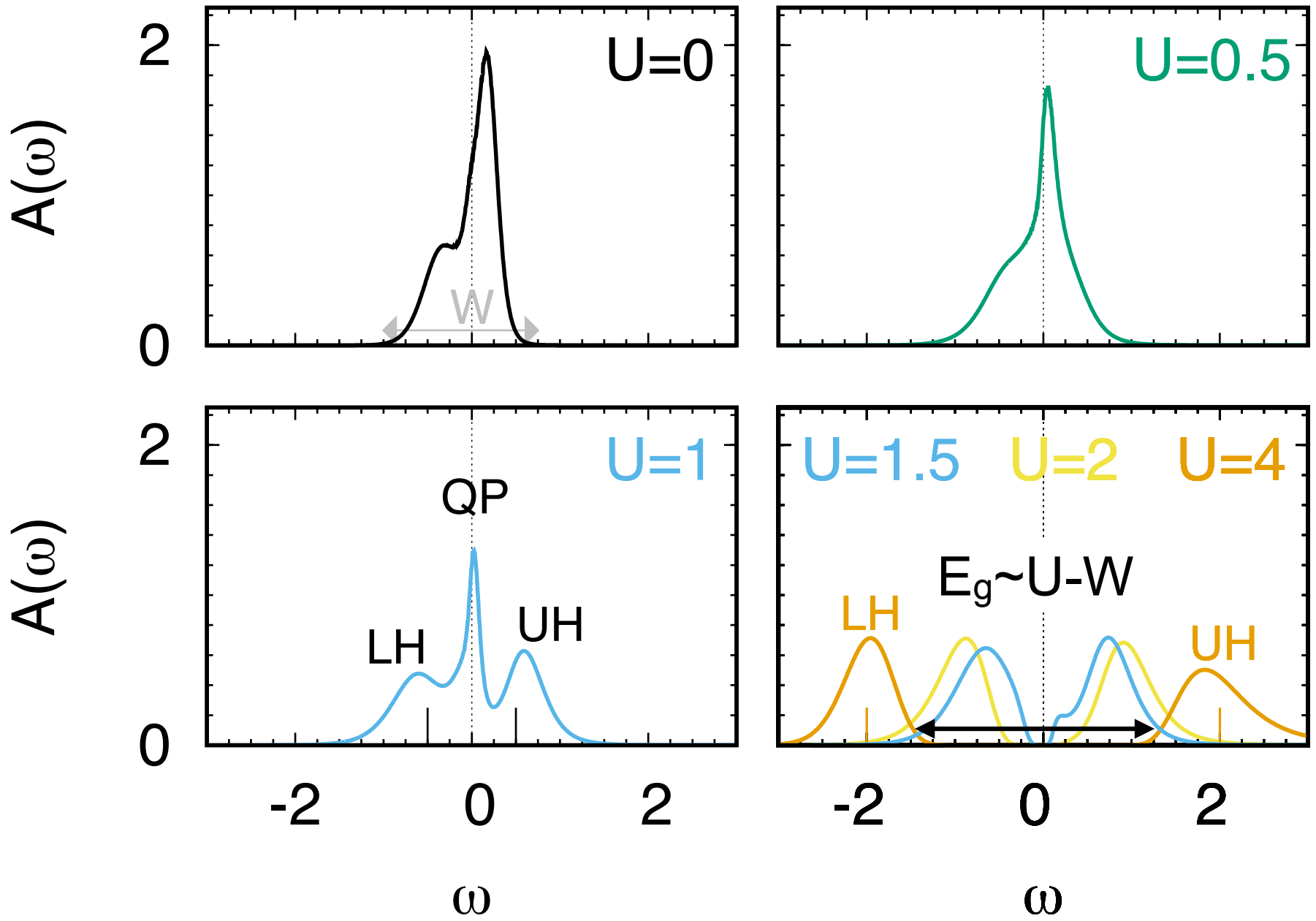
a real-system case: $VOMoO_4$





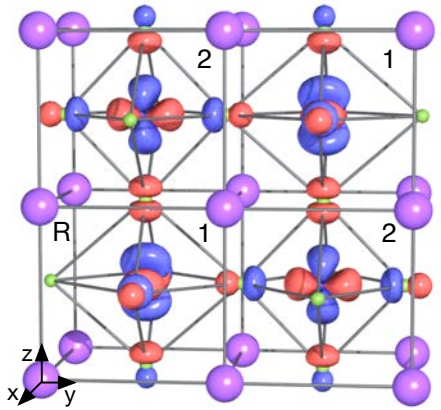
Amin Kiani and Eva Pavarini, Phys. Rev. B **94**, 075112 (2016)

a real-system: $VOMoO_4$

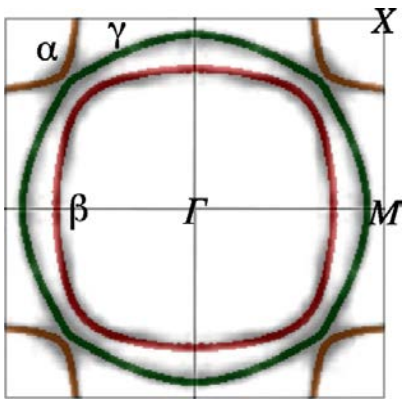


what can we do?

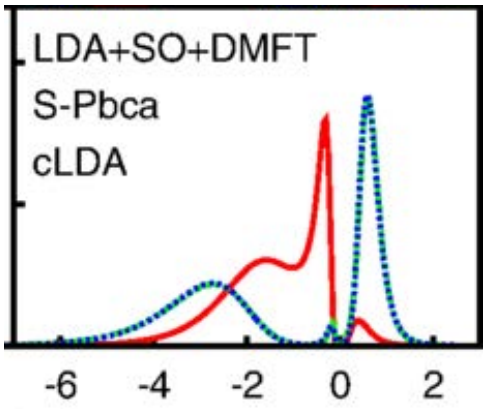
orbital order



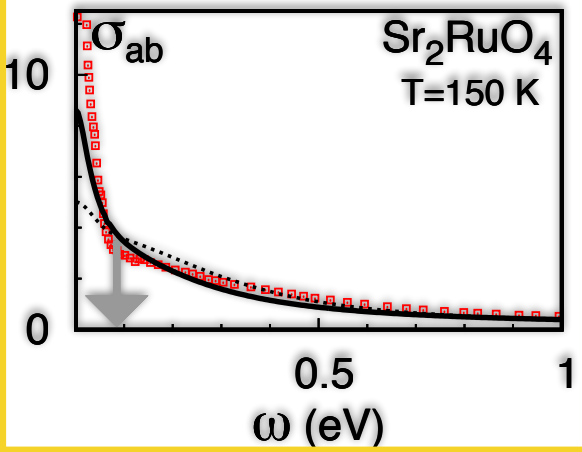
Fermi surface



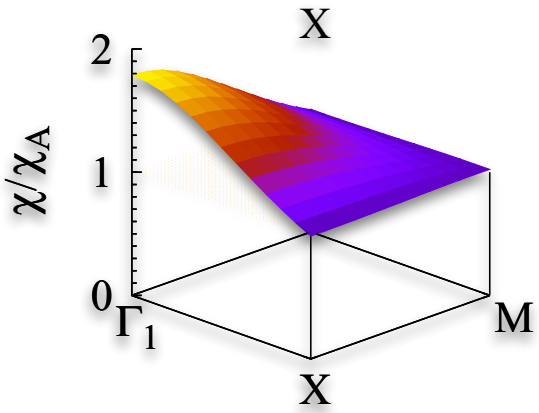
spin-orbit



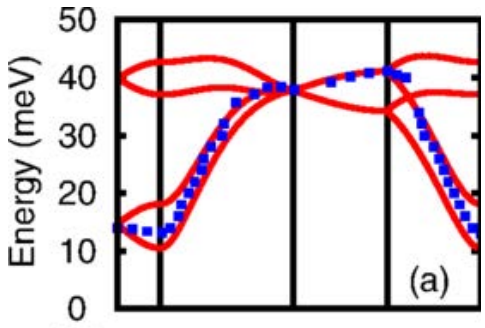
conductivity



response functions



spin waves

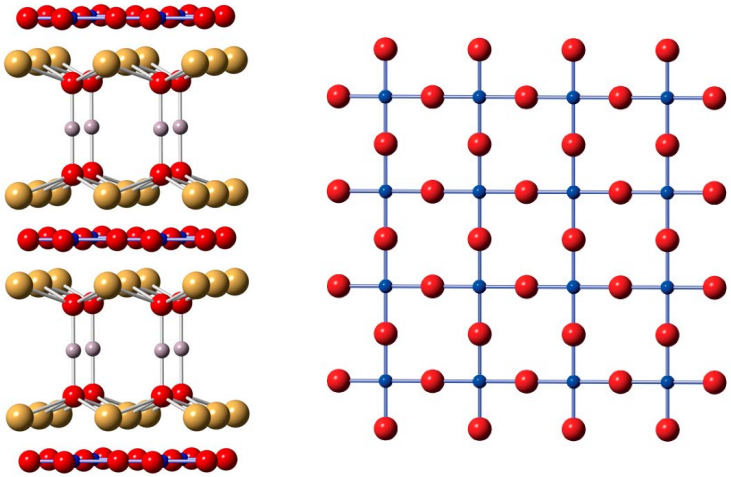


many fundamental problems still open!

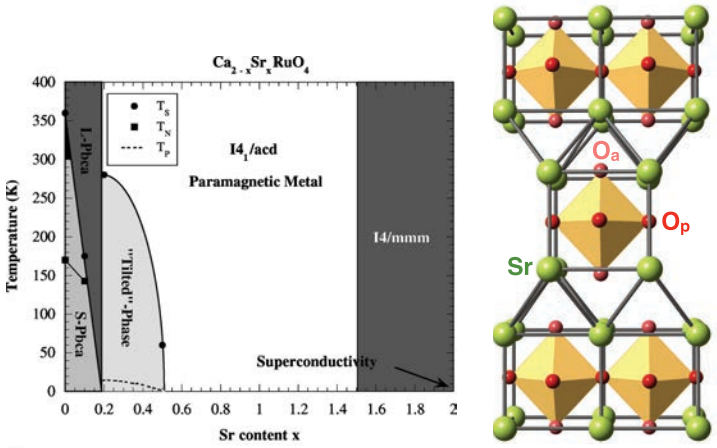
many fundamental problems still open!

high-temperature superconductivity

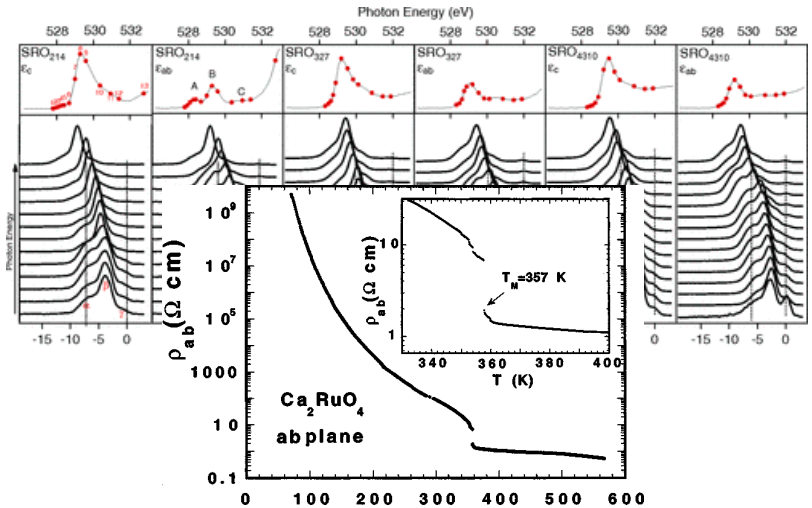
$HgBa_2CuO_4$



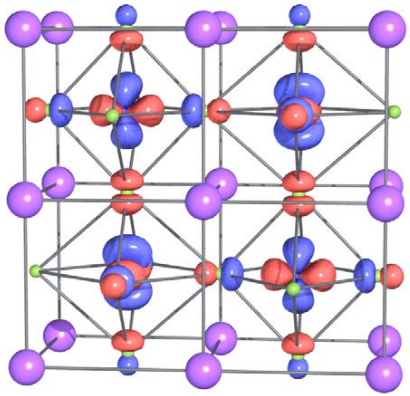
unconventional superconductivity



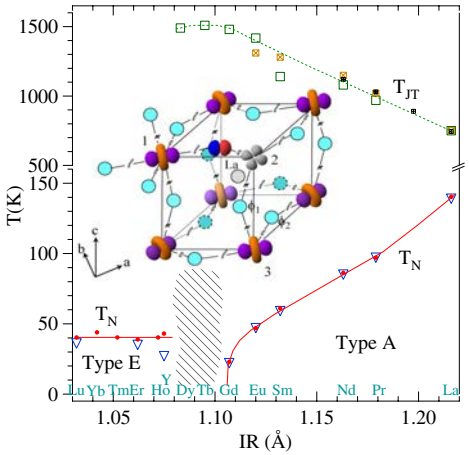
the metal-insulator transition



orbital order



order-to-disorder



what can be a seminar topic?

topics for seminars

- theory: the many-body problem
- model building: tight-binding theory
- model building: Wannier functions
- model building: DFT/LDA bands
- model building: Coulomb tensor
- model solving: DMFT self-consistent loop
- model solving: Hartree-Fock approximation
- model solving: Monte Carlo method
- model solving: 2-site problem, DMFT vs exact solution
- physics: the metal-insulator transition

seminar example

- model building: tight-binding theory

- motivation
- atomic orbitals
- definition of hopping integrals and overlaps
- the case of a linear chain
- the case of a square lattice: HTSCs
- the case of an hexagonal lattice: graphene

- outlook: build model for real material

seminar example

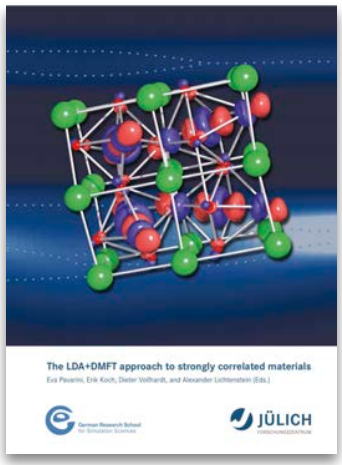
- model solving: Monte Carlo method
- motivation
- random numbers and random number generators
- statistical errors
- application: integrals
- applications: Ising model
- outlook: quantum Monte Carlo

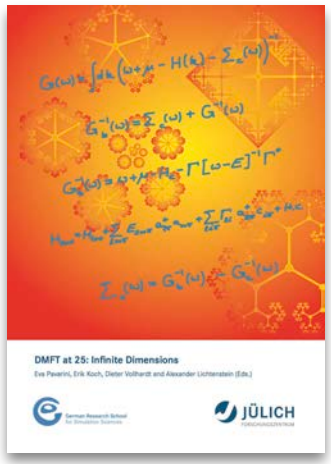
what should you bring?

- motivation
  - interest in physics
  - interest in quantum mechanics
  - interest in computational science
  - interest in mathematics
- knowledge (for physics focus)
  - functions, analysis
  - linear algebra
  - basic statistical mechanics
  - one programming language
  - quantum mechanics
- knowledge (for seminar)
  - functions, analysis
  - linear algebra
  - understand programming
  - basics quantum mechanics

summer term: mandatory (physics)

Computational Many-Body Physics



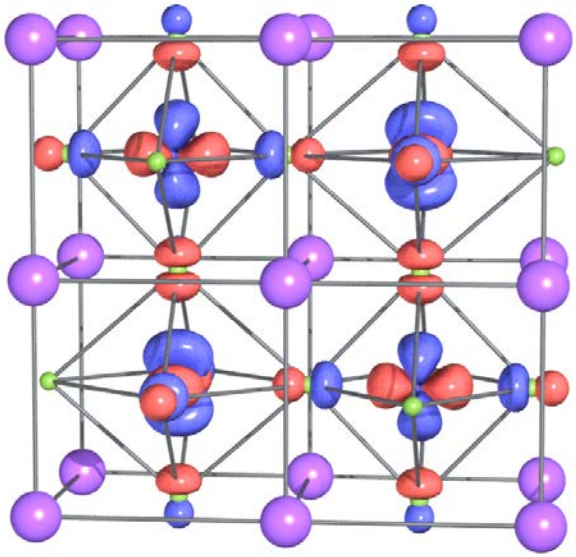


- Solid state physics as many-body problem
- Second quantization
- Electron gas
- Hubbard model and *t*-*J* model
- Two-site Hubbard model
- Matsubara formalism and many-body perturbation theory
- Green function and self-energy
- Mean-field/Hartree-Fock method
- Fermi-liquid theory
- Dynamical mean field theory (DMFT)
- Mott transition

http://iffwww.iff.kfa-juelich.de/~pavarini/SS/lecture.html

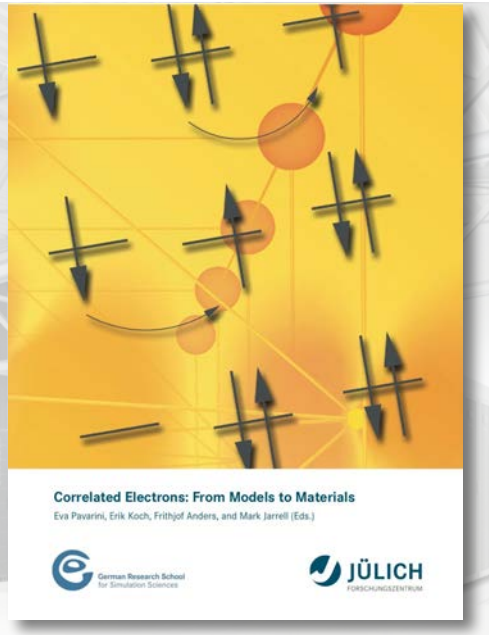
summer term: elective

Correlated Electrons



- Many-electrons in atoms, ions, and molecules
  - direct exchange and Hund's rules
  - kinetic exchange and antiferromagnetism
- crystal-field theory
  - Symmetries in solids
  - JahnTeller effect
- Mott transition and the Hubbard model
  - second quantization and configuration representation
  - limiting cases of the Hubbard model
- Mott insulators
  - t-J model and orbital ordering

www.cond-mat.de/teaching/correl/

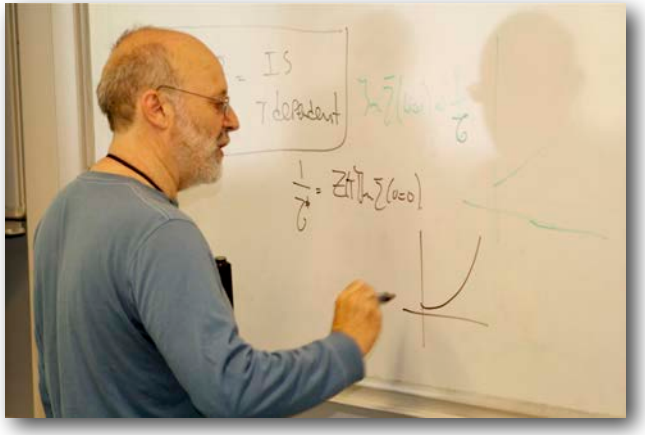


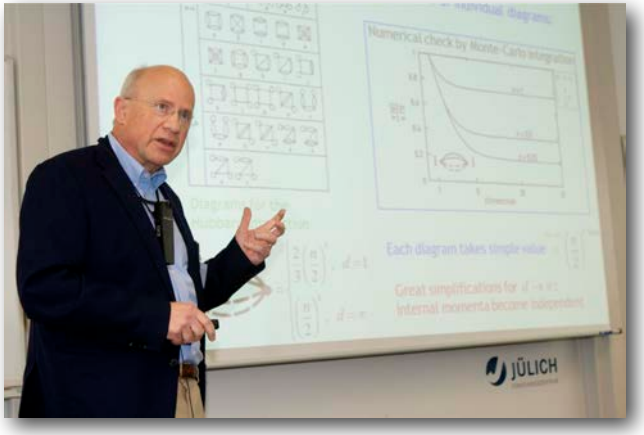
Autumn School on Correlated Electrons

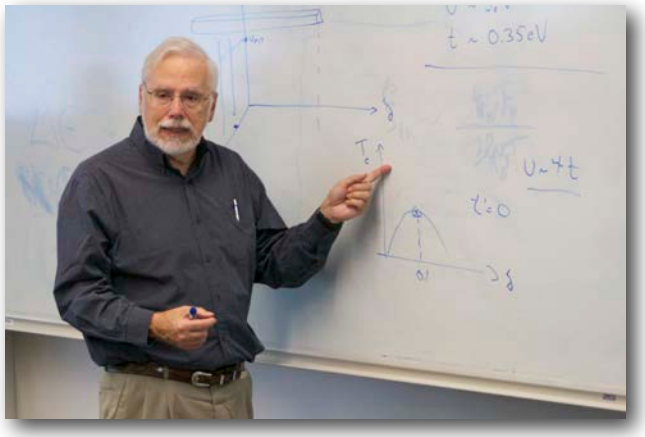
every year in september

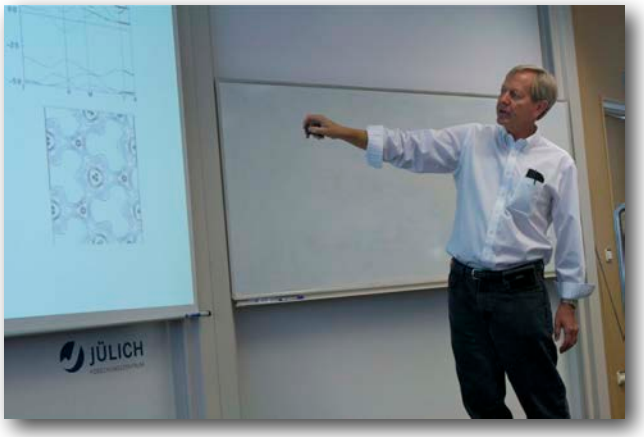
17-21 September 201, Forschungszentrum Jülich

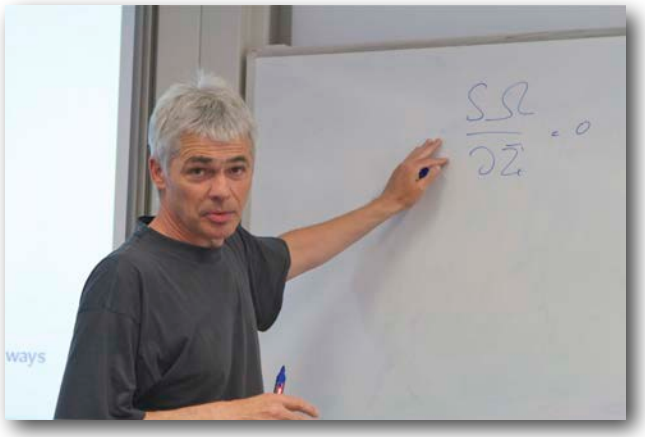
world leading lecturers

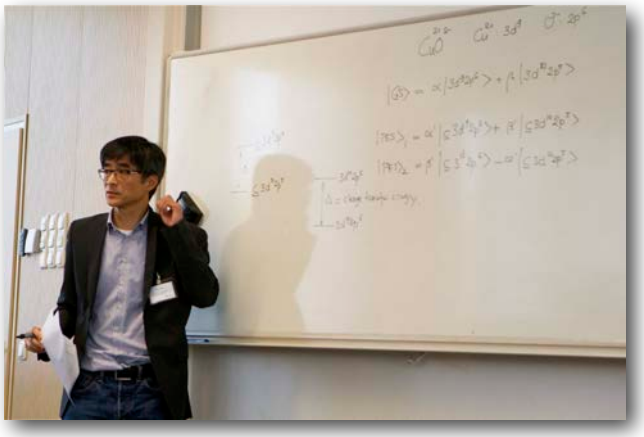












questions time

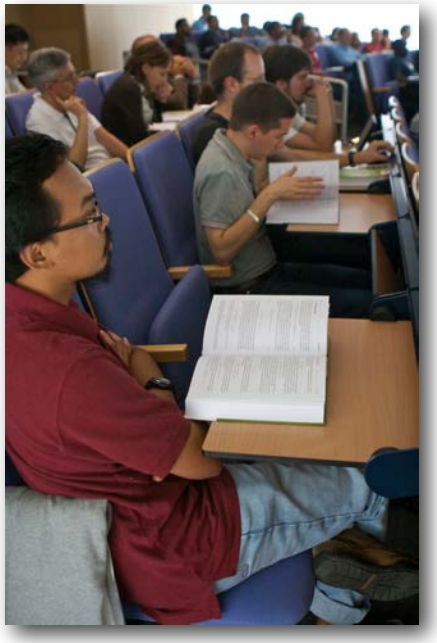








popular lecture notes

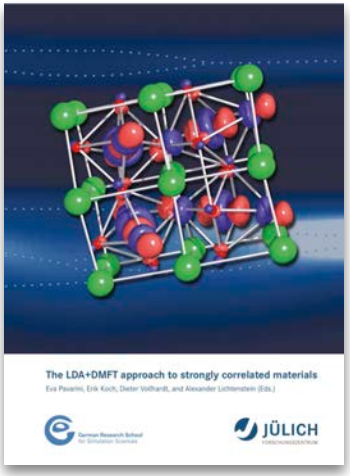




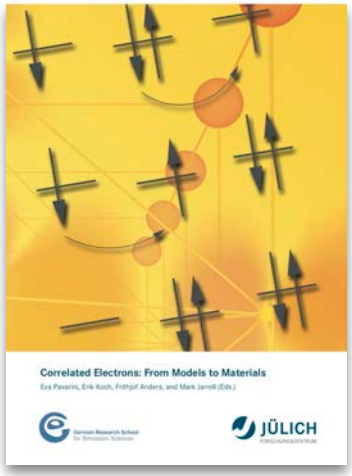


Autumn School on Correlated Electrons

http://www.cond-mat.de/events/correl.html



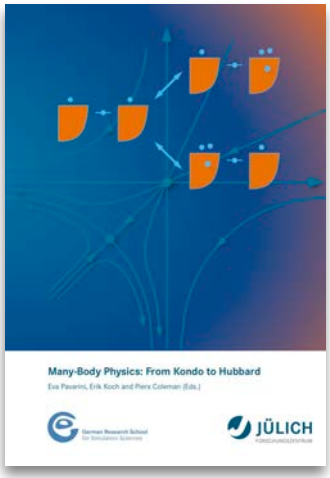
2011



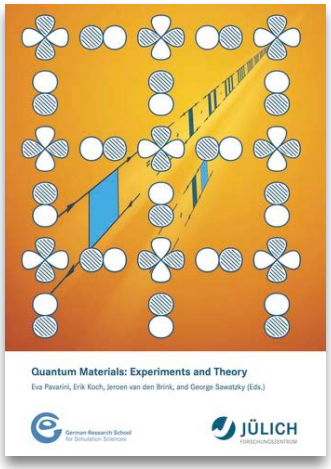
2012

2013

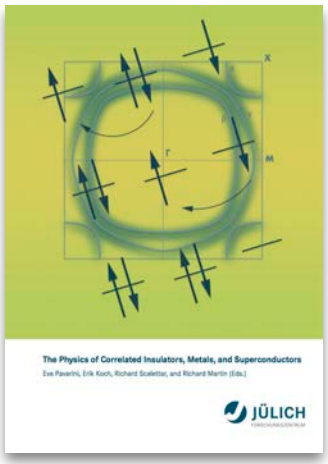
2014



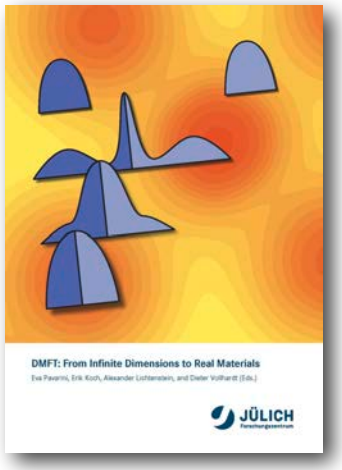
2015



2016



2017

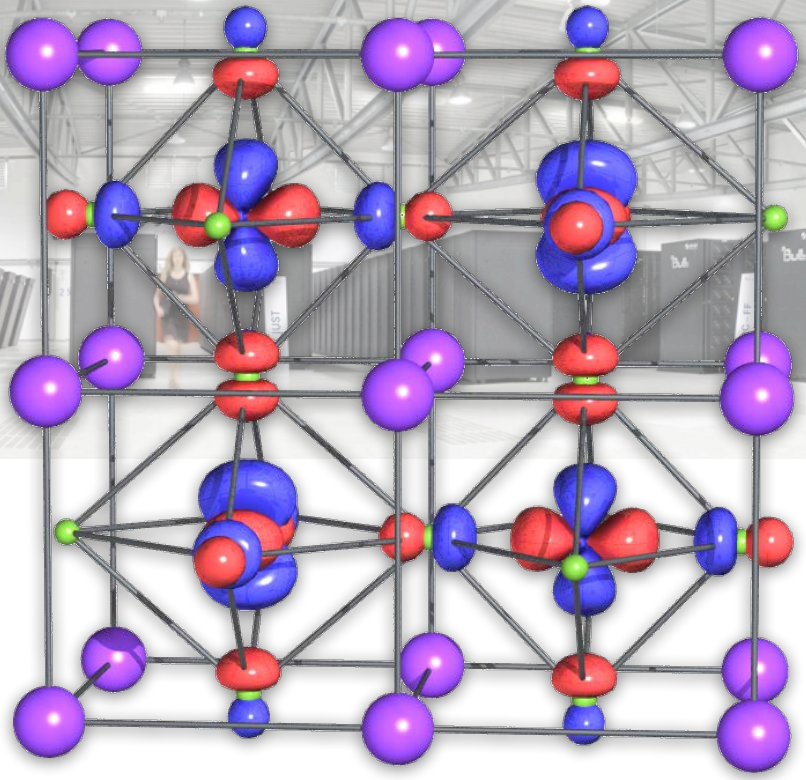


2018

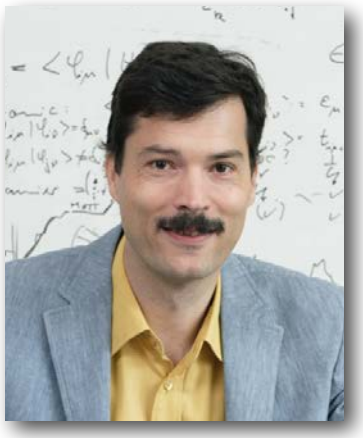
physics of strongly-correlated systems

http://iffwww.iff.kfa-juelich.de/~pavarini/group.html

http://www.grs-sim.de/research/computational-materials-science/team/koch.html



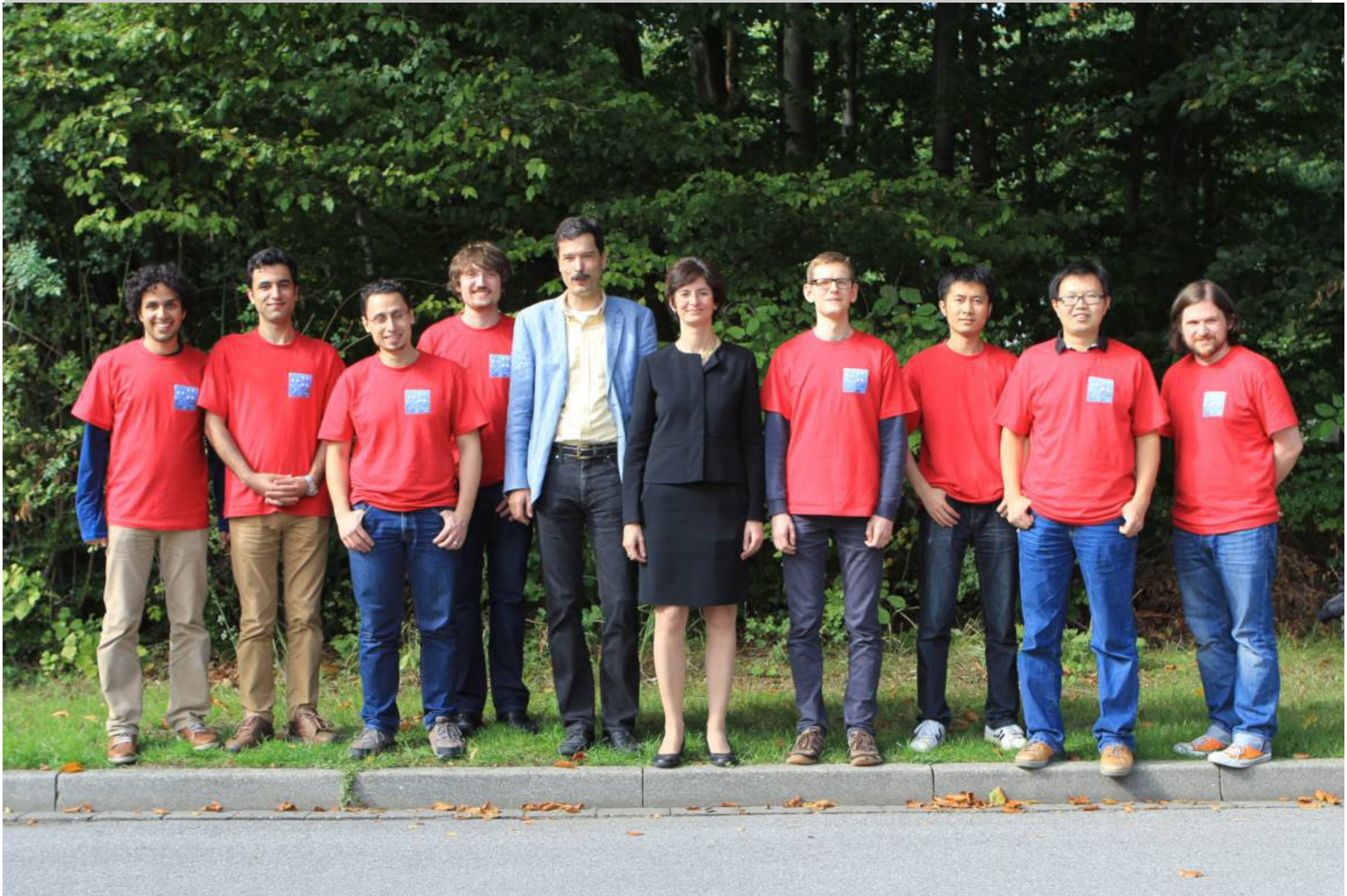
Erik Koch



E.Koch@fz-juelich.de

Eva Pavarini

E.Pavarini@fz-juelich.de



thank you!