LECTURE

THE NUMERICAL RENORMALIZATION GROUP (NRG)

Classic Reading:

K.G. Wilson, Rev. Mod. Phys. 47, 773 (1975)

H.R. Krishna-murthy, J.W. Wilkins and K.G. Wilson, Phys. Rev. B 21, 1003 (R80)

R. Bulla, T.A. Costi and T. Pruschke, Rev. Mod. Phys. 80, 395 (2008)

Outline:

I Kondo and Anderson models

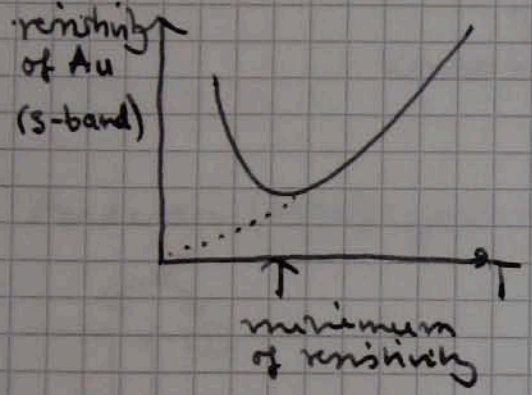
II NRG
1. Logarithmic discretization
2. Mapping to semi-infinite chain
3. Iterative diagonalization
4. RG flow

III Observables
1. Thermodynamics
2. Dynamics

I Kondo and Anderson model

- Metals with magnetic impurities
  ↑ internal degree of freedom – no simple pot. scattering!
- quantum dots
- dissipative quantum systems

de Haas, de Boer, van den Berg (1934)



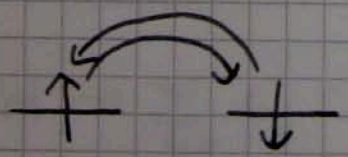
impurity effect of Fe (d-orbital)

Zener (1951): s-d-Hamiltonian aka Kondo model

Au: well delocalized; Fe: strongly localized single electron (spin)

low imp. concentration: <u>single-impurity</u> model

$$H_{sd\ (Kondo)} = \underbrace{\sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma}}_{\text{Au conduction band}} + J \sum_{kk'} \left(S^+ c^+_{k\downarrow} c_{k'\uparrow} + S^- c^+_{k\uparrow} c_{k'\downarrow} + S^z \left(c^+_{k\uparrow} c_{k'\uparrow} - c^+_{k\downarrow} c_{k'\downarrow} \right) \right)$$



on-site repulsion (forces single occupation): virtual second-order process (cf. Heisenberg model) ⇒

$J > 0$ (AFM) favors singlet formation

Kondo (1964): all terms (but leading) in perturbation series logarithmically divergent at $T \to 0$

↑ "Kondo problem"

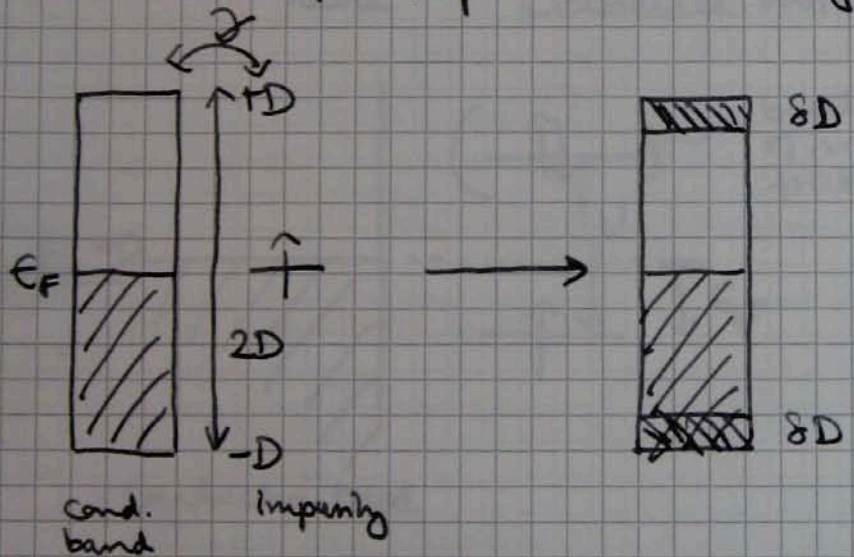
$$R_{imp} = \alpha J^2 (1 - \beta J \ln T) + \dots$$

with "normal" contributions: minimum of resistivity

divergence scale: $T_K \sim e^{-1/2\rho J}$

↑ Kondo temperature ↑ density of states for conduction electrons

Anderson (1970): poor man's scaling



- treat coupling to extreme part of spectrum perturbatively (ok for small J)
- integrate out and incorporate effect into Hamiltonian
- (rescale Hamiltonian to maintain bandwidth)

Hamiltonian retains structure:

$$H \to \sum_{\underline{k}\sigma} \epsilon_{\underline{k}} c^\dagger_{\underline{k}\sigma} c_{\underline{k}\sigma} + J(D) \sum_{\underline{k}\underline{k}'} \left(S^+ c^\dagger_{\underline{k}\downarrow} c_{\underline{k}'\uparrow} + \text{h.c.} + \dots \right)$$

↑ grows exponentially with $D \downarrow$

perturbative ansatz breaks down, but indicates perfect screening of local moment into a singlet; nonmagnetic ground state; problem: exp. many electrons involved!!

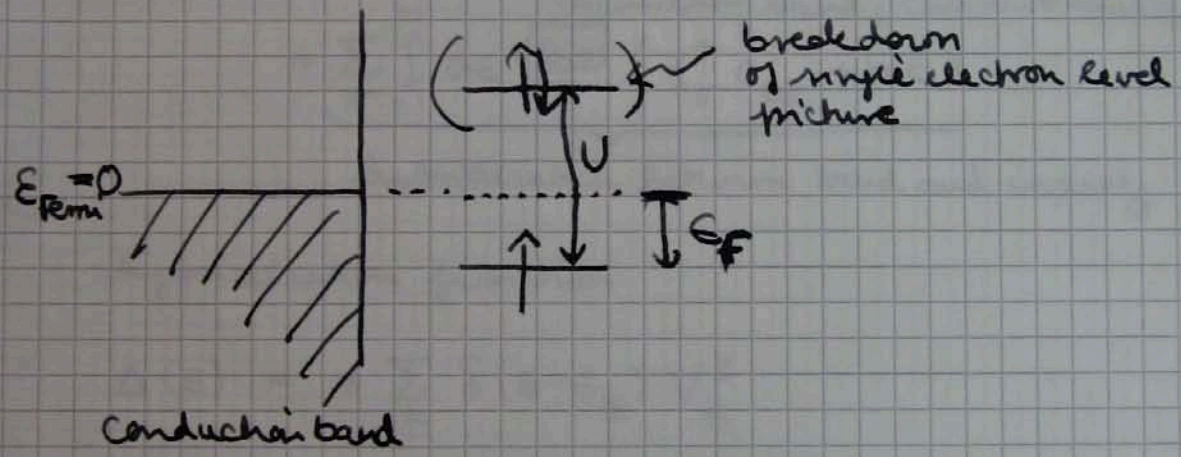
more realistic model: Anderson(-Wolff) model (1961)

take charge fluctuations into account
(i.e. zero, double occupancies)

$$H_{And} = \underbrace{\sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{\text{conduction band}} + \sum_{k\sigma} V_k \left(f^\dagger_\sigma c_{k\sigma} + \text{h.c.} \right)$$

V_k: hopping amplitude band–impurity; f: denotes impurity site

$$+ \underbrace{\epsilon_f n_f}_{\text{energy level}} + \underbrace{U n_{f\uparrow} n_{f\downarrow}}_{\substack{\text{on-site repulsion} \\ \text{(localized orbital)}}}$$



symmetric Anderson model: $\uparrow\downarrow$ and $\uparrow, \downarrow$ have same distance to Fermi energy $\boxed{-U/2 = \epsilon_f}$

Kondo model follows through Schrieffer-Wolff transformation in appropriate limit (U large)

$$J \sim \frac{V_k^2}{U}$$

cf. Hubbard → Heisenberg

II NRG

1. Logarithmic discretization

Consider SIAM.

- change from momentum to energy representation: <u>s-wave approximation</u>
- rescale bandwidth $D \to 1$

effective <u>1D</u> problem

$$H_{And} = H_{imp} + \underbrace{\sum_\sigma \int_{-1}^{+1} d\epsilon\ \epsilon\ c^\dagger_{\epsilon\sigma} c_{\epsilon\sigma}}_{\text{conduction band, constant density of states}} + \underbrace{\sum_\sigma \int_{-1}^{+1} d\epsilon \sqrt{\frac{\Delta(\epsilon)}{\pi}} \left(f^\dagger_\sigma c_{\epsilon\sigma} + \text{h.c.} \right)}_{\text{hybridization between band and impurity}}$$

hybridization function

$$\Delta(\epsilon) = \pi \sum_{\underline{k}} \delta(\epsilon - \epsilon_{\underline{k}})\, V^2_{\underline{k}}$$

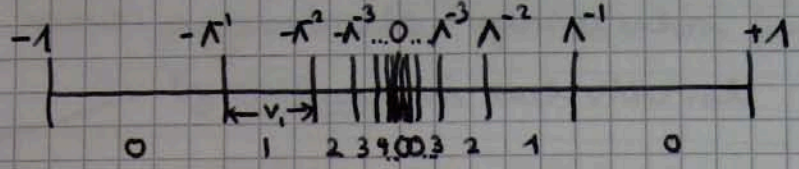
assume <u>half-filling</u> of band: $\epsilon_F = 0$

- physics of "Kondo problem" happens at low temperatures $\hat{=}$ low energies
- poor man's scaling indicates exponentially growing relevance of low energy contributions

<u>Logarithmic discretization</u>:

reformulate problem with exponentially strong focus on $\epsilon \to \epsilon_F = 0$.

discretization parameter $\Lambda > 1$ (typical value: $\Lambda = 2$)



conduction band

$$n = 0, 1, \dots, \infty \quad \begin{cases} [\Lambda^{-(n+1)}, \Lambda^n] & \epsilon > 0 \\ [-\Lambda^{-n}, -\Lambda^{-(n+1)}] & \epsilon < 0 \end{cases}$$

width: $v_n = \Lambda^{-n}(1 - \Lambda^{-1})$

construction of complete basis as a combination of bases in each interval, expressed in Fourier space:

in interval n: $\omega_n = \frac{2\pi}{v_n}$ fundamental Fourier frequency

basis wave functions

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

$p \in \mathbb{Z}$: complete set in interval

$$c_{\epsilon\sigma} = \sum_{np} a_{np\sigma} \psi^{+}_{np}(\epsilon) + b_{np\sigma} \psi^{-}_{np}(\epsilon)$$

$$a_{np\sigma} = \int_{-1}^{+1} d\epsilon \, (\psi^{+}_{np}(\epsilon))^* c_{\epsilon\sigma}$$

$$b_{np\sigma} = \int_{-1}^{+1} d\epsilon \, (\psi^{-}_{np}(\epsilon))^* c_{\epsilon\sigma}$$

fermionic operators: $\{a_{np\sigma}, a^{\dagger}_{n'p'\sigma'}\} = \delta_{nn'}\delta_{pp'}\delta_{\sigma\sigma'}$

$\{b_{np\sigma}, b^{\dagger}_{n'p'\sigma'}\} = \delta_{nn'}\delta_{pp'}\delta_{\sigma\sigma'}$

so far, no approximation!

now: approximate hybridization function $\Delta(\epsilon)$ by constant in each interval — exact for $\Lambda \to 1$

then: impurity couples only to $p = 0$ states

$$\int_{-1}^{+1} d\epsilon \sqrt{\Delta(\epsilon)}\, c_{\epsilon\sigma}$$

$$= \sum_{np} \left(a_{np\sigma} \int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} d\epsilon \sqrt{\Delta(\epsilon)} \frac{e^{i\omega_{np}\epsilon}}{\sqrt{v_n}} + b_{np\sigma} \int_{-\Lambda^{-n}}^{-\Lambda^{-(n+1)}} d\epsilon \sqrt{\Delta(\epsilon)} \frac{e^{-i\omega_{np}\epsilon}}{\sqrt{v_n}} \right)$$

$$= \sum_{n} \Big(a_{no\sigma} \underbrace{\int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} d\epsilon \sqrt{\Delta(\epsilon)} \frac{1}{\sqrt{v_n}}}_{=: \gamma_n^+} + b_{no\sigma} \underbrace{\int_{-\Lambda^{-n}}^{-\Lambda^{-(n+1)}} d\epsilon \sqrt{\Delta(\epsilon)} \frac{1}{\sqrt{v_n}}}_{=: \gamma_n^-} \Big)$$

$$d_{o\sigma} := \frac{1}{\sqrt{\xi_0}} \int_{-1}^{+1} d\epsilon \sqrt{\Delta(\epsilon)}\, c_{\epsilon\sigma} = \frac{1}{\sqrt{\xi_0}} \sum_n \left(\gamma_n^+ a_{no\sigma} + \gamma_n^- b_{no\sigma} \right)$$

with normalization ξ_0 to assure $\{d_{o\sigma}, d_{o\sigma'}^\dagger\} = \delta_{\sigma\sigma'}$

$$\xi_0 = \sum_n \left((\gamma_n^+)^2 + (\gamma_n^-)^2 \right) \qquad \xi_0 = 2\Delta \text{ if } \Delta(\omega) = \Delta$$

$d_{o\sigma} \hat{=}$ maximally localized state $d_{o\sigma}^\dagger |0\rangle$

We can neglect $p \neq 0$ in the hybridization.

It turns out:

in $c_{\epsilon\sigma}^\dagger c_{\epsilon\sigma} \to \sum_{pp'} (a,b)_{npo}^\dagger (a,b)_{np'\sigma}$ $p, p' \neq 0$ terms

don't contribute much for $\Lambda = 2$; vanish exactly for $\Lambda \to 1$

Finally, logarithmic discretization therefore yields

$$H_{And} = H_{imp} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma (f_\sigma^+ d_{0\sigma} + h.c.)$$

$$+ \frac{1+\Lambda^{-1}}{2} \sum_{n=0,\sigma}^{\infty} \Lambda^{-n} \left(a_{n\sigma}^+ a_{n\sigma} - b_{n\sigma}^+ b_{n\sigma} \right)$$

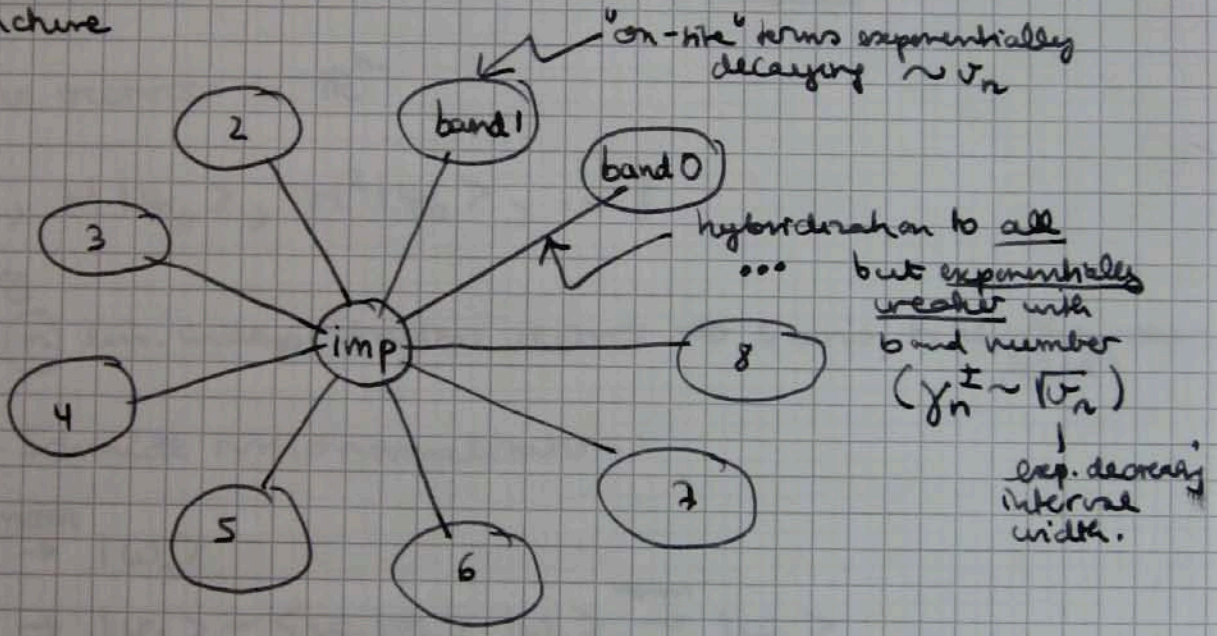
neg. energy $\epsilon < 0$

mean energy in interval n.

$p=0$ index dropped

terms exponentially decreasing

but still intractable because $d_{0\sigma}$ has complicated a,b structure

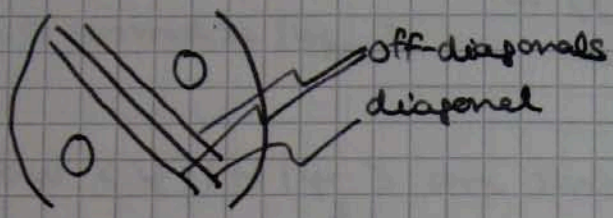


<u>separation of energy scales</u> ~ <u>iterative diagonalization!</u>

II. 2. Mapping to semi-infinite chain

Any Hamiltonian can be brought iteratively into tridiagonal form

i.e. basis $\{|i\rangle\}$ such that

$H_{ij} =$ 

procedure: Lanczos diagonalization $\hat{=}$ Gram-Schmidt orthonormalization of Krylov vectors

Krylov vectors: in $\mathbb{R}^n$

$\{|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, \dots\}$

↑ arbitrary

max. (n) lin. indep. Krylov vectors ⇒ basis, to be orthonormalized!

Gram-Schmidt orthonormalization:

$|v_1\rangle \xrightarrow{\text{norm}} |w_1\rangle$

$|v_2\rangle \to |v_2\rangle - \langle w_1|v_2\rangle \cdot |w_1\rangle \xrightarrow{\text{norm}} |w_2\rangle$

$|v_3\rangle \to |v_3\rangle - \underbrace{\langle w_1|v_3\rangle \cdot |w_1\rangle - \langle w_2|v_3\rangle \cdot |w_1\rangle}_{\Rightarrow\ -\sum_{i<j} \langle w_i|v_j\rangle |w_i\rangle} \xrightarrow{\text{norm}} |w_3\rangle$

...

gets important simplification on Krylov vectors!

Orthogonality to basis vectors "more than 2 index numbers away" automatically ensured (show by ind.)

leads to Lanczos recursion:

$$t_n |\psi_{n+1}\rangle = H|\psi_n\rangle - \underbrace{\langle\psi_n|H|\psi_n\rangle}_{\epsilon_n \text{ (diagonal)}}|\psi_n\rangle - \underbrace{\langle\psi_{n-1}|H|\psi_n\rangle}_{t_{n-1} \text{ (off-diagonal)}}|\psi_{n-1}\rangle$$

t_n: chosen to normalize $|\psi_{n+1}\rangle$

all other $\langle\psi_i|H|\psi_j\rangle$ are strictly 0 $\Rightarrow$ tridiagonal form of H in ONB $\{|\psi_n\rangle\}$

start by $|\psi_0\rangle := d_0^\dagger|0\rangle$ (suppress 0)

define d_n by $|\psi_n\rangle =: d_n^\dagger|0\rangle$

OK - so we can tridiagonalize any H, in particular H_{And}. Why is this useful?

- <u>normally</u>, because spectrum of iteratively generated tridiagonal Hamiltonian converges quickly to <u>extreme</u> eigenvalues of original Hamiltonian $\Rightarrow$ <u>exact diagonalization</u>
- <u>here</u> because Lanczos tridiagonalization generates tridiagonal Hamiltonian with (essentially) <u>exact total</u> spectrum because of energy scale separation — in a sense to be seen ...

$$H = \sum_{n=0}^{\infty} \Lambda^{-n} \left(a_n^\dagger a_n - b_n^\dagger b_n \right) \qquad \text{(in each spin sector)}$$

$$\downarrow$$

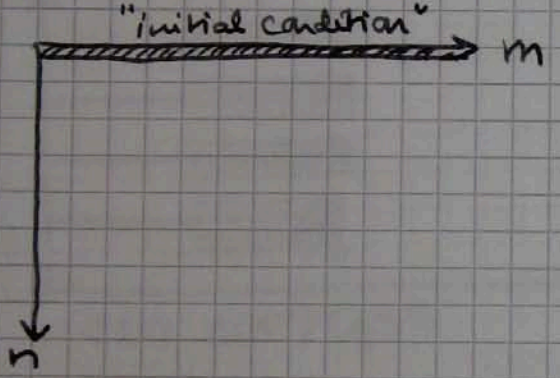
$$H = \sum_{n=0}^{\infty} t_n \left(d_n^\dagger d_{n+1} + \text{h.c.} \right) + \epsilon_n d_n^\dagger d_n$$

$$d_n^\dagger = \sum_m u_{nm} a_m^\dagger + v_{nm} b_m^\dagger \qquad \text{(unitary trafo!)}$$

to make contact to hybridization term:

$$|\psi_0\rangle = d_0^\dagger |0\rangle \quad \text{hence} \quad u_{0m} = \frac{\gamma_m^+}{\sqrt{\xi_0}} \quad v_{0m} = \frac{\gamma_m^-}{\sqrt{\xi_0}}$$

as start of Lanczos iteration.



$$t_{-1} = 0$$

$$\epsilon_n = 0 \quad \text{if } \Delta(\epsilon) = \Delta(-\epsilon)$$

one finds

$$\epsilon_n = \sum_m \Lambda^{-m} \left(u_{nm}^2 - v_{nm}^2 \right)$$

$$t_n^2 = \sum_m \Big[\left(\Lambda^{-m} u_{nm} - \epsilon_{n-1} u_{(n-1)m} - \epsilon_n u_{nm} \right)^2 + \left(-\Lambda^{-m} v_{nm} - \epsilon_{n-1} v_{(n-1)m} - \epsilon_n v_{nm} \right)^2 \Big]$$

$$t_{n-1} = \sum_m \Lambda^{-m} \left(u_{(n-1)m} u_{nm} - v_{(n-1)m} v_{nm} \right)$$

$$u_{(n+1)m} = \frac{1}{t_n} \left(\Lambda^{-m} u_{nm} - t_{n-1} u_{(n-1)m} - \epsilon_n u_{nm} \right)$$

$$v_{(n+1)m} = \frac{1}{t_n} \left(-\Lambda^{-m} v_{nm} - t_{n-1} v_{(n-1)m} - \epsilon_n v_{nm} \right)$$

} recursion set.

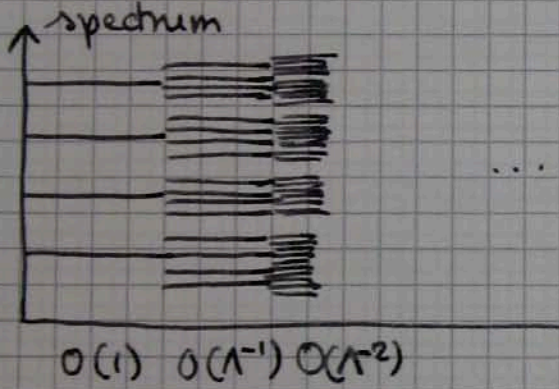
exact for $\Delta(\omega) = \Delta$

$$\epsilon_n = 0$$

$$t_n = \frac{(1+\Lambda^{-1})(1-\Lambda^{-n-1})}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}\Lambda^{-n/2}$$

$$\to \tfrac{1}{2}(1+\Lambda^{-1})\Lambda^{-n/2}$$ exponentially decaying

The exponential decay of t_n as $\Lambda^{-n/2}$ results from iterative diagonalization: at each application of H, the leading term "diagonalized away" diminishes as Λ^{-1}.



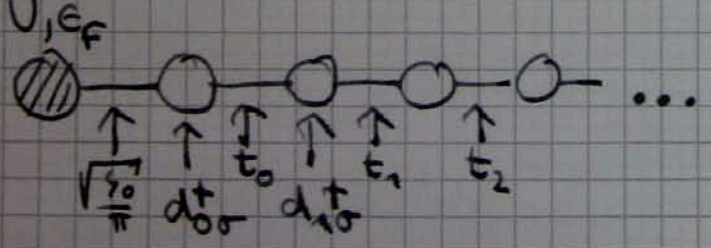
here: energies "wrong" by Λ^{-n}

density of states approx. correct (if correctly normalized)

resulting Hamiltonian: <u>semi-infinite chain</u>

$$H = \epsilon_f n_f + U n_{f\uparrow} n_{f\downarrow} + \sqrt{\frac{t_0}{\pi}} \sum_\sigma \left(d_\sigma^\dagger d_{0\sigma} + \text{h.c.} \right)$$

$$+ \sum_{n=0}^{\infty} t_n \left(d_{n\sigma}^\dagger d_{(n+1)\sigma} + \text{h.c.} \right) \qquad \text{(assuming } \epsilon_n = 0\text{)}$$



$$t_n \sim \Lambda^{-n/2}$$

physical interpretation:

$d^{+}_{n\sigma}|0\rangle$ creates wave packets with energy at Fermi surface, centered at impurity, with spatial extent $\Lambda^{n/2}$

we neglect states far away from impurity and far away from Fermi surface $\Rightarrow$ a massive physically motivated approximation specific to the problem has happened!

II.3. Iterative diagonalization of the semi-infinite chain

- $H = H_{imp} + H_{hyb} + \sum_{n=0,\sigma}^{\infty} t_n (d_{n\sigma}^{\dagger} d_{n+1,\sigma} + h.c.)$

  is still too complex for exact treatment:

  $t_n \sim \Lambda^{-n/2}$ sets energy and <u>temperature</u> scale;
  for typical Kondo-like problem (fixed T_K)
  $n \sim 50 \dots 60$ implied

  # states: $4^n \gtrsim 2^{100} \gtrsim 10^{30}$ inaccessible!

  full spectra for matrices $O(1000)$

- scales of coefficients vary exponentially:
  numerically potentially problematic ...?

$$H_N := \Lambda^{(N-1)/2} \Big\{ \epsilon_f n_f + U n_{f\uparrow} n_{f\downarrow} + \sqrt{\frac{\xi_0}{\pi}} \sum_{\sigma} (f_{\sigma}^{\dagger} d_{0\sigma} + h.c.) + \sum_{n=0,\sigma}^{N-1} t_n (d_{n\sigma}^{\dagger} d_{(n+1)\sigma} + h.c.) \Big\}$$

↑ makes low-lying excitations of $O(1)$

$$H_0 = \Lambda^{-1/2} \Big\{ \epsilon_f n_f + U n_{f\uparrow} n_{f\downarrow} + \sqrt{\frac{\xi_0}{\pi}} \sum_{\sigma} (f_{\sigma}^{\dagger} d_{0\sigma} + h.c.) \Big\}$$

$$H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N$$

$$\boxed{H_{N+1} = \Lambda^{1/2} H_N + \sum_{\sigma} \Lambda^{N/2} t_N (d_{N\sigma}^{\dagger} d_{(N+1)\sigma} + h.c.)}$$

RG transformation equations.

give Hamiltonian block-diagonal structure by use of good quantum numbers

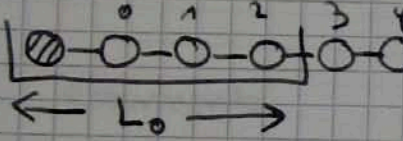
$|Q, S, S^z, r\rangle$ ← labels states in subspace

$$Q_N = \sum_{n=0,\sigma}^{N} (d^\dagger_{n\sigma} d_{n\sigma} - \tfrac{1}{2}) + \sum_\sigma (f^\dagger_\sigma f_\sigma - \tfrac{1}{2})$$ charge w/r half-filling

$$S^i_N = \tfrac{1}{2} \sum_{n=0,\mu\nu}^{N} d^\dagger_{n\mu} \sigma^i_{\mu\nu} d_{n\nu} + \tfrac{1}{2} \sum_{\mu\nu} f^\dagger_\mu \sigma^i_{\mu\nu} f_\nu$$

total spin S: more difficult / not first choice

approximate analysis: fix M ($O(1000)$)

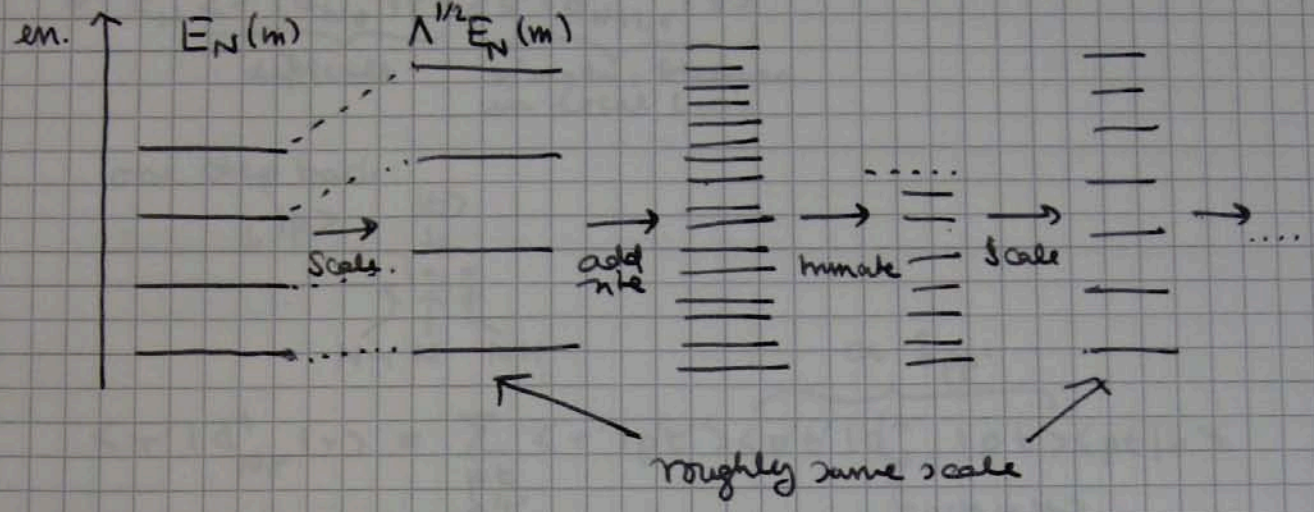


$4^{L_0} > M > 4^{L_0-1}$

0. $L = L_0$
1. diagonalize H_{L-2} (system length L): $\{|m\rangle_{L-2}\}$; $E^{(m)}_{L-2}$
2. <u>retain M lowest-energy states</u>
   (physically motivated truncation)
3. rescale $E^{(m)}_{L-2}$ by $\Lambda^{1/2}$
4. build $\{|\underbrace{m\ n}_{\#: 4M}\rangle\}$ ($|n\rangle$ + local states)
5. $L \to L+1$; express H_{L-2} in $\{|mn\rangle\}$ basis; goto 1.

many-particle energy flow:

$$H_N |m\rangle_N = E_N(m) |m\rangle_N$$

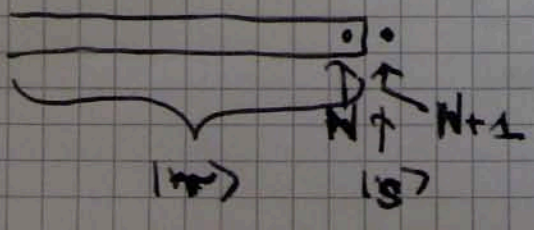


comments:

- check quality by varying M
- to make $\Lambda \to 1$, M has to go up!
  (sep. of energy scales vanishes)
- obtain approximation to many-particle spectrum of Hamiltonian in exp. decreasing energy window

technical excursion: calculation of <u>matrix elements</u>
(needed also for observables)

consider $t_N \, d^\dagger_{N\sigma} \, d_{N+1,\sigma}$ (cf. DMRG!)

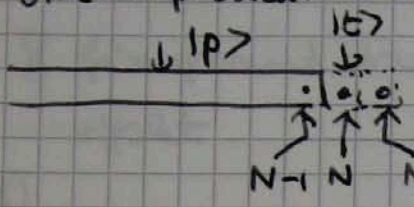


express this expression in basis $|rs\rangle$

$$\langle r's'| t_N d^\dagger_{N\sigma} d_{N+1,\sigma} |rs\rangle$$

$$= t_N \underbrace{\langle r'| d^\dagger_{N\sigma} |r\rangle}_{\text{difficult}} \underbrace{\langle s'| d_{N+1,\sigma} |s\rangle}_{\text{simple, because in local basis}}$$

one step back:



$$\langle r'| d^\dagger_{N\sigma} |r\rangle = \sum_{\substack{pt \\ p't'}} \langle r'|p't'\rangle \underbrace{\langle p't'| d^\dagger_{N\sigma} |pt\rangle}_{\propto \delta_{pp'}} \langle pt|r\rangle$$

↑ acts on $|t\rangle$

$$= \sum_{ptt'} \underbrace{\langle r'|pt'\rangle}_{\text{known from last truncation. (reduced unitary transformation)}} \langle r'| d^\dagger_{Nr} |t\rangle \underbrace{\langle pt|r\rangle}_{\text{known from last truncation. (reduced unitary transformation)}}$$

easy to write up!

So, any observable can be built up as

- when site "added", calculate $\langle s_N | O | s'_N \rangle$
  - observable in local basis
- express in new basis as

$$\langle r_N | O | r'_N \rangle = \sum_{\substack{r_{N-1} \\ s_N, s'_N}} \langle r_N | r_{N-1} s_N \rangle \langle s_N | O | s'_N \rangle \langle r_{N-1} s'_N | r'_N \rangle$$

- update as

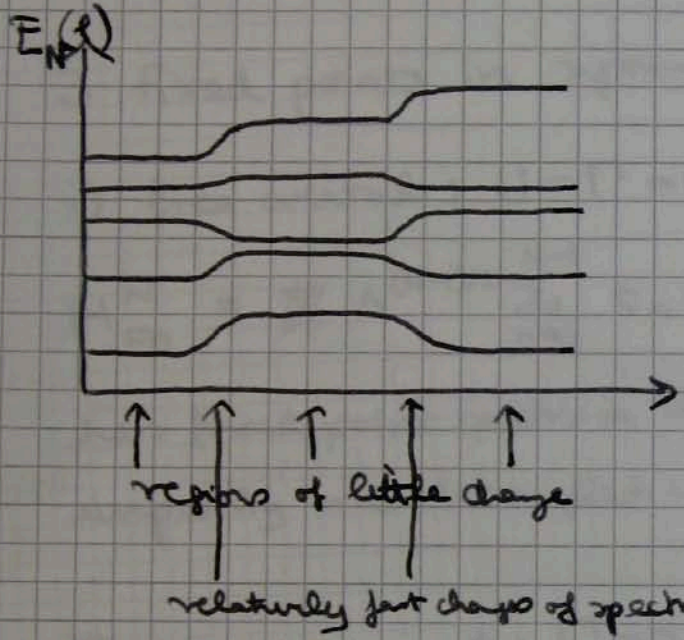
$$\langle r_{N+1} | O | r'_{N+1} \rangle = \sum_{r_N, r'_N} \langle r_{N+1} | r_N s_{N+1} \rangle \langle r_N | O | r'_N \rangle \langle r'_N s_{N+1} | r'_{N+1} \rangle$$

s_{N+1} ← because diagonal!

II.4. RG flow

What if we plot energies vs. NRG iteration?

- Only plot even or odd iterations – at half-filling, spectrum changes quite substantially (fermions!)
- fix ground state energy to be zero at each step via offset



typical picture:
"railway track picture"

invariance of spectrum under rescaling: RG fixed points?

RG: normally, consider flow of Hamiltonian parameters
$\{K\} \to \{K'\}$ under RG trafo (decimation, rescaling)

here: parameter sets change (new coupling) → consider spectra instead (as plotted!)

RG equation:

$$H_{N+1} = \Lambda^{1/2} H_N + \sum_\sigma \underbrace{\Lambda^{N/2} t_N}_{O(1)} (d^\dagger_{N\sigma} d_{(N+1)\sigma} + h.c.) \underbrace{- E^0_{N+1}}_{\text{to make GS energy } 0}$$

$O(\Lambda^{-N/2})$

abbreviate:

$\mathcal{H}_{N+1} = \mathcal{T}[\mathcal{H}_N]$ maps $E_N(\ell) \to E_{N+1}(\ell)$

RG trafo

fixed point $\mathcal{H}^* = \mathcal{T}[\mathcal{H}^*]$; here $H^* = \mathcal{T}^2[H^*]$

3 fixed points in symmetric Anderson model:

i) free orbital: $U = \Gamma = 0$

$$H^N_{FO} = \Lambda^{(N-1)/2} \sum_{n=0}^{N-1} t_n (d^\dagger_{n\sigma} d_{(n+1)\sigma} + h.c.)$$

has fixed point spectrum under RG; corresponds to impurity site decoupled with 4 deg. states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$.

ii) local moment: $\Gamma = 0$, $U \to \infty$

$$H^N_{LM} = \Lambda^{(N-1)/2} \Big(\sum_{n=0}^{N-1} \sum_\sigma t_n (d^\dagger_{n\sigma} d_{(n+1)\sigma} + h.c.) + \frac{\Gamma}{U} \sum_{\mu\nu} d^\dagger_{0\mu} \vec{\sigma}_{\mu\nu} d_{0\nu} \cdot \vec{\tau} \Big)$$

Spin $\frac{1}{2}$ on impurity couples to 1st band shell (Kondo!)

iii) strong coupling: $U = 0$; $\Gamma \to \infty$

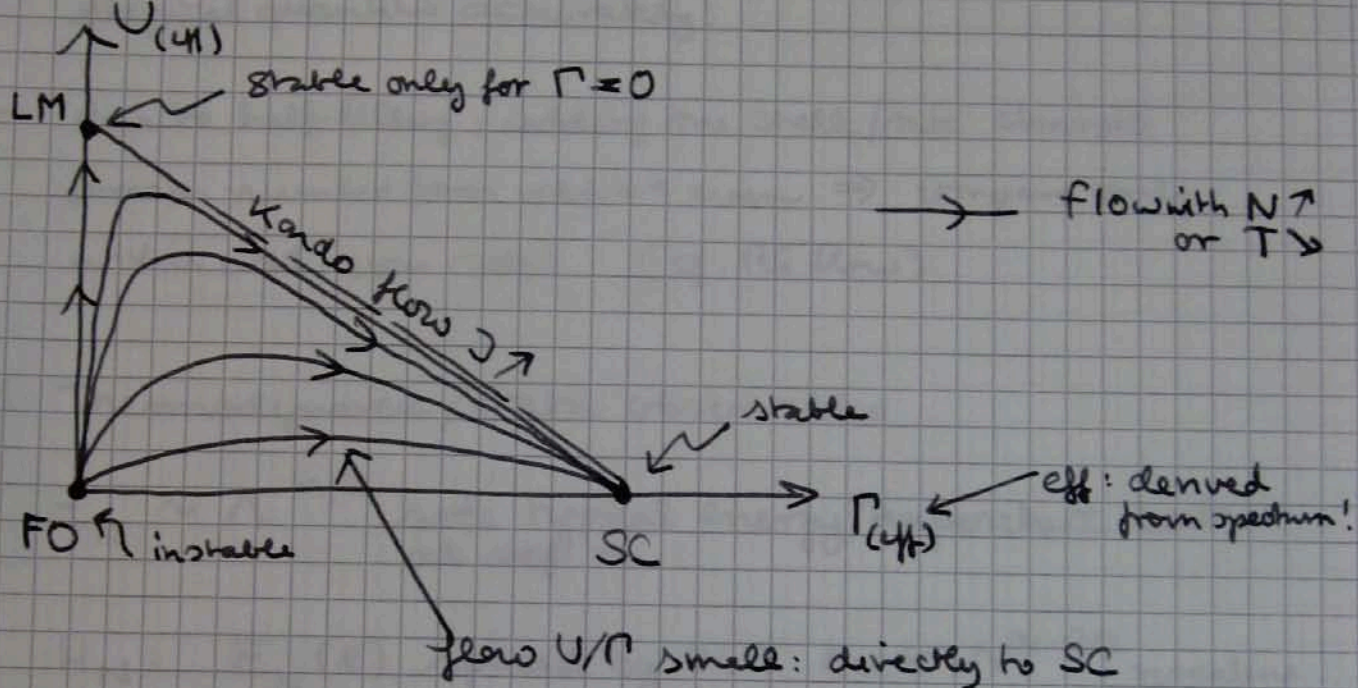
$$H^N_{SC} = \Lambda^{(N-1)/2} \sum_{n=1,\sigma}^{N-1} t_n (d^\dagger_{n\sigma} d_{(n+1)\sigma} + h.c.)$$

imp. / 1st band shell are paired off as singlet and decouple completely (perfect screening)

in the picture showed, flow from FO → LM → SC as N grows (and effective T is lowered, see III.)

Close to fixed points, little change to H → hence almost stationary spectrum

flow diagram for Anderson model:



III. Observables

General remarks

- We have consistently discarded information about the conduction band ⇒ we can only calculate <u>impurity</u> contributions to physical quantities accurately!
- due to half-filling, adding one shell/site changes fermion number from odd ↔ even ⇒ compare only within odd, even sets! (cf. RG flow)

1. Thermodynamic/static observables

$t_n \sim \Lambda^{-n/2}$ sets typical energy/temperature scale at step n.

H_N: $E_N(\ell)$ spaced by $O(1)$ due to $\Lambda^{(N-1)/2}$ rescaling

$$\underbrace{E_N(\ell) - E_N(0)}_{\text{high-lying excitations}} \gg \underbrace{\Lambda^{(N-1)/2} k_B T}_{\text{restore true scale}}$$

will not contribute much!

⇒ for $\beta_N = (k_B T_N)^{-1}$ with $\beta_N \Lambda^{-(N-1)/2} = \bar{\beta} \doteq O(1)$ H_N approximates for full H

modifications to ~~foot~~ levels in further NRG steps will only affect lowest-lying states:

$$\underbrace{E_N(\ell) - E_N(0)}_{\text{lowest-lying states will be further modified}} \ll \Lambda^{(N-1)/2} k_B T_N$$

H_N allows thermodynamics at scale $k_B T_N = \Lambda^{-(N+1)/2}$

expressions:

$$S/k_B = \beta \langle H \rangle + \ln Z$$

$$C/k_B = \beta^2 (\langle H^2 \rangle - \langle H \rangle^2)$$

or

$$C = \frac{\partial \langle H \rangle}{\partial T}$$

} dilemma: precision of $\langle H^2 \rangle$ vs precision of num. derivative

$$\chi = \beta (\langle (S^z_{tot})^2 \rangle - \langle S^z_{tot} \rangle^2)$$

or response to inf. ext. field

$$\chi_{imp}(T) = \chi(T) - \chi^{(0)}(T)$$
$$S_{imp}(T) = S(T) - S^{(0)}(T)$$
$$C_{imp}(T) = C(T) - C^{(0)}(T)$$

↑ calculated for tridiagonal Ham.

$$H^N_{(0)} = \sum_{n=0,\sigma}^{N-1} t_n (c^+_{n\sigma} \xi_{(n+1)\sigma} + \text{h.c.}) + \sum_{n=0,\sigma}^{N} \epsilon_n c^+_{n\sigma} c_{n\sigma}$$

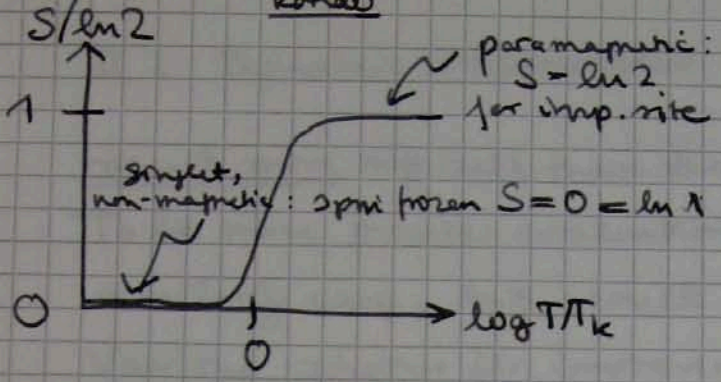
↖ if applicable.

For $T \to 0$, also analytically.

improve on N odd, even problem: averaging

- $O^{(N-1)}, O^{(N)}, O^{(N+1)}$ for $T = T_{N-1}, T_N, T_{N+1}$
- $$O(T_N) \approx \frac{1}{2} \Big(\underbrace{O^{(N)}}_{\text{value for } T_N} + \underbrace{O^{(N-1)} + \frac{O^{(N+1)} - O^{(N-1)}}{T_{N+1} - T_{N-1}} \cdot (T_N - T_{N-1})}_{\text{interpolated value for } T_N} \Big)$$

Kondo



how good is Kondo?

calculate local occupancy in Anderson-model

$$n_\sigma(T_N) \sim \frac{1}{Z^{(N)}} \sum_{QS^z r} e^{-\beta E_N(QS^z r)} \underbrace{{}_N\langle QS^z r|\, f^\dagger_\sigma f_\sigma\, |QS^z r\rangle_N}_{\text{construction of matrix elements as explained in II.3.}}$$

Z-averaging:

finite Λ → discretization introduces arbitrary cuts

idea: vary position of cuts

- $x_n = \Lambda^{-n}_{n\geq 1} \longrightarrow x_n = \Lambda^{-n+z} \quad z \in [0,1)$
- for fixed z: do NRG calc. for $T_N = \Lambda^{-(N-1)/2}\frac{1}{\beta}$
- average over different z

often, just 2 values of z sufficient to remove spurious oscillations in quantities

(Oliveira & Oliveira, 1994)

III.2. Dynamic observables

<u>much more</u> difficult than thermodynamic case!
To be more precise: evaluation in most simple approaches similarly easy, but results are much less accurate.
Various schemes for improvement exist!

Green's function

$$G_\sigma(t-t') = -i\theta(t-t') \langle [f_\sigma(t), d_\sigma^+(t')]_+ \rangle_{\rho(T)}$$

($t-t'$: homogeneous in time; $\rho(T)$: density operator at temp. T)

$$f_\sigma(t) = e^{iHt} f_\sigma(0) e^{-iHt}$$ Heisenberg

$$G_\sigma(\omega, T) = \int_{-\infty}^{+\infty} d(t-t')\, e^{i\omega(t-t')}\, G_\sigma(t-t')$$ FT

$$A_\sigma(\omega, T) = -\frac{1}{\pi} \operatorname{Im} G_\sigma(\omega, T)$$ <u>spectral density</u>

assume <u>complete</u> spectrum known $\{|r\rangle\}$; E_r

$$\rho(T) = \frac{1}{Z(T)} \sum_r e^{-\beta E_r} |r\rangle\langle r|$$

$$Z(T) = \sum_r e^{-\beta E_r}$$

After some calculation: Lehmann representation

$$A_\sigma(\omega, T) = \frac{1}{Z(T)} \sum_{rr'} |M_{rr'}|^2 \left(e^{-E_r/k_BT} + e^{-E_{r'}/k_BT}\right) \cdot \delta\left(\omega - (E_r - E_{r'})\right)$$

with $M_{rr'} = \langle r | f_\sigma | r' \rangle$

Consider cases $T=0$ (easy) and $T>0$ (problematic) separately.

T=0 : Lehmann representation occurs from expr. like

$$\langle f_\sigma f_\sigma^+ \rangle_\beta = \sum_r \langle r | f_\sigma f_\sigma^+ | r \rangle e^{-\beta E_r}$$

$$= \sum_{rr'} \underbrace{\langle r | f_\sigma | r' \rangle \langle r' | f_\sigma^+ | r \rangle}_{|M_{rr'}|^2} e^{-\beta E_r}$$

↑ insert 1

now $\sum_r$ collapses to just $|0\rangle$ (ground state)

$$A_\sigma(\omega, T=0) = \frac{1}{Z(0)} \left(\sum_r |M_{r0}|^2 \delta(\omega - (E_r - E_0)) + \sum_{r'} |M_{0r'}|^2 \delta(\omega - (E_{r'} - E_0)) \right)$$

g.s. deg.

assume $E_0 = 0$

evaluate with approximate H_N:

$$A_\sigma^{(N)}(\omega, T=0) = \frac{1}{Z(0)} \left(\sum_r |M_{r0}^{(N)}|^2 \delta(\omega - E_N(r)) + \sum_{r'} |M_{0r'}^{(N)}|^2 \delta(\omega - E_N(r')) \right)$$

the characteristic frequency for ~~H_N~~ H_N is (mean of limits)

$$\omega_N \sim \frac{1}{2}(1 + \Lambda^{-1}) \Lambda^{-(N-1)/2}$$

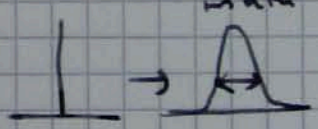
realistic results for frequency in range

$$\omega_N \leq \omega \leq K(\Lambda)\omega_N$$

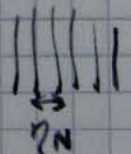
↑ order 5-10 for $\Lambda = 1.5\text{-}2$, $M = 500\text{-}1000$.

peaks are δ-functions ⇒ <u>smoothening</u> to obtain continuous curve:

$$\delta(\omega \mp E_N(r)) \to P(\omega \mp E_N(r))$$



width $\eta_N \sim \omega_N$ ← energy level distance scale



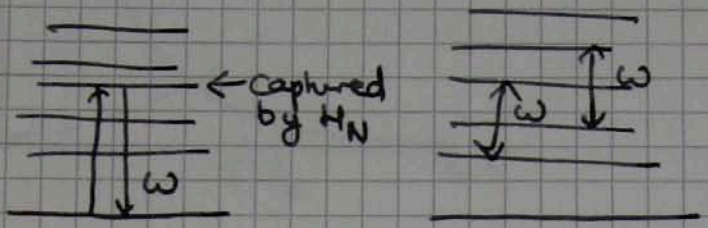
typical (but not unique) choice:

$$P_{Gauss}(\omega \pm \bar{E}_N(r)) = \frac{1}{\eta_N \sqrt{\pi}} e^{-[(\omega \pm E_N(r))/\eta_N]^2}$$

(Gaussian broadening)

$T>0$:

compare $T=0$ and $T>0$



contributions from all excited states

$\omega \approx \omega_N$ no longer captured just by H_N.

but: "higher" contributions suppressed by Boltzmann factor

so, for high frequencies (energies) we can do as if only ground-state matters:

$\omega = 2\omega_N > k_B T$: $\quad A_\sigma(\omega, T) \simeq A_\sigma^{(N)}(\omega, T)$

problem occurs for low frequencies: assume thermal fluctuations "wash out" "higher" contributions

$\omega = 2\omega_N < k_B T$: $\quad A_\sigma(\omega, T) \cong A_\sigma^{(M)}(\omega, T)$

M defined from $\omega_M \sim k_B T$.

transport: $\dfrac{1}{\tau_{tr}(\omega,T)} = \dfrac{2 n_i \Delta}{N_F} A_\sigma(\omega, T)$

τ_{tr}: transport time

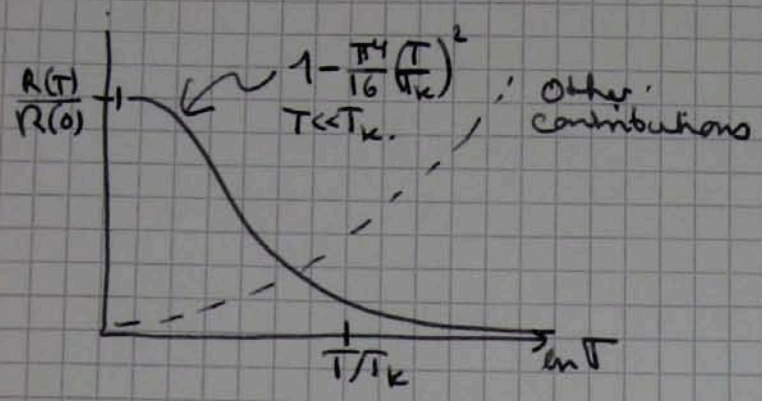
n_i : impurity concentration

Δ : hybridization

N_F : density of states

resistivity: $R(T) = \left[e^2 \int d\omega \left(-\dfrac{\partial f}{\partial \omega}\right) \tau_{tr}(\omega, T) \right]^{-1}$

f: Fermi function derivative


R(T)/R(0)
1
$1-\frac{\pi^4}{16}\left(\frac{T}{T_K}\right)^2$
$T \ll T_K$.
: Other contributions
T/T_K
ln T