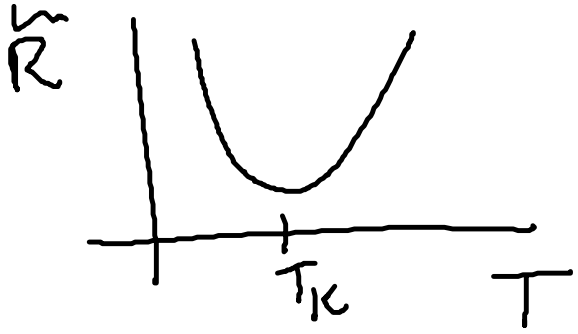


Spin-flip scattering

1964 Kondo :

ferromagnetism in metals (Zener)

Ref.: "Theory of magnetism" Yoshida Springer

Model Hamiltonian

Magnetic impurity with spin S (here spin $\frac{1}{2}$) coupled to a gas of free electrons.

Impurity creation operator $d^\dagger_\sigma$, $\sigma = \uparrow, \downarrow$

Imp. Spin operators

$$S^z = \frac{1}{2}\left(d^\dagger_\uparrow d_\uparrow - d^\dagger_\downarrow d_\downarrow \right)$$

$$S^+ = d^\dagger_\uparrow d_\downarrow, \quad S^- = d^\dagger_\downarrow d_\uparrow .$$

$$S^x = \frac{1}{2}\left(S^+ + S^-\right), \quad S^y = \frac{1}{2i}\left(S^+ - S^-\right)$$

$$H_B \equiv \sum_{\underline{k},\sigma} \left(\varepsilon_{\underline{k}} - \mu\right) a^\dagger_{\underline{k}\sigma} a_{\underline{k}\sigma}$$

μ: chem. Potential

Impurity at $\underline{x} = 0$. Band electron spin operators

$\Psi, \Psi^\dagger$ electron field operators

$$s^+_0 \equiv \Psi^\dagger_\uparrow(x=0)\,\Psi_\downarrow(x=0)$$

$$= \frac{1}{\left(\sqrt{\Omega^2}\right)} \sum_{\underline{k}\,\underline{k}'} a^\dagger_{\underline{k}\uparrow} a_{\underline{k}'\downarrow}$$

(expansion into plane waves)

Ω : Volume

The total Kondo Hamiltonian H_K

$$H_K = H_B + 2J \hat{\underline{S}} \cdot \hat{\underline{S}}_0$$

careful

J : coupling

$J < 0$: ferromagnetic exchange coupling

$J > 0$: antiferromagnetic coupling

Exchange interaction :

QM of molecules "Statistical Mechanics" by R. Feynman.

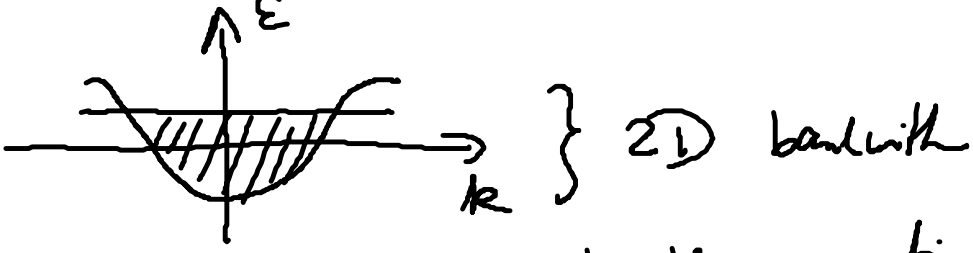
$$\underline{S} \cdot \underline{s}_0 = S^z s_0^z + \frac{1}{2}\left(S^+ s_0^- + S^- s_0^+\right) \quad (\ddot{u}A)$$

$$H_K = \sum_{k\sigma} (\varepsilon_k - \mu) a^\dagger_{k\sigma} a_{k\sigma} + H_{s-d}$$

$$H_{s-d} \equiv + \frac{J}{\Omega} \sum_{k k'} \Big[S^z \left(a^\dagger_{k\uparrow} a_{k'\uparrow} - a^\dagger_{k\downarrow} a_{k'\downarrow} \right)$$

$$+ S^+ a^\dagger_{k\downarrow} a_{k'\uparrow} + S^- a^\dagger_{k\uparrow} a_{k'\downarrow} \Big]$$

all momenta k within the band are coupled to the impurity

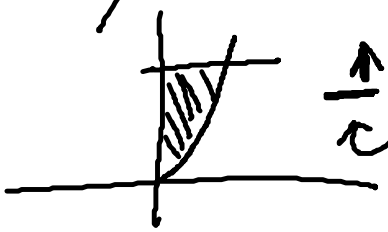


all energies couple to the magnetic impurity •

- Sign convention $-2J\vec{S}\cdot\vec{s}_0$
  $+2J\vec{S}\cdot\vec{s}_0$

"s-d" Hamiltonian

- Kondo Model can be derived from the SIAM (Single Impurity Anderson Model) by Schrieffer-Wolff.



$\frac{1}{\epsilon}$ interaction term U.

Kondo Hamiltonian + many-Body Physics

Why is it difficult?

The impurity forces us to study the band electrons as a many-body problem.

Example: two electrons with spin ↑
scatter at impurity (spin ↓)
1st electron scatters, but
then second can't spin-flip scatter.

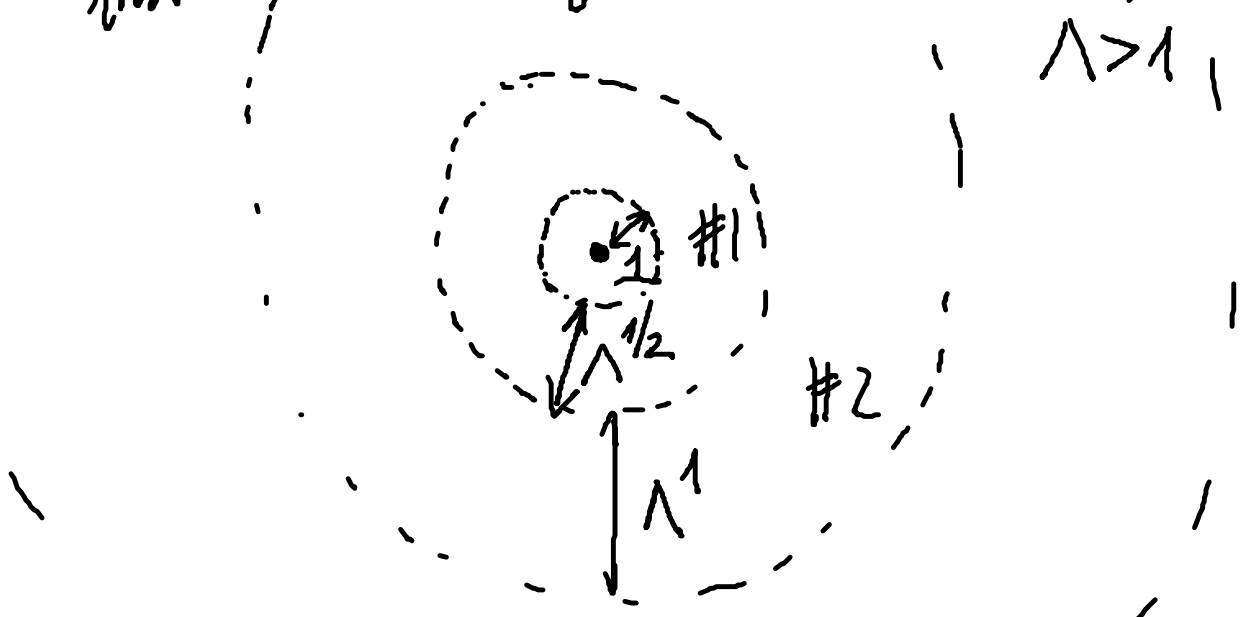
An exact numerical diagonalisation is impossible:

- Hilbert space is too large
- too many single particle states
- too many electrons.

Key ideas: 1) Find a (very) good basis of single particle states in which to diagonalise.

Usual plane-wave basis is not suitable here.
Instead we use a basis similar to Wannier functions: this emphasises the interaction between the impurity and the band electrons.

- first state has strong overlap with the impurity



"onion-like" shell structure : Kondo basis

2) Strategy:

- First solve impurity coupled to the first Kondo state $\Rightarrow$ a few eigenvalues
- Add the second layer, solve combined problem
- Numerical problem: $n=0$: $2^3 = 8$ states (8×8 matrix)

2nd: 2^{3+2n} : becomes very big!

(each onion shell has $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$)

Procedure: Renormalisation group "language"

within one step (adding one shell)
one moves from H_N to H_{N+1}

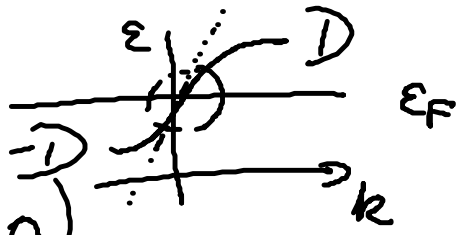
RG-step $H_{N+1} = R[H_N]$

R: renorm. group transformation

Details:

Spherical symmetry: Expand $\psi^\dagger_\sigma(0)$ $\psi_\sigma(0)$ into $Y_{lm}(\varphi, \theta)$.
The impurity only couples to s-waves.
Energies $\varepsilon_{\underline{k}} = \varepsilon_{|k|}$

We write $\varepsilon_{\underline{k}} = \varepsilon_F + \left(k - k_F\right)\frac{\partial \varepsilon_k}{\partial k} + \ldots$



Energies counted from ε_F ($k_F = 0$)
re-defining units

$$\varepsilon_{\underline{k}} = k_{\underline{}} = \varepsilon \qquad \text{(Check)}$$

$$H_K = \sum_{\sigma} \int_{-D}^{D} d\varepsilon\, \varepsilon\, a^{+}_{\varepsilon\sigma} a_{\varepsilon\sigma} + \left(2J \hat{\underline{S}}\, \hat{\underline{s}}_0\right)$$

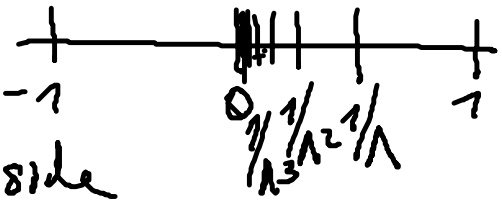
Wilson: • Divide energy band into
discrete intervals.

• Logarithmic discretisation

$D = 1$

Λ

$k \Rightarrow$



both on positive + negative side

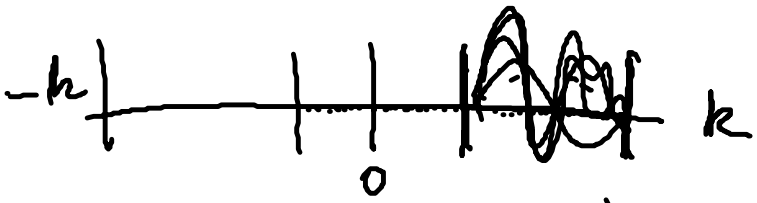
e.g. $\Lambda = 2$

intervals in the energy band:

$$\left[-\Lambda^{-n}, -\Lambda^{-(n+1)}\right] \; ; \; \left[\Lambda^{-(n+1)}, \Lambda^{-n}\right]$$

$n = 0, 1, 2, \ldots$

Transformation from $a^{+}_{\varepsilon\sigma} \longrightarrow$ discrete index

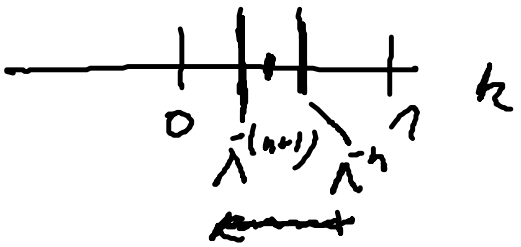


For each interval, introduce a basis for a Fourier series, introduce functions

$$\psi^{\pm}_{np}(\varepsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i \omega_n p \varepsilon} & \Lambda^{-(n+1)} < \pm\varepsilon < \Lambda^{-n} \\ 0 & \text{else} \end{cases}$$

$p = 0, \pm 1, \pm 2 \qquad \omega_n = 2\pi / d_n$

$d_n = \underbrace{\Lambda^{-n}(1 - \Lambda^{-1})}$,



Expand the electron operator

$$a_{\varepsilon\sigma} = \sum_{np} \left[a_{np\sigma} \psi^{+}_{np}(\varepsilon) + b_{np\sigma} \psi^{-}_{np}(\varepsilon) \right]$$