DFT+DMFT及其在重费米子体系的应用

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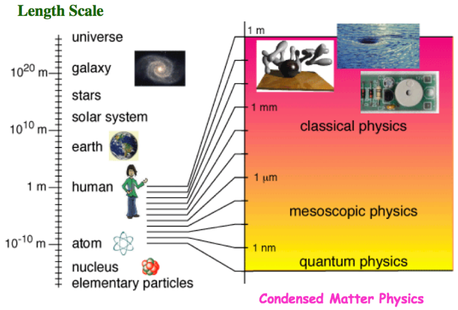
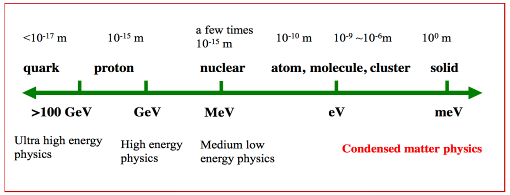
国家自然科学基金委员会 National Natural Science Foundation of China

Density Functional Theory

Condensed Matter Physics

Condensed matter physics is the science that studies microscopically the **structures**, laws of motion and macroscopic properties of condensed matter composed of **interacting many particles**.

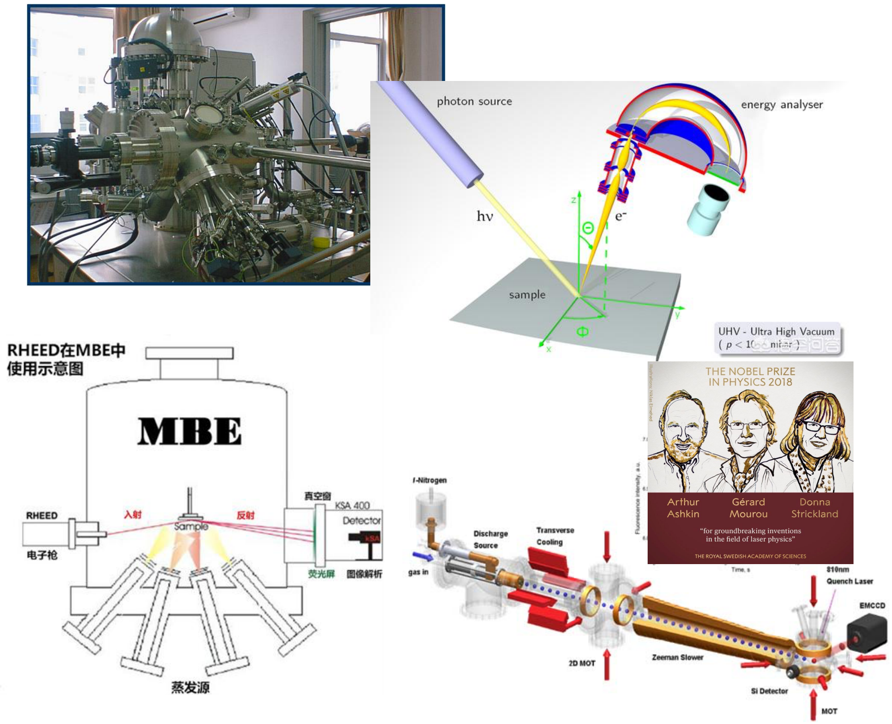


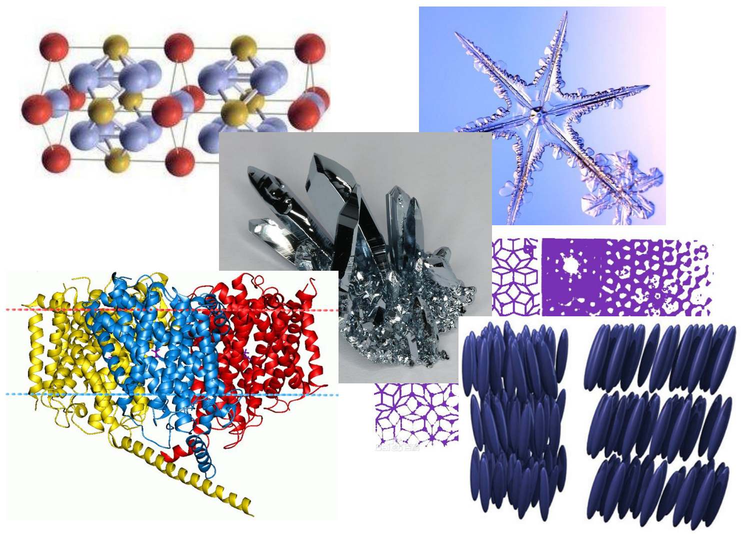


形形色色的实验探测手段

✓存在大量不同的物质宏观状态

✓微观上是复杂的相互作用多电子体系



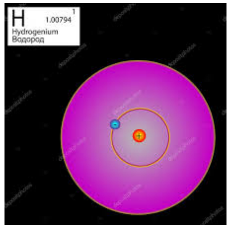


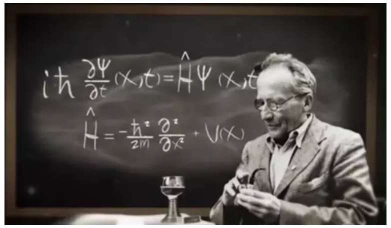
自然界中的各种宏观物态

HOW TO DEAL WITH THE COMPLEX SYSTEMS FOR THEORETICAL EXPLORING?

Density Functional Theory

Quantum mechanism





利用薛定谔方程求解量子力学问题

A quantum many body problem

$$\hat{H}=\sum_i -\frac{\hbar^2}{2M_i}\nabla^2_{R_i}-\sum_i \frac{\hbar^2}{2m_e}\nabla^2_{r_i}-\frac{1}{4\pi\varepsilon_0}\sum_{i,j}\frac{e^2 Z_i}{|R_i-r_j|}+\frac{1}{8\pi\varepsilon_0}\sum_{i\neq j}\frac{e^2}{|r_i-r_j|}+\frac{1}{8\pi\varepsilon_0}\sum_{i\neq j}\frac{e^2 Z_i Z_j}{|R_i-R_j|}$$

Born-Oppenheimer approximation

$$\hat{H}(r_i,R_\alpha)=\hat{H}^{el}_{R_\alpha}(r_i)$$

Time-independent Schrödinger equation

$$\hat{H}^{el}\psi_n(x_1,x_2,\cdots,x_n)=E_n\psi_n(x_1,x_2,\cdots,x_n)$$

$$\hat{H}^{el}=-\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla^2_{r_i}-\frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{n}\sum_{\alpha}\frac{Z_\alpha e^2}{|R_\alpha-r_i|}+\frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{n}\sum_{j>i}\frac{e^2}{|r_i-r_j|}$$

Electronic energy: functional of Ψ_n

$$E_n[\psi_n]=\frac{\langle\psi_n(x_1,\cdots,x_n)|\hat{H}^{el}|\psi_n(x_1,\cdots,x_n)\rangle}{\langle\psi_n(x_1,\cdots,x_n)|\psi_n(x_1,\cdots,x_n)\rangle}$$

Density functional theory

Use the electron density ρ(r) as the basic variable, instead of the n-electron wave-function $\Psi_n(x_1,\cdots,x_n)$.

Hohenberg and Kohn (1964)

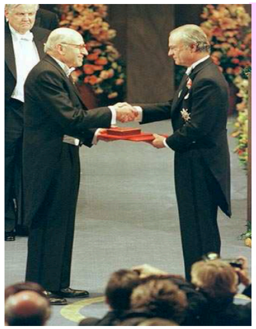
The Ground-State properties of any system of n-interacting particles are rigourously deduced from the electron density distribution ρ(r).

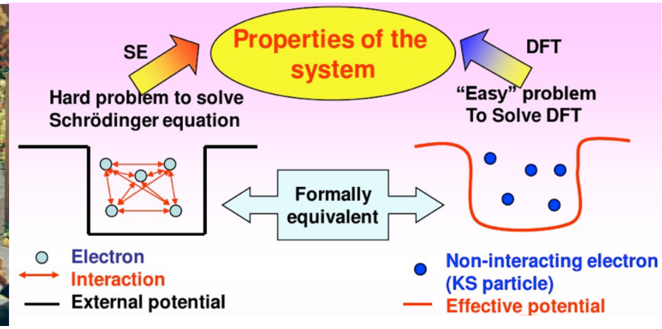
Theorem HK1: There is a unique correspondence $v(r)\longleftrightarrow\rho(r)$

$$E_v[\rho]=\int\rho(r)v(r)dr+F_{HK}[\rho]$$

Theorem HK2: ρ(r) minimizes E[ρ]

$$E_v[\rho]=\min_\rho\left\{F_{HK}[\rho]+\int\rho(r)v(r)\right\}$$





Kohn–Sham Equation

A quantum many body problem:

$$\hat{H} = \hat{T} + \hat{V}_{Ne} + \hat{V}_{ee}$$

$T[\rho]$ unknown $V_{ne}[\rho]$ known $V_{ee}[\rho]$ unknown

We are still left with the many-body problem ...
We need a trick to solve this equation

Using an auxiliary system of n non-interacting particles for which the kinetic energy is know:

$$\rho_s(r) = \sum_{i=1}^{n} \left|\phi_i(r)^2\right| \qquad E[\rho] = T_0[\rho] + V_{Ne}[p] + V_H[\rho] + V_{xc}[\rho]$$

Kohn-Sham equation:

$$\sum_{i=1}^{n} \left\{ -\frac{1}{2m_e}\nabla_i^2 + V_{eff}(r) \right\} \phi_i(r) = \sum_{i=1}^{n} \varepsilon_i \phi_i(r)$$

The exchange-correlation functional

$$E_{xc}[\rho] = \int \varepsilon_{xc}[\rho]\rho(r)dr$$

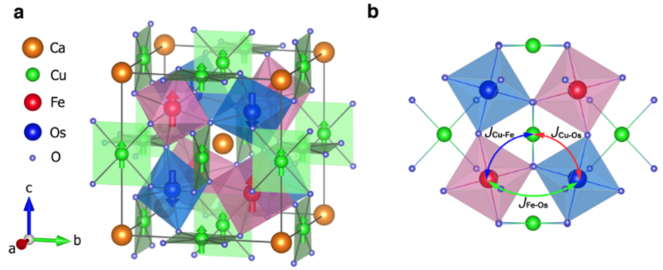
- Local Density Approximation (LDA)
- Generalized Gradient Approximation (GGA)
- Meta Generalized Gradient Approximation (meta-GGA)

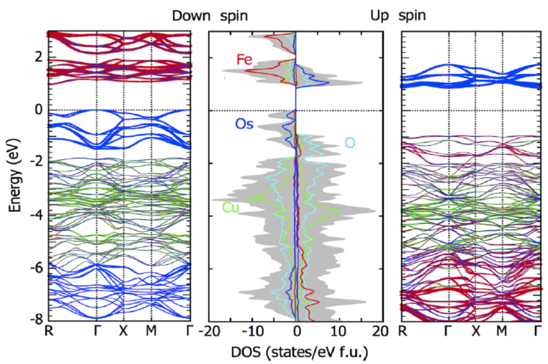
$$\epsilon_{xc}[\rho] = f(\rho, \nabla\rho, \Delta\rho, \ldots)$$

Success of Density Functional Theory

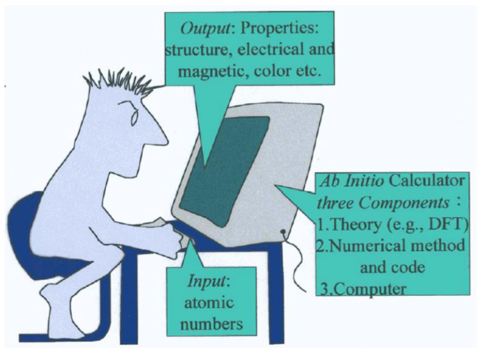
传统的磁性与自旋态的研究

$CaCu_3Fe_2Os_2O_{12}$





$$H = \sum_{\langle ij \rangle} J_{ij} S_i \cdot S_j$$

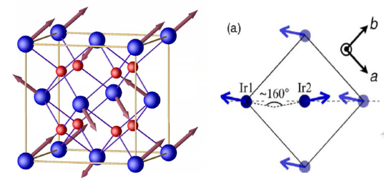


Phys. Rev. B 94, 024414 (2016)
Phys. Rev. Materials 1, 024406 (2017)

J. Phys.: Condens. Matter **29,** 244001 (2017)
Sci. Rep. **7**, 14178 (2017)

复杂磁性(非共线磁性)与奇异物态（超导）的研究

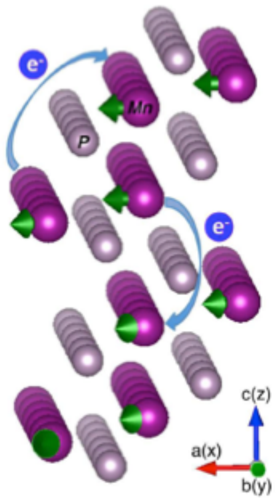
Canted AFM



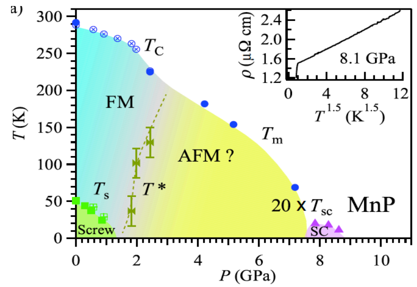
Spin spirals

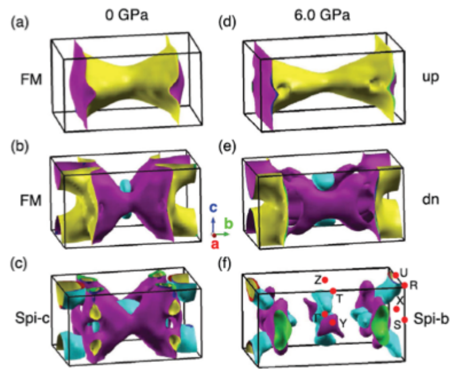
"Generalized Bloch Theorem"

$$\psi_k(r) = e^{ik\cdot r} \begin{pmatrix} e^{\frac{-iq\cdot r}{2}} u_k^{\uparrow}(r) \\ e^{\frac{iq\cdot r}{2}} u_k^{\downarrow}(r) \end{pmatrix}$$



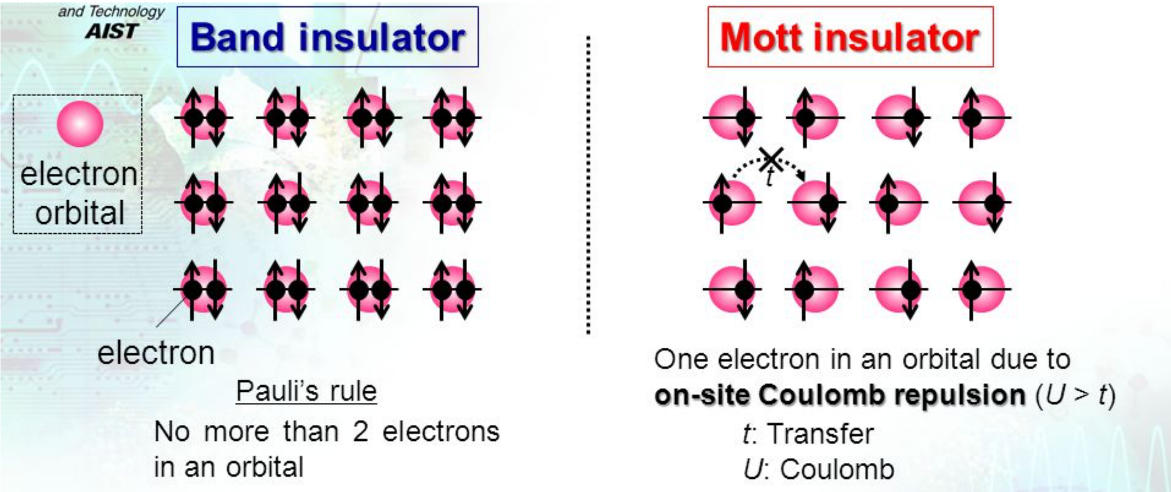
MnP

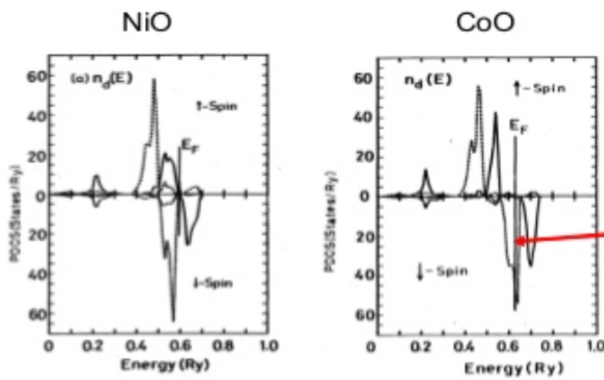




Breakdown of Density Functional Theory

The role of electronic correlations: localization versus itinerancy



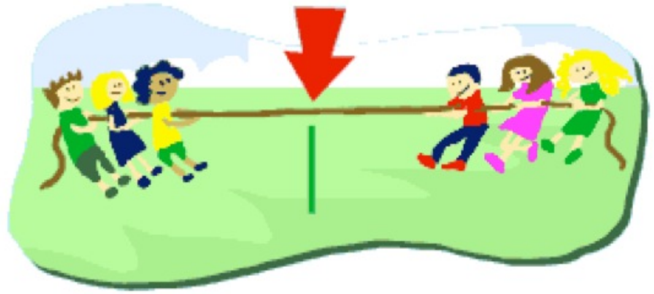


NiO and CoO are experimentally wide gap insulators (Mott insulators) but LSDA gave small gap insulator for NiO and metal for CoO with partially filled t_{2g} spin-down electronic subshell

多体关联效应

$$H = H_{kinetic} + H_U$$

Coulomb X Kinetic

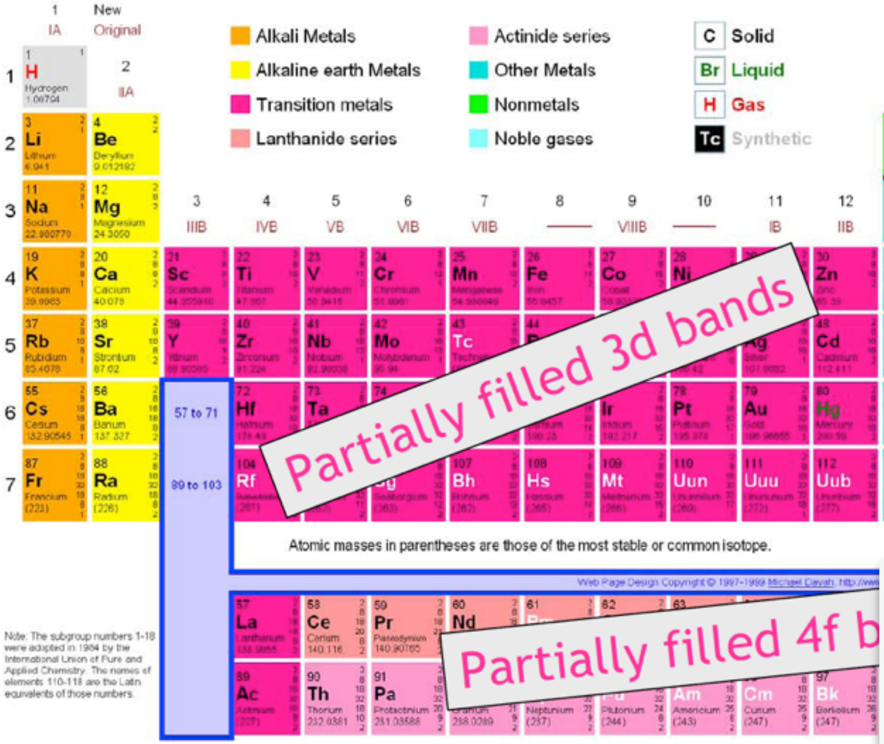


局域 versus 巡游

有趣的物理往往都发生在两者交界， 如 高温超导 等等

缺乏共识，需要进行严格的数值求解以进行裁决！

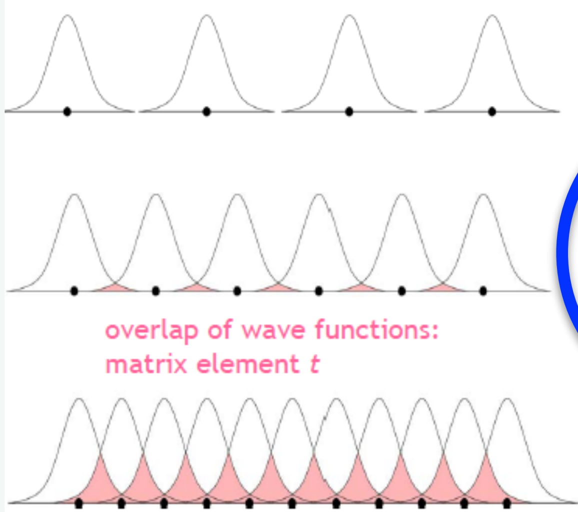
Breakdown of Density Functional Theory



Narrow 3d, 4f orbitals

Strong electronic correlation

Electronic Bands in Solids

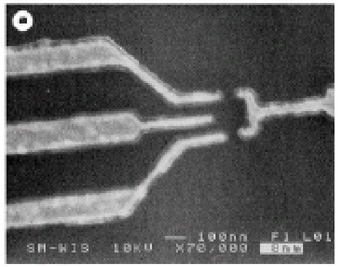


Property	Energy levels	Character, Repre-sentation	Example
Insu-lator	Atomic levels	Localized electrons $n_{i\sigma}$	Solid Ne NaCl
Corre-lated metal	Narrow bands	$n_{i\sigma} \leftrightarrow n_{k\sigma}$	Tran-sition + rare earth metals (Ni, V_2O_3, Ce
Simple metal	Broad bands	Extended waves $n_{k\sigma}$	Na, Al

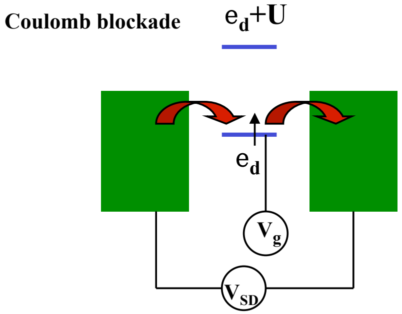
The Kondo problem

Single Impurity Kondo Problem

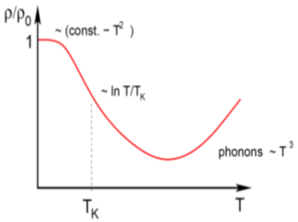
Kondo effect in quantum dot

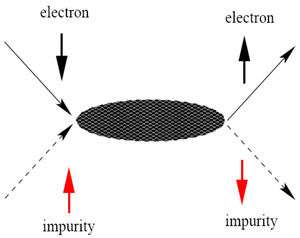


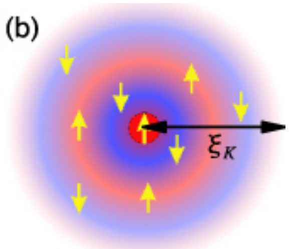
single quantum dot



Kondo effect



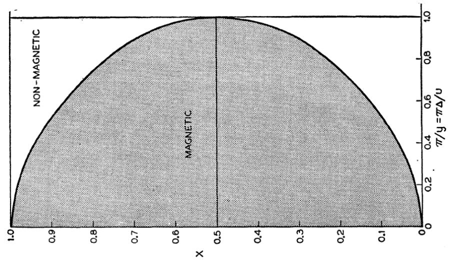




At low temperature, spin-flip scattering between conduction band and impurity site become important.

Anderson impurity model

$$H = \sum_{ks} \epsilon_k c^\dagger_{ks} c_{ks} + \sum_{s} \epsilon_d d^\dagger_s d_s + U n_{d\uparrow} n_{d\downarrow} + \sum_{ks} V c^\dagger_{ks} d_s + h.c$$

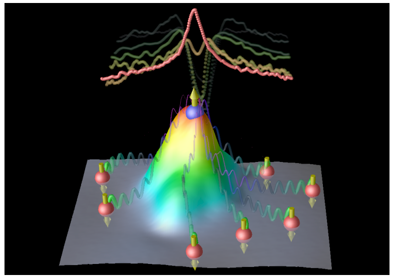


HOW TO SOLVE ANDERSON IMPURITY MODEL NUMERICALLY?

- Renormalization group approach
- Continues-time quantum Monte Carlo
- One-crossing approximation

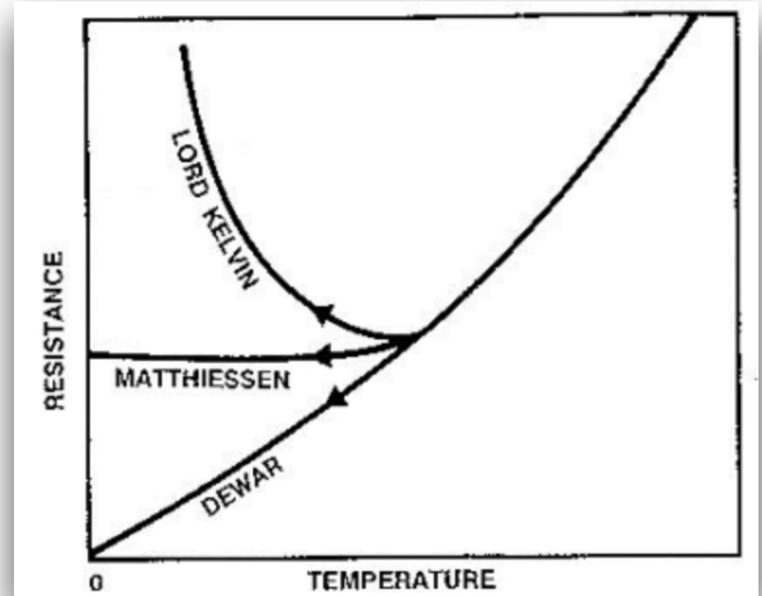
We usually call these numerical methods as "impurity solver", which is the most important in DMFT calculations.

Single Impurity Kondo Problem

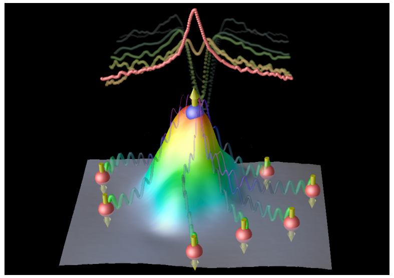


- **Historic development of Kondo**
  - ✓ (19th Century) Electron behavior @ T➔0

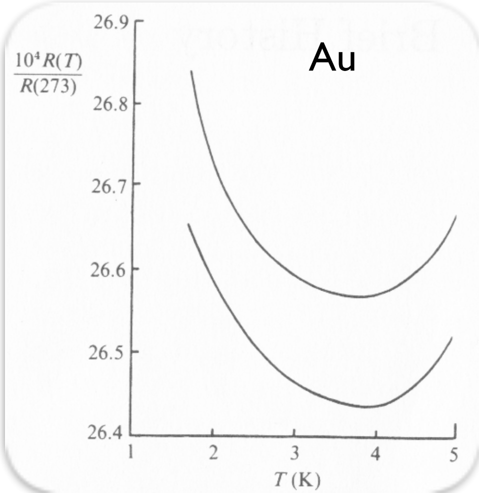
lnT	Kondo/2D WL
T	Non-Fermi liquid
T^2	Fermi liquid
T^5	Phonon scattering
$e^{-\Delta/T}$	Insulator/Semiconductor
$e^{T^{-1/n}}$	VRH (Semiconductor)
...	...



Single Impurity Kondo Problem

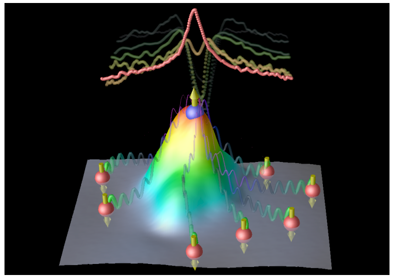


- **Historic development of Kondo**
  - ✓ (19th Century) Electron behavior @ T→0
  - ✓ Liquification & Resistance measurement
  - ✓ 1911-1957 Superconductivity EXP→THEO
  - ✓ 1934 Resistivity minima



de Haas, de Boer and van den Berg, 1934

Single Impurity Kondo Problem



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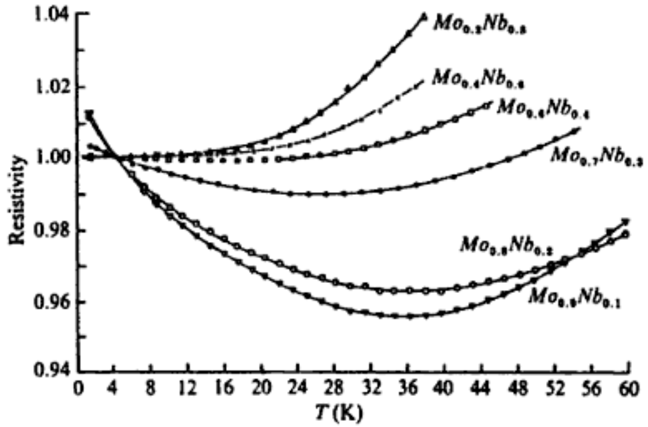
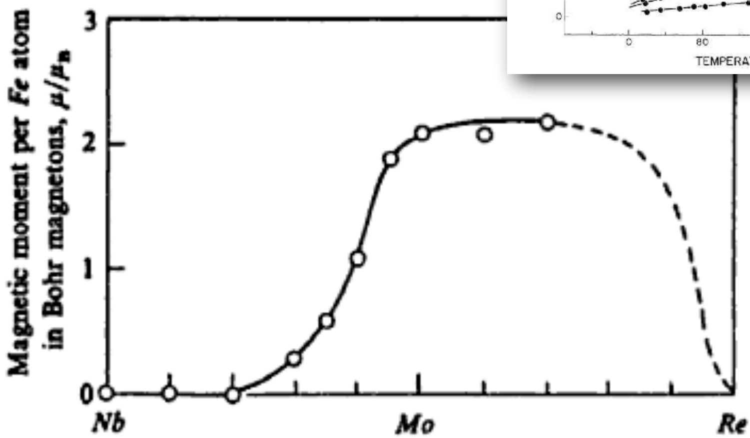


Figure 2.6 Resistance minima for *Fe* in a series of *Mo–Nb* alloys (from Sarachik et al, 1964). Compare the depths of the minima with the corresponding moments in figure 1.8.



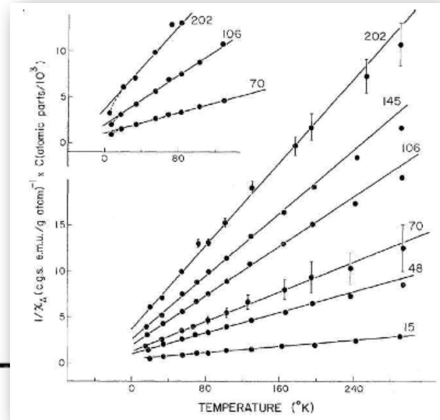
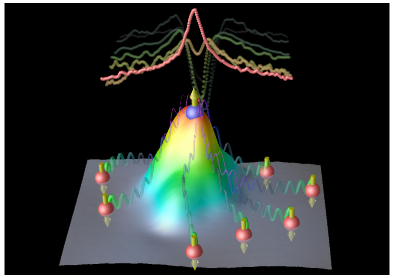


Figure 1.8. The magnetic moment in μ_B of *Fe* in various *Mo–Nb* and *Mo–Re* alloys as a function of alloy composition (Clogston et al, 1962).

Smoking gun:* Resistance minima ☛ *Magnetic impurity

Single Impurity Kondo Problem



Progress of Theoretical Physics, Vol. 32, No. 1, July 1964

Resistance Minimum in Dilute Magnetic Alloys

Jun KONDO

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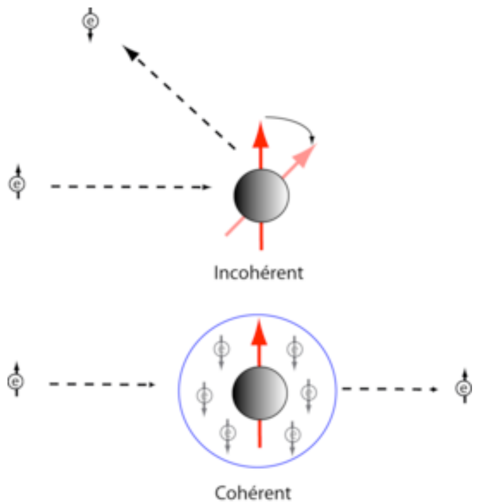
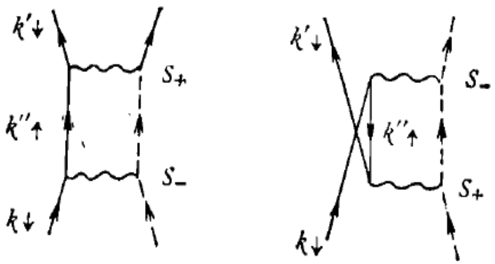
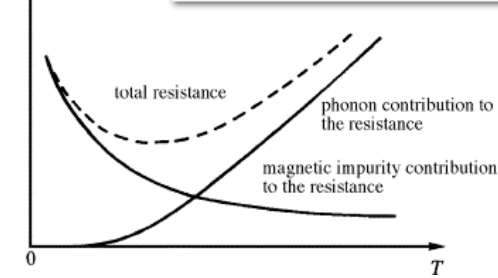
(Received March 19, 1964)

- **Historic development of Kondo**
  - ✓ (19th Century) Electron behavior @ T→0
  - ✓ Liquification & Resistance measurement
  - ✓ 1911-1957 Superconductivity EXP→THEO
  - ✓ 1934 Resistivity minima
  - ✓ 1964 Kondo effect (logarithmic resistivity)



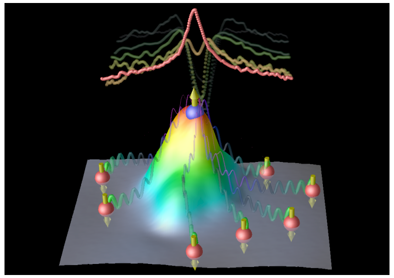


$$R(T) = aT^5 + c_{imp}R_0 - c_{imp}R_1 \ln(k_B T / D)$$



$$H_{sd} = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k},\mathbf{k}'}(S^+ c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} + S^- c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\downarrow} + S_z(c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\uparrow} - c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\downarrow}))$$

Single Impurity Kondo Problem



The renormalization group: Critical phenomena and the Kondo problem*†

Kenneth G. Wilson

Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850

This review covers several topics involving renormalization group ideas. The solution of the *s*-wave Kondo Hamiltonian, describing a single magnetic impurity in a nonmagnetic metal, is explained in detail. See Secs. VII–IX. "Block spin" methods, applied to the two dimensional Ising model, are explained in Sec. VI. The first three sections give a relatively short review of basic renormalization group ideas, mainly in the context of critical phenomena. The relationship of the modern renormalization group to the older problems of divergences in statistical mechanics and field theory and field theoretic renormalization is discussed in Sec. IV. In Sec. V the special case of "marginal variables" is discussed in detail, along with the relationship of the modern renormalization group to its original formulation by Gell-Mann and Low and others.

- **Historic development of Kondo**
  - ✓ (19th Century) Electron behavior @ T→0
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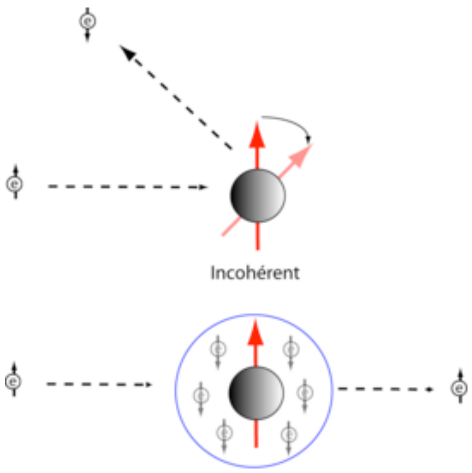
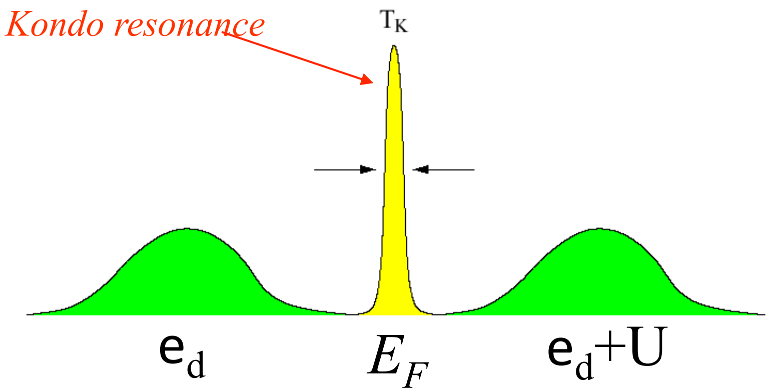
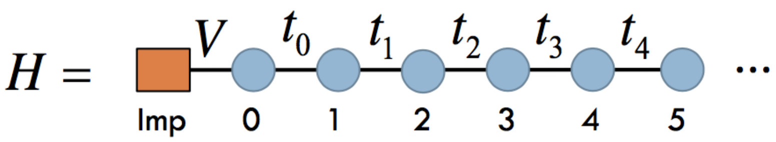




Numerical renormalization group (NRG)

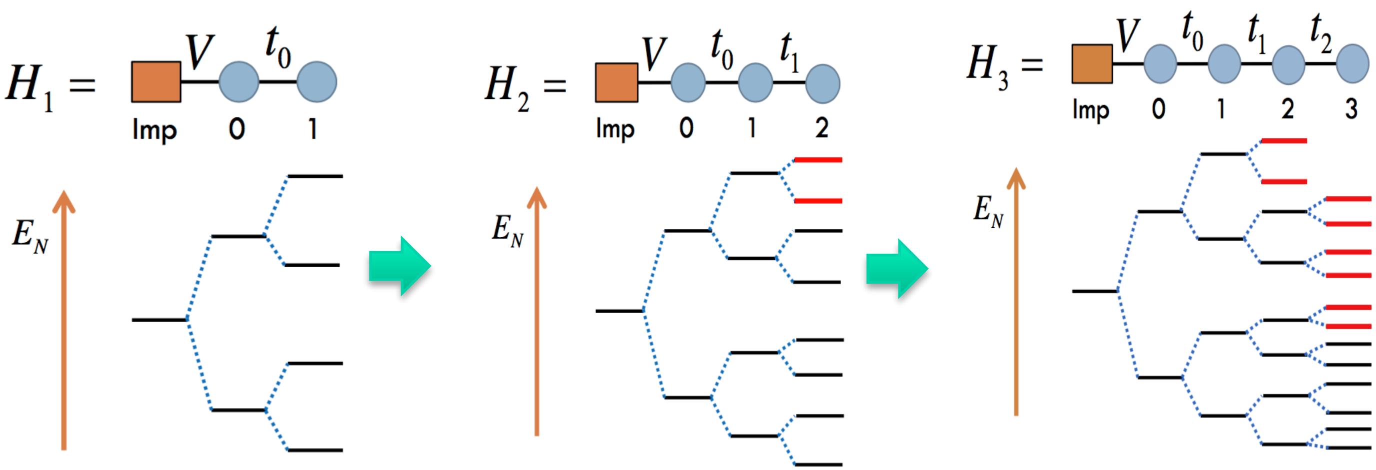
- **Reduce the Hilbert space by throwing away high energy states**



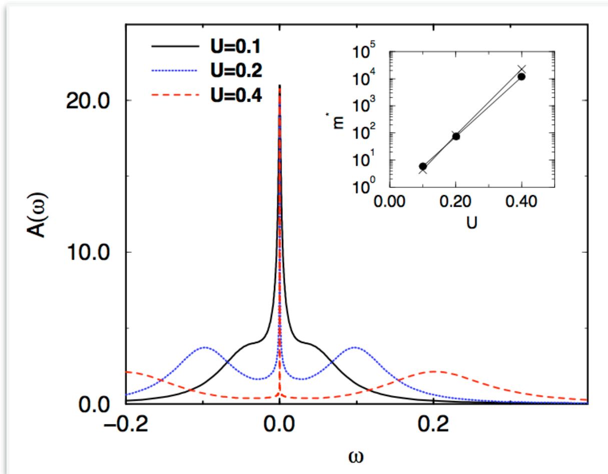
$$H_{N+1} = H_N + H_{N+1}^{hop}$$
$$H_{N+1}^{hop} = \sum_{\sigma} t_N c_{N\sigma}^{\dagger} c_{(N+1)\sigma} + \text{H.c.}$$

K. G. Wilson
Nobel prize 1982

Iterative diagonalization & Truncation (keep fixed number of low energy states)



require separation of energy scales ($t_{N+1}/t_N \sim \Lambda < 1$)

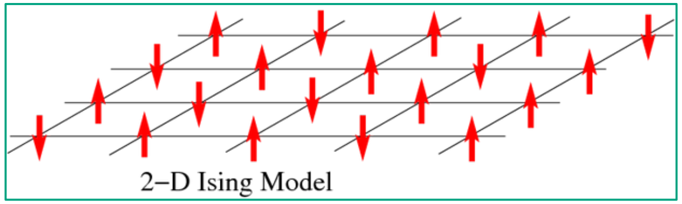


这解决了强关联物理的一大问题，即单格点（0维）的Kondo问题！

Monte Carlo Simulation

Classical Monte Carlo

$$H = -J\sum_{<i,j>} S_i S_j - h\sum_i S_i$$



对任一位形，H({S_i})为一数

对自旋空间的所有位形按照权重取样

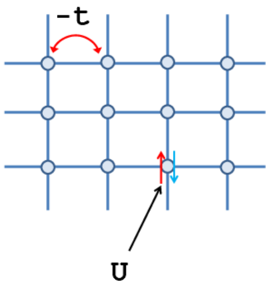
$$Z = \sum_{\{S_i\}} e^{-\beta H(\{S_i\})}, \quad \langle m\rangle = \sum_{\{S_i\}} \frac{1}{Z} e^{-\beta H(\{S_i\})} m(\{S_i\}) = \sum_{\{S_i\}} w(\{S_i\}) m(\{S_i\})$$

Metropolis algorithm

- 随机选择z，翻转自旋： $\{\overline{S}_i\} = (S_1^k, S_2^k, \ldots, -S_z^k, \ldots, S_N^k)$
- 计算前后权重的比值： $\alpha = \dfrac{w(\{\overline{S}_i\})}{w(\{S_i\}_k)} = e^{-\beta(H(\{\overline{S}_i\}) - H(\{S_i\}_k))} = e^{-\beta\Delta E}$
- 选择随机数γ，若$\alpha \geq \gamma$，接受新位形，否则拒绝！

Quantum Monte Carlo (QMC)

$$H = U\sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} - t\sum_{<ij>\sigma} c_{i\sigma}^\dagger c_{j\sigma}$$



对任一状态，H({S_i})不是数，
需要构造新的位形空间！

多种处理方法

☑辅助场QMC：引入合适的经典辅助场，将费米子态积掉，得到辅助场的有效作用量，在辅助场的位形空间进行取样。

Hubbard-Stratonovich变换：

$$\exp\left[-\Delta\tau U\left(n_\uparrow n_\downarrow - \frac{1}{2}(n_\uparrow + n_\downarrow)\right)\right] = \frac{1}{2}\mathrm{Tr}_\sigma[\exp[\lambda\sigma(n_\uparrow - n_\downarrow)]$$

$$Z = \sum_{\{\sigma_i\}} D(\{\sigma_i\})$$

After integrate out the "free" fermions, sample $\{\sigma\}$ with the Metropolis algorithm

☑连续时间QMC：在配分函数中将动能t项或相互作用U项做微扰展开，以自由电子(t)或孤立原子(U)为背景，对微扰展开项进行取样。

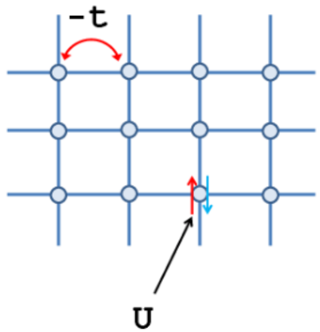
From the single impurity problem to the lattice problem

Dynamical Mean Field Theory

Lattice model

Considering the Hubbard model

$$H = -\sum_{<ij>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

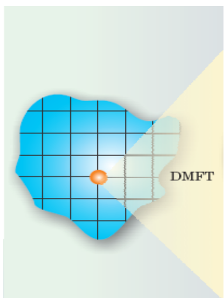


The action is:

$$S = \int_0^{\beta} d\tau [\sum_{i,\sigma} c^{*}_{i\sigma}(\tau)(\frac{\partial}{\partial \tau} - \mu) c_{i\sigma}(\tau) - \sum_{<i,j>\sigma} t_{i,j} c^{*}_{i\sigma}(\tau) c_{j\sigma}(\tau) + \sum_{i} H_i^{on-site}(\tau)]$$

When we integrating out of the other site:

$$S_{eff} = -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{\sigma} c^{\dagger}_{o\sigma}(\tau) g_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^{\beta} d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

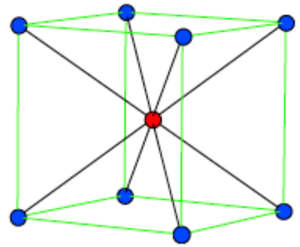


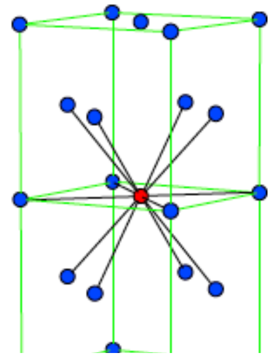
$$G(\tau - \tau') = -< T c_{o\sigma}(\tau) c_{o\sigma}{}^{\dagger}(\tau') >_{S_{eff}}$$

$$\Sigma(iw_n) = G_0^{-1}(iw_n) - G^{-1}(iw_n)$$

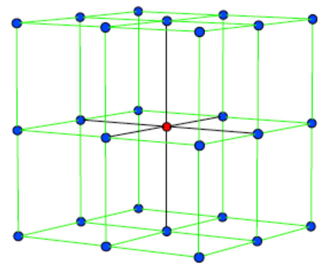
Coordination number Z

Z=8 (body-centered cubic)



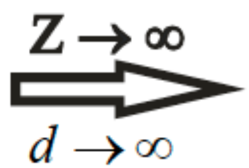


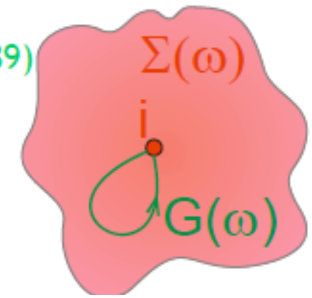
Z=12 (face-centered cubic)



Z=6 (simple cubic)

Metzner + Vollhardt (1989)



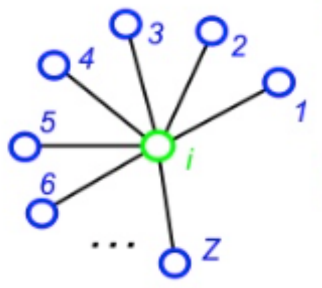


$$\Sigma(\mathrm{k}, \omega) = \Sigma(\omega)$$

“Single-site” mean-field theory with full many-body dynamics

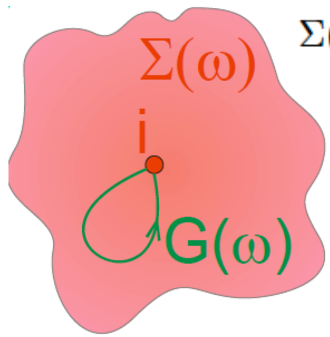
Dynamical Mean Field Theory

Mapping the lattice Hubbard model to an impurity Anderson model



$d \rightarrow \infty$

Metzner, Vollhardt (1989)



$\Sigma(\mathbf{k},\omega) = \Sigma(\omega)$

Hubbard model

$$H = -\sum_{<ij>,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Impurity Anderson model

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} V_{k\sigma} (c_{k\sigma}^{\dagger} d_{\sigma} + h.c.)$$

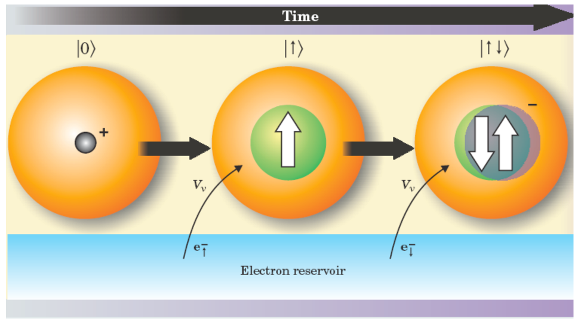
Non-interacting conduction (*s*-) electrons
+
single *d*-orbital ("impurity")
+
s,*d*-hybridization

An equivalent formulation obtained by integrating the fermions

$$S_{imp} = -\int_0^{\beta} d_{\sigma}^{\dagger}(\tau) G_{0\sigma}^{-1}(\tau - \tau') d_{\sigma}(\tau') + \int_0^{\beta} d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

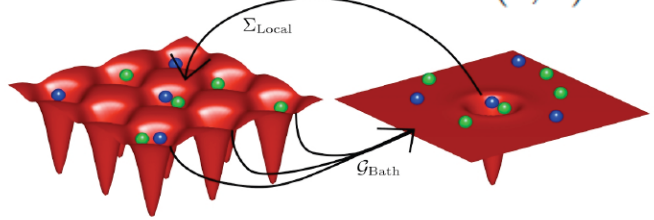
Hybridization function: $\Delta_{\sigma}(i\omega_n) \equiv \sum_{k} \frac{|V_{k\sigma}|^2}{i\omega_n - \varepsilon_{k\sigma}}$

Bath function: $G_{0\sigma}^{-1}(i\omega_n) \equiv i\omega_n + \varepsilon_d - \Delta_{\sigma}(i\omega_n)$



Dynamical Mean Field Theory

$$\Sigma(\mathbf{k},\omega)=\Sigma(\omega)$$



Dynamical mean-field theory

Dynamical mean field theory self-consistent equation

$$\begin{cases}
S_{eff}=-\int_0^{\beta}d\tau\int_0^{\beta}d\tau'\sum_{\sigma}c_{o\sigma}^{\dagger}(\tau)g_0^{-1}(\tau-\tau')c_{0\sigma}(\tau')+U\int_0^{\beta}d\tau n_{o\uparrow}(\tau)n_{o\downarrow}(\tau) \\
G(\tau-\tau')=-<Tc_{o\sigma}(\tau)c_{o\sigma}^{\dagger}(\tau')>_{S_{eff}} \\
\Sigma(iw_n)=G_0^{-1}(iw_n)-G^{-1}(iw_n) \\
G(k,iw_n)=\dfrac{1}{iw_n+\mu-\varepsilon_k-\Sigma(iw_n)}
\end{cases}$$

$\mathcal{G}_0 \longrightarrow$ Impurity Solver $\longrightarrow G$

$\uparrow$ $\downarrow$

$\mathcal{G}_0^{-1}=\bar{G}^{-1}+\Sigma$ $\qquad$ $\Sigma=\mathcal{G}_0^{-1}-G^{-1}$

$\nwarrow$ $\swarrow$

$$\bar{G}=\int_{-\infty}^{\infty}\mathrm{d}\epsilon\,\frac{D(\epsilon)}{\mathrm{i}\omega_n+\mu-\epsilon-\Sigma}$$

周期性Anderson模型

$$H=\sum_{ij,\sigma}t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\varepsilon_d\sum_{i\sigma}n_{i\sigma}^{d}+U\sum_{i}n_{i\uparrow}^{d}n_{i\downarrow}^{d}+\sum_{ij,\sigma}(V_{ij}c_{i\sigma}^{\dagger}d_{j\sigma}+h.c)$$

Effective impurity model defined by hybridization function is solved with an “impurity ” solver, e.g. QMC, NRG,ED…

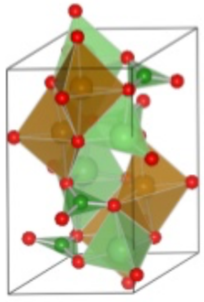
Density Functional Theory

+

Dynamical Mean-Field Theory

Framework: DFT+DMFT

Density Functional Theory



+

+

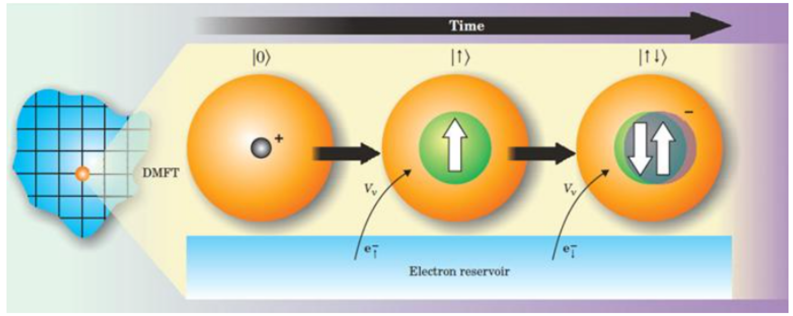
$$i\hbar \frac{d\Psi(\{r_i\};t)}{dt} = \hat{H}\Psi(\{r_i\};t)$$

$$H = \sum_{i=1}^{N_e} \nabla_i^2 + \sum_{i=1}^{N_e} V_{nuclear}(r_i) + \sum_{i=1}^{N_e} V_{effective}(r_i)$$

- **A framework for materials calculations**
  - ✓ Kohn-Hohenberg theorem
  - ✓ Kohn-Sham equation

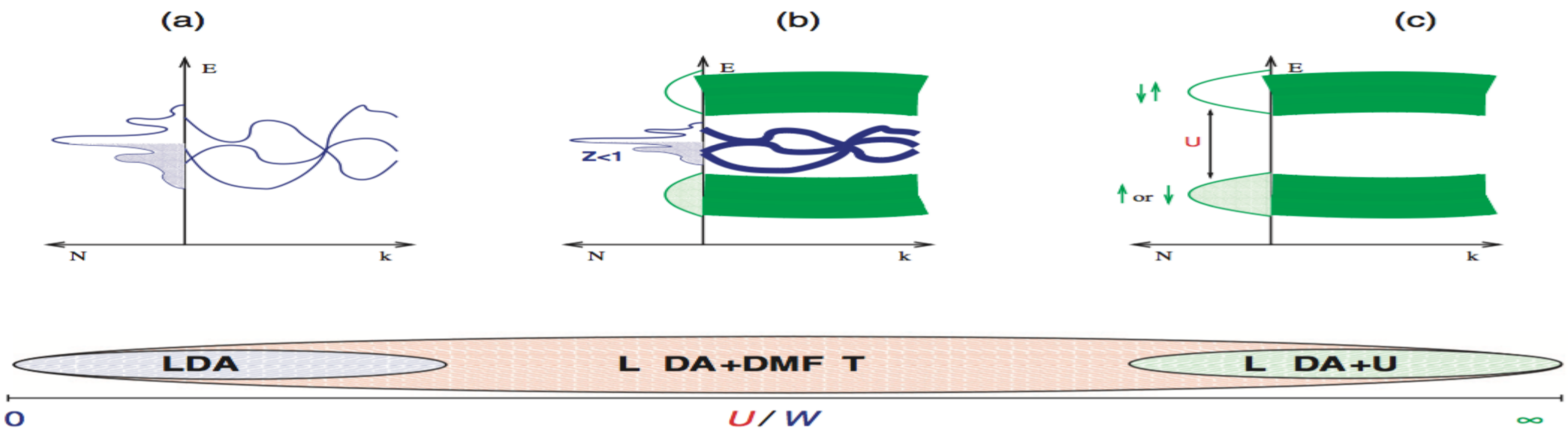
    WIEN2k package; WIEN2Wannier
  - ✓ Electronic/magnetic/structural/orbital
  - ✓ Ground state tuning; Materials design

Dynamical Mean-Field THeory



- **Strongly correlated electron systems**
  - ✓ Kondo and Mott physics beyond DFT
  - ✓ Non-perturbative; time-consuming

    NRG/QMC/CTQMC/NCA/OCA/IPT
  - ✓ Quantum phase transitions
  - ✓ Quantum criticality & Non-Fermi liquid



Framework: DFT+DMFT

(1) Calculate LDA band structure

$$\varepsilon_{lml'm'}(k) \rightarrow \hat{H}_{LDA}$$

(2) Supplement LDA band by local Coulomb interaction (only for correlated bands)

$$\hat{\mathcal{H}} = \underbrace{\sum_{\mathbf{k}\,lm\,l'm'\sigma} \epsilon_{lm\,l'm'}(\mathbf{k})\,\hat{c}^{\dagger}_{\mathbf{k}lm\sigma}\,\hat{c}_{\mathbf{k}l'm'\sigma}}_{\text{LDA}} \underbrace{- \sum_{\substack{i=i_d,\\ \ell=\ell_d}} \sum_{m\sigma} \Delta\varepsilon_d \hat{n}_{i\ell m\sigma}}_{\text{double counting correction}}$$

$$\underbrace{+ \sum_{\substack{i=i_d,\\ l=l_d}} \sum_{m\sigma,m'\sigma'}{}' \frac{U^{\sigma\sigma'}_{mm'}}{2} \hat{n}_{ilm\sigma}\hat{n}_{ilm'\sigma'}}_{\text{local Coulomb interaction}} \underbrace{- \sum_{\substack{i=i_d,\\ l=l_d}} \sum_{m\sigma,m'\sigma'} J_{mm'}\hat{c}^{\dagger}_{ilm\sigma}\hat{c}^{\dagger}_{ilm'\sigma'}\hat{c}_{ilm'\sigma}\hat{c}_{ilm\sigma'}}_{\text{Hund's rule coupling}}$$

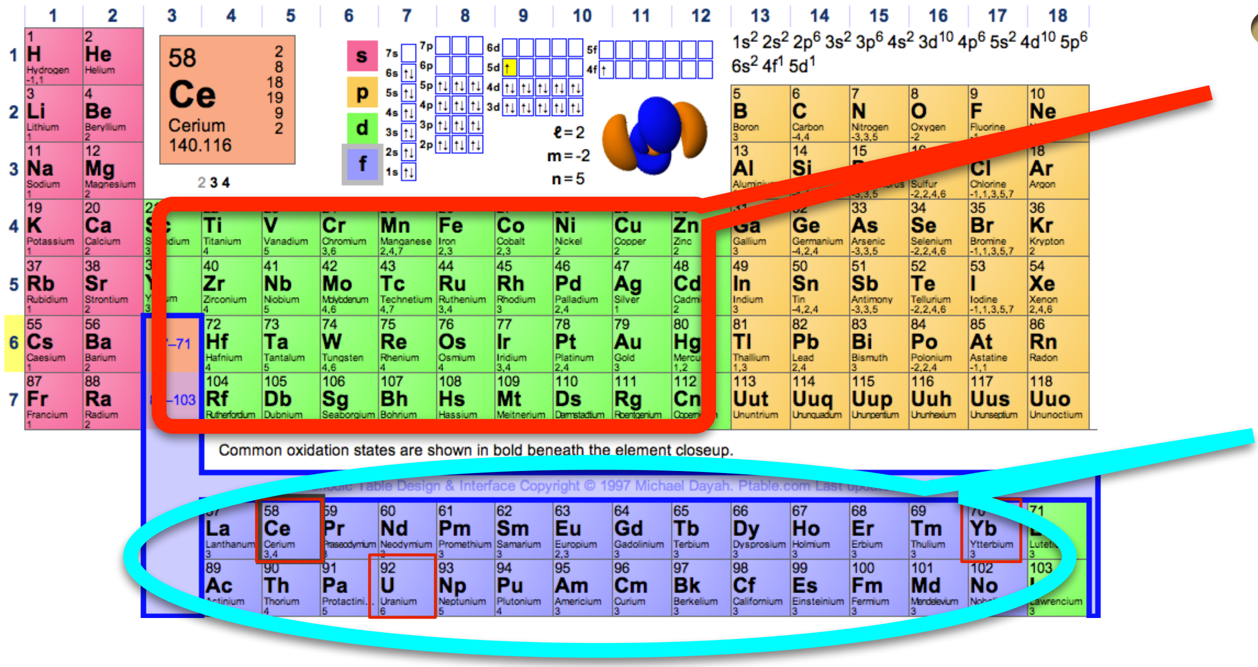
(3) Solve model by DMFT with impurity solver

$$G = -\frac{1}{Z}\int \mathcal{D}[\psi\psi^*]\psi\psi^* e^{\psi^*[G^{-1}+\Sigma]\psi - U\psi^*\psi\psi^*\psi + J\psi^*\psi\psi^*\psi}$$

$$G^{\sigma}_{mm'}(\omega) = \frac{1}{V_B}\int d^3k \left[(\omega - \Sigma^{\sigma}(\omega))\delta_{m,m'} - \left(H^{0\,eff}_{LDA}(\mathbf{k})\right)_{m,m'}\right]^{-1}$$

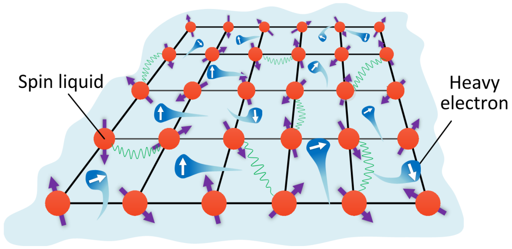
Application to the Kondo lattice

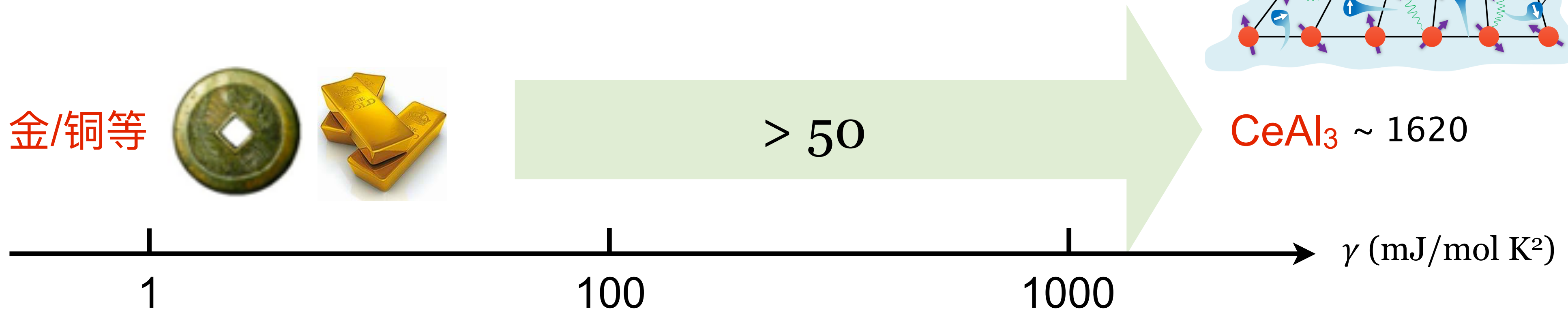
Heavy Fermion Materials



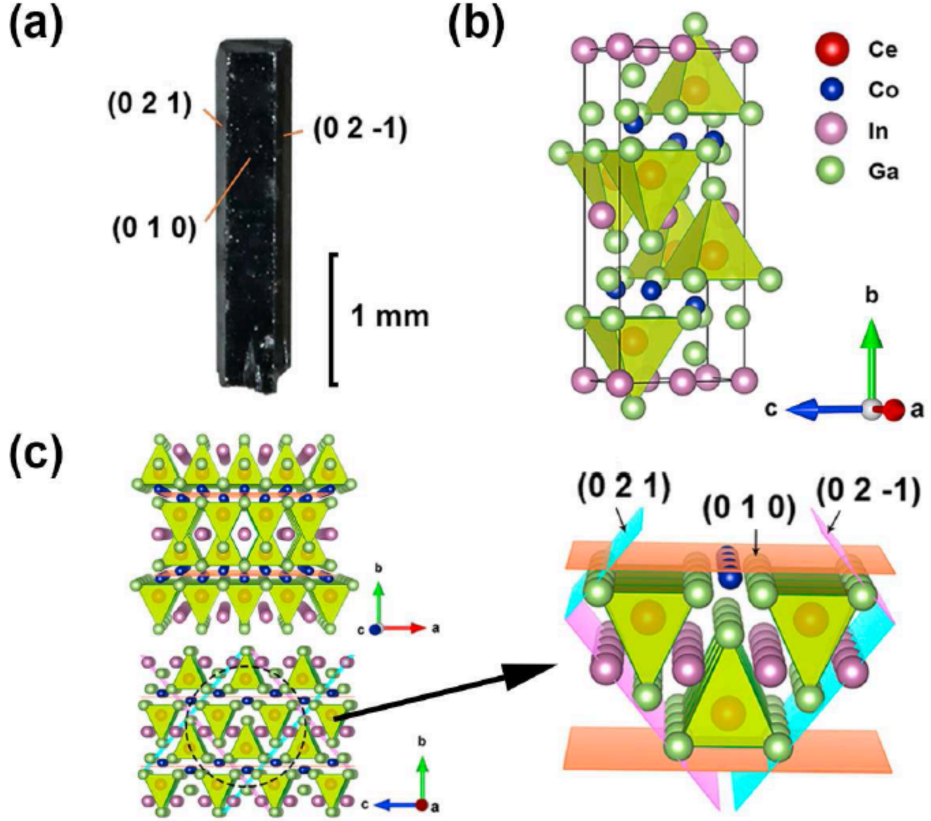
- **Transition metal oxides**
  - ✓ Hubbard model
  - ✓ Mott physics
  - ✓ Energy scale: 10-100 meV
- **Heavy fermion intermetallics**
  - ✓ Anderson model
  - ✓ Kondo lattice physics
  - ✓ Energy scale: 1-10 meV

Mostly f-electron intermetallics of Ce, U, or Yb

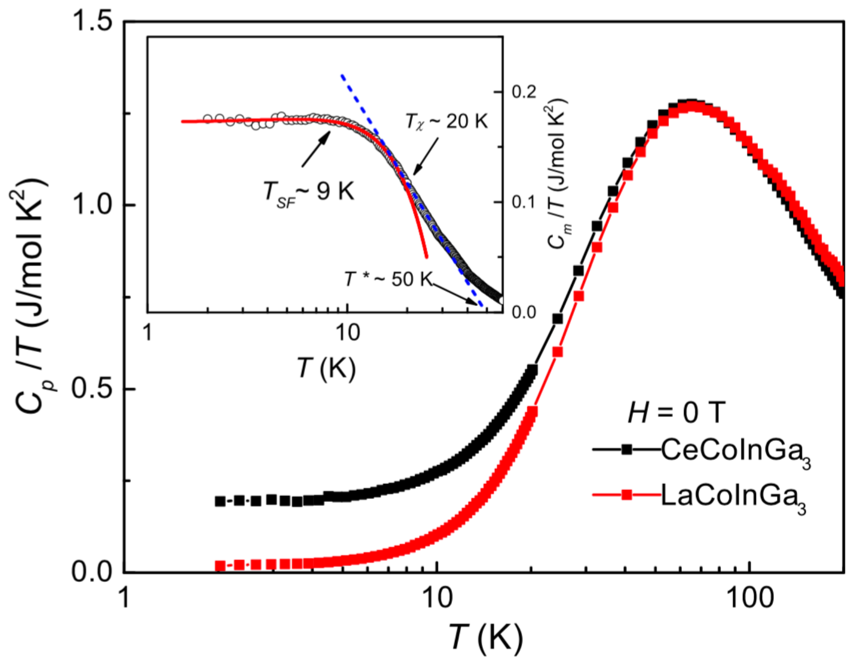




Kondo lattice $CeCoInGa_3$



Phys. Rev. B 98, 115119 (2018).



Typical heavy fermion system !

金/铜等

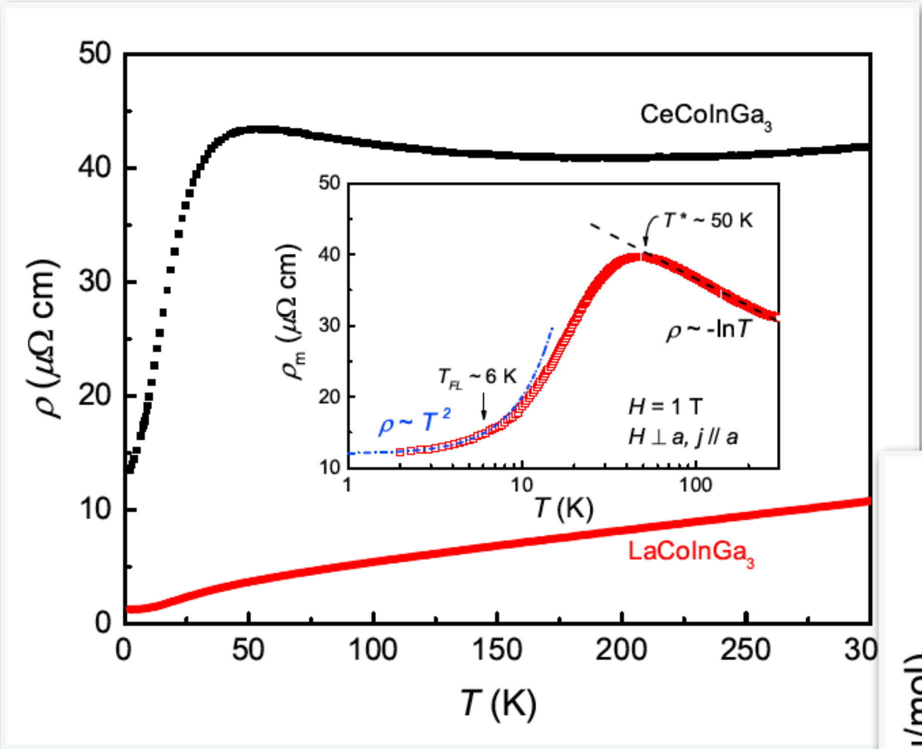
> 50

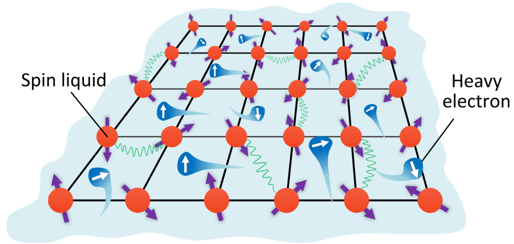
$CeAl_3$ ~ 1620

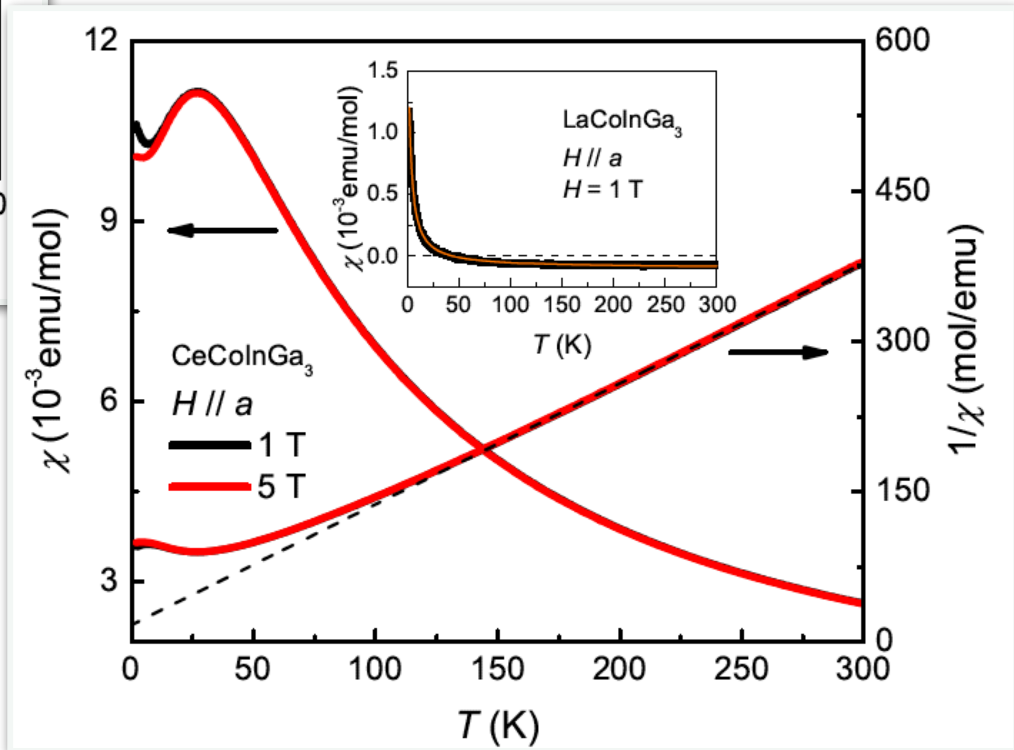
1 — 100 — 1000 — γ (mJ/mol K²)

Kondo lattice $CeCoInGa_3$

Phys. Rev. B 98, 115119 (2018).





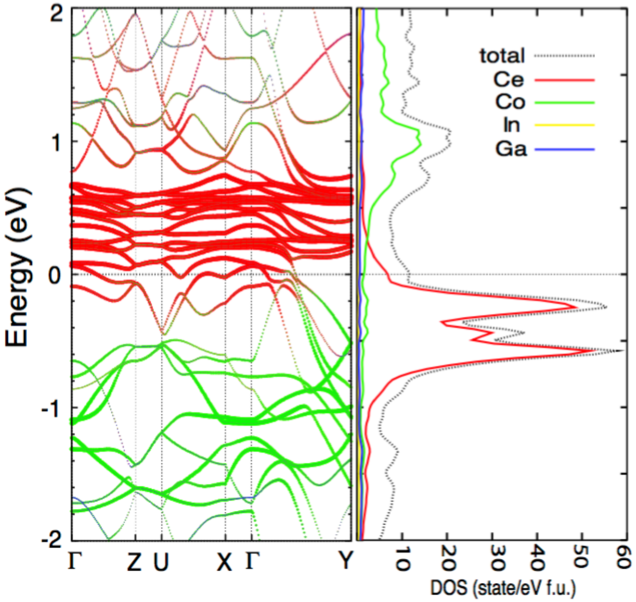


Transition from high-T local spin to low-T metallic electrons ——

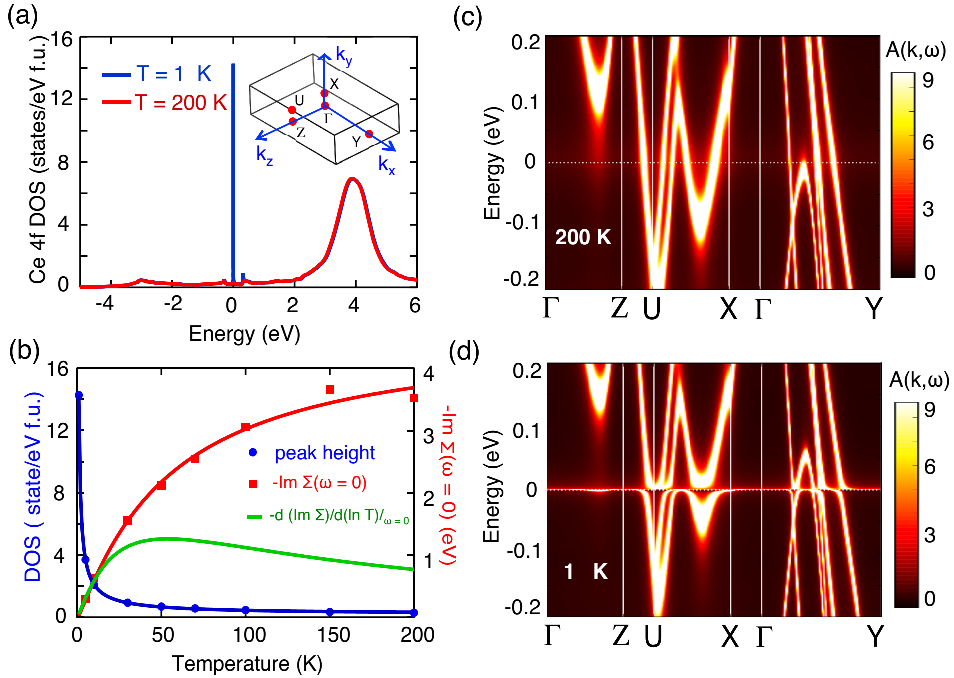
Kondo-like physics!

Kondo lattice CeCoInGa3

DFT results



DFT+DMFT calculations

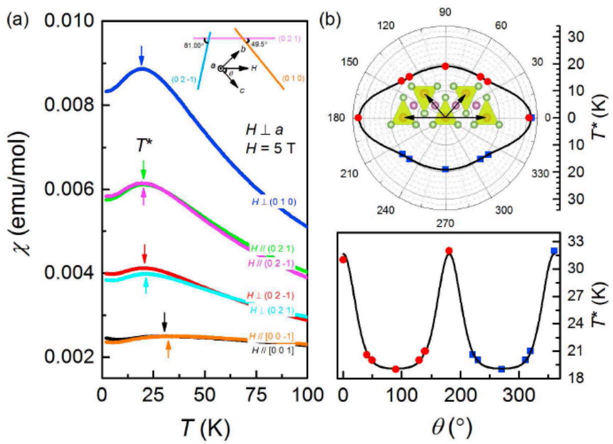


The failure of DFT: There is no flat band and large density of states at the Fermi level !

The success of DFT+DMFT:

- Typical heavy fermion evolution with temperature can be well captured.
- The anisotropic hybridization gap agree well with experiments.

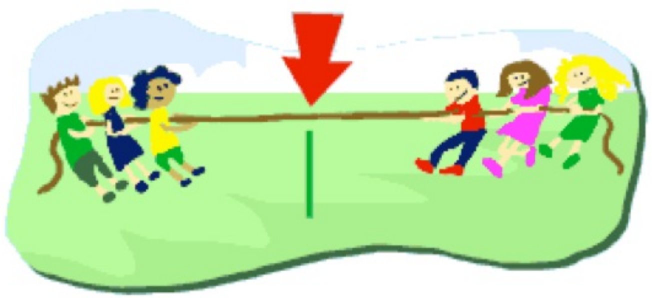
Anisotropic hybridization

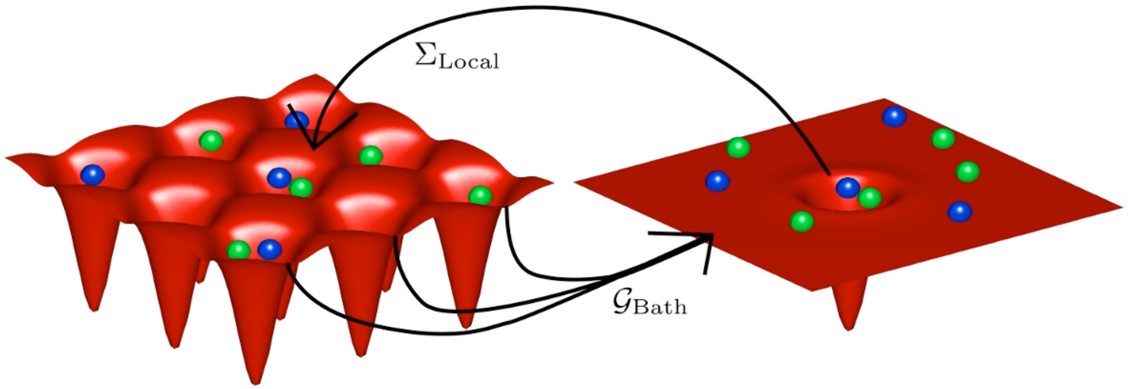


Summary

有趣的物理往往都发生在局域和巡游的边界：高温超导、庞磁阻等等

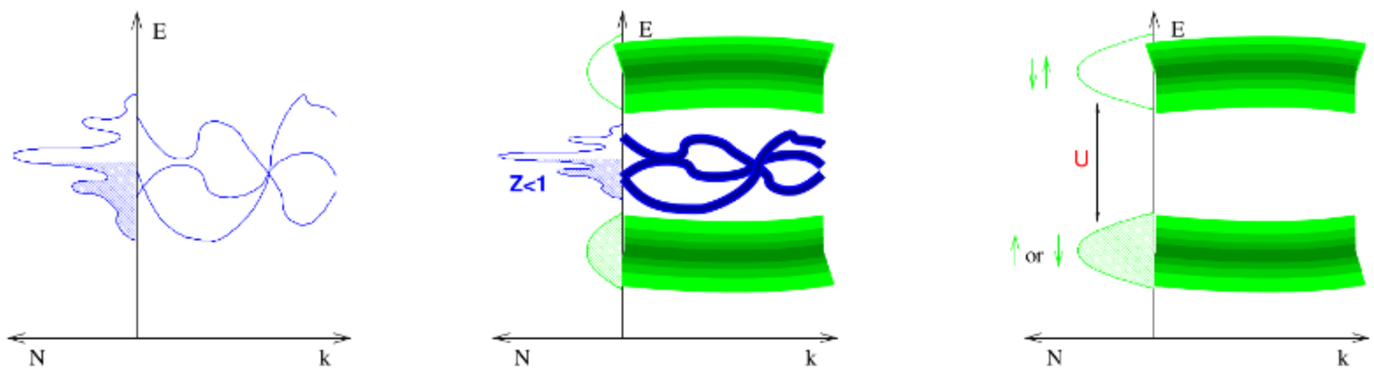
Coulomb X Hybridization

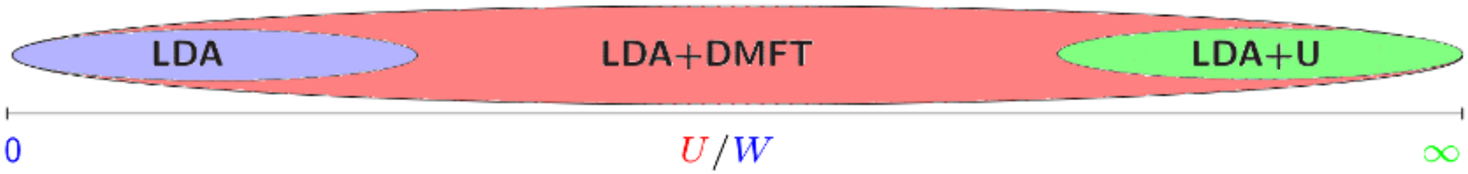




localization vs itinerancy

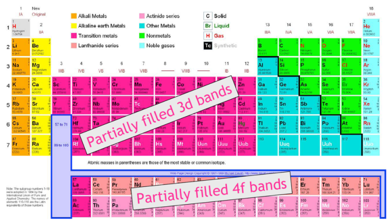
Dynamical mean-field theory

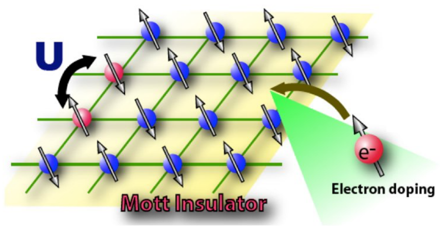


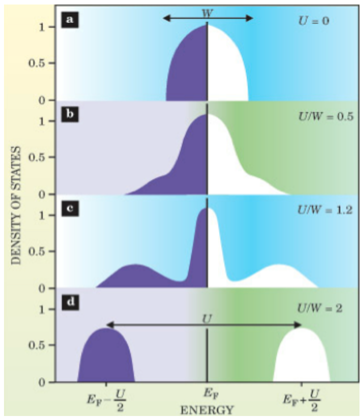


Correlation in Condensed Matter Physics

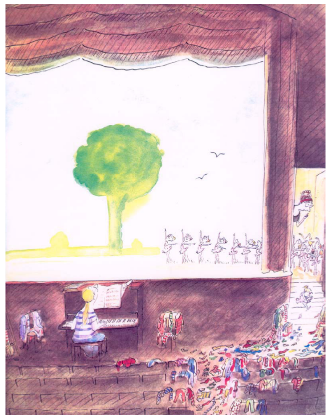
Mott insulator

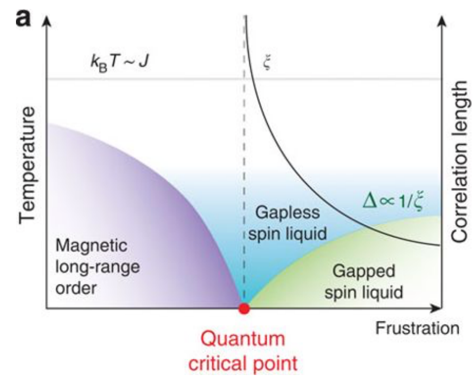






Correlations & long-range order



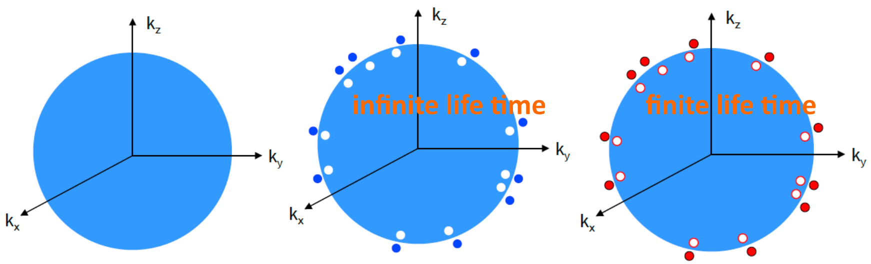


Quasiparticles

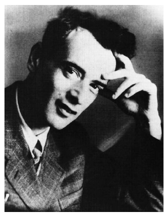
Ground state: Fermi gas

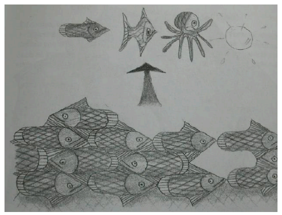
Excited states (T>0)

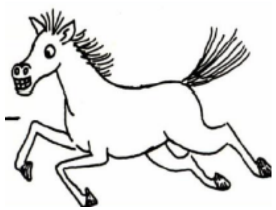
Landau Fermi liquid

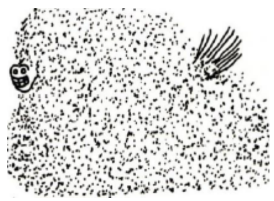


A quasiparticle has an effective mass, selfenergy (energy and lifetime)

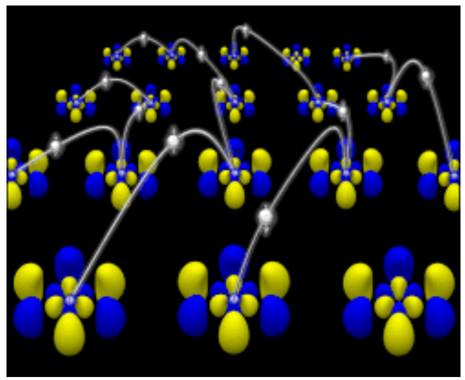


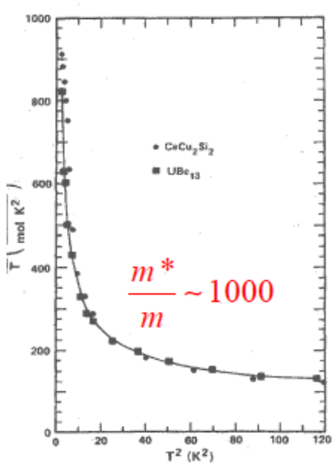






Exotic quantum state





$$\lim_{T \to 0} \frac{C_V}{T} = \gamma \propto \frac{m^*}{m}, \quad v_F = \frac{\hbar k_F}{m^*}$$

UBe_{13}, $CeCu_2Si_2$

Stewart *et al.* (1983, 1984)