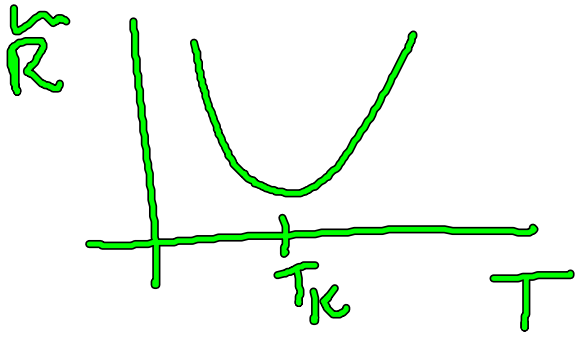


Spin-flip scattering

1964 Kondo :

ferromagnetism in metals (Zener)

Ref: "Theory of magnetism" Yoshida

Springer

Model Hamiltonian

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

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

Imp. Spin operators

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

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

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

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

μ: chem. Potential

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

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

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

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

(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

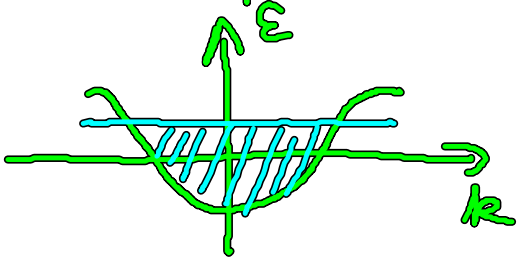
"statistical mechanics" by R. Feynman.

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

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

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

all momenta k within the band are coupled to the impurity



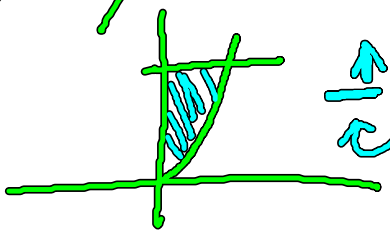
} 2D bandwidth

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.



$\frac{1}{r}$ interaction term.

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 ↓)
1 of A 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 $\Rightarrow$ 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 $\mathcal{H}_N$ to $\mathcal{H}_{N+1}$

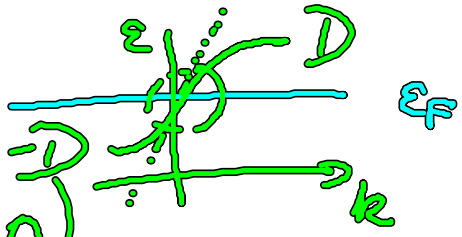
RG-step $\mathcal{H}_{N+1} = R[\mathcal{H}_N]$

R: renorm. group transformation

Details:

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

We work $\varepsilon_k = \varepsilon_F + (k-k_F)\frac{\partial \varepsilon_k}{\partial k} + \dots$



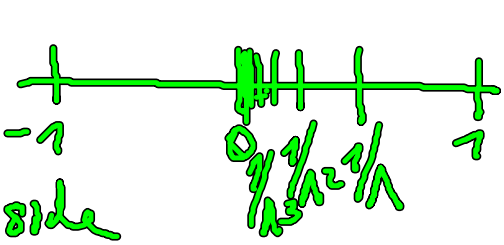
Energies counted from ε_F re-defining units $(k_F = 0)$

$\varepsilon_k = k_F = \varepsilon$ (Check)

$$H_K = \sum_\sigma \int_{-D}^{D} d\varepsilon\, \varepsilon\, a^\dagger_{\varepsilon\sigma} a_{\varepsilon\sigma} + (\dots \hat{S}\hat{S}_0)$$

Wilson: • Divide energy band into discrete intervals. $D = 1$

• Logarithmic discretisation



both on positive + negative side

e.g. $\Lambda = 2$

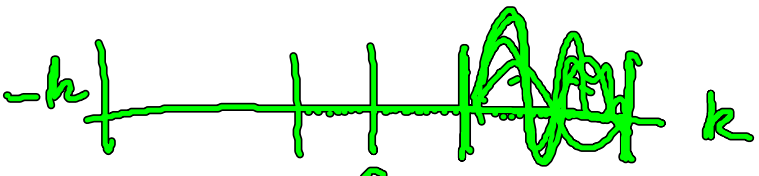
intervals in the energy band:

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

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

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

$\varepsilon = k$



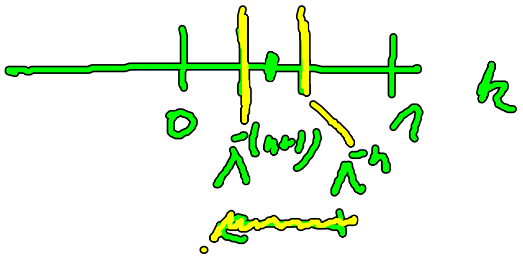
For each interval, introduce a basis

for a Fourier series, introduce functions

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

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

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



Expand the electron operator

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