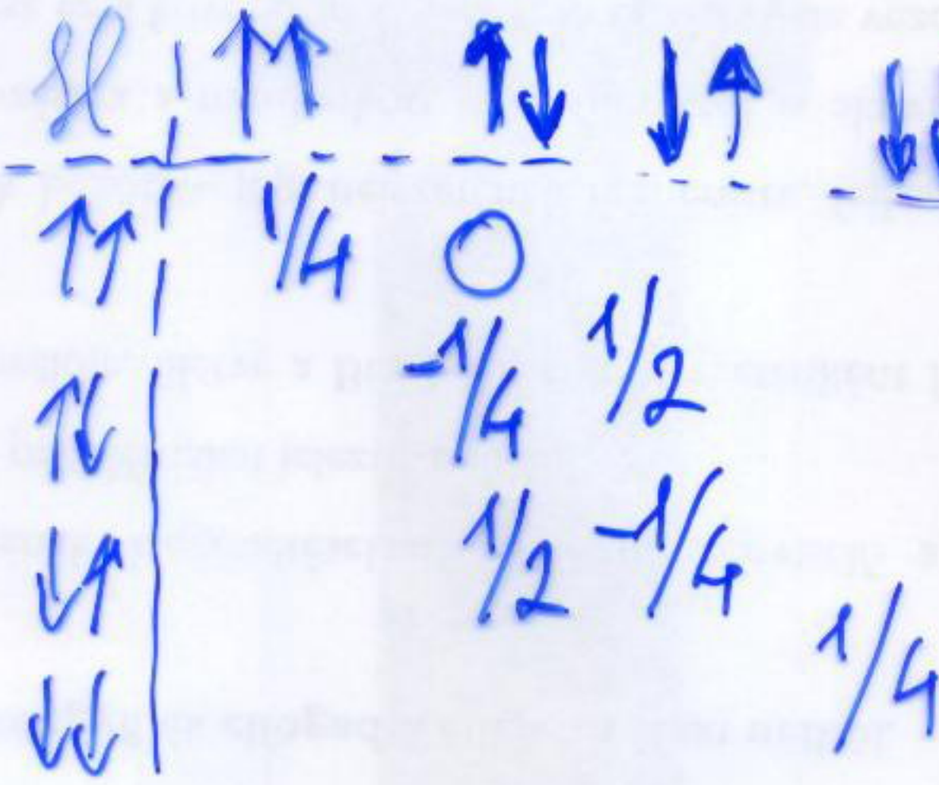
BRG

$q=2$ $S=1/2$ Heisenberg model

$$\mathcal{H}^{(n)} = \frac{J^{(n)}}{2}\left(S_i^{+(n)} S_{i+1}^{+(n)} + S_i^{-(n)} S_{i+1}^{+(n)}\right) + \Delta\, S_i^{z(n)} S_{i+1}^{z(n)}$$

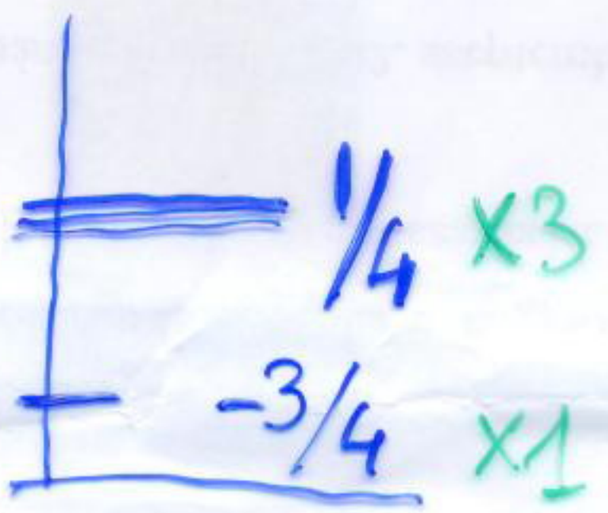
- for 2 sites:



$$S^z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} \qquad S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

- diagonalization → $E_\alpha^{(2)}$, $\psi_\alpha^{(2)}$

$\alpha = 1, 2, 3, 4$



$\psi_4 = \uparrow\uparrow$

$\psi_3 = \downarrow\downarrow$

$\psi_2 \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$

$\psi_1 = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$

- Renormalization of operators

$$A^{(l+1)} = O A^{(l)} O^+$$

in general case

$$O \equiv [M', M*q]$$

$$O = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad M'$$

if $M=2$ which one to keep?

cut at some point

Numerical renormalization Group (NRG)

- Single impurity Anderson model (SIAM)
- -"- Kondo model

SIAM (1961): spherically symmetric strongly correlated impurity in an uncorrelated non-magnetic metal

$$H = \varepsilon_d \sum_\sigma n_\sigma^d + U n_\uparrow^d n_\downarrow^d + \sum_{k\sigma} V_{kd} c_{k\sigma}^\dagger d_{k\sigma} + H.C.) + \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma}$$

- impurity with energy ε_d, $n_\sigma^d = d_\sigma^\dagger d_\sigma$

  U local Coulomb interaction

- hybridization $V_{k,d}$ allows scattering from all momentum states

- hybridization function: $\Delta(w) = \pi \sum_k |V_{kd}|^2 \delta(w - \varepsilon_k)$
- density of states of the conduction band $s(w) = \sum_k \delta(w - \varepsilon_k)$; s-wave & orbitally symmetric case

for numerical treatment model is mapped onto a linear chain using a Lanczos tridiagonalization procedure:

- define localized Wannier state:

$$|0,\sigma\rangle \equiv f_{0\sigma}^{+}|\psi_{vac}\rangle \;,\; f_{0,\sigma} = \frac{1}{V}\sum_{k} V_{kd}\, c_{k\sigma}$$

main object is to transform hybridization into a local term

$$V \equiv \left(\sum_{k} |V_{kd}|^{2}\right)^{1/2} \;;\; H_c = \sum_{k} \varepsilon_k c_{k\sigma}^{+} c_{k\sigma}$$

- sequence of orthogonal states generated by H_c:

$$|1\rangle = \frac{1}{\lambda_0}\left[H_c|0\rangle - |0\rangle\langle 0|H_c|0\rangle\right]$$

$$|n+1\rangle = \frac{1}{\lambda_n}\{H_c|n\rangle - |n\rangle\langle n|H_c|n\rangle - |n-1\rangle\langle n-1|H_c|n\rangle\}$$

$$\tilde{\mathcal{H}} = \varepsilon_d n_{\ell}^{d} + U n_{\ell\uparrow}^{d} n_{\ell\downarrow}^{d} + V\sum_{k\sigma}\left(f_{0\sigma}^{+} d_{\sigma} + H.C.\right) + \sum_{n=0,\sigma}^{\infty}\left[\varepsilon_n f_{n,\sigma}^{+} f_{n,\sigma} + \lambda_n\left(f_{n,\sigma}^{+} f_{n+1,\sigma} + H.C.\right)\right]$$

where $\lambda_n = \langle n+1 | H_c | n \rangle$, $\varepsilon_n = \langle n | H_c | n \rangle$

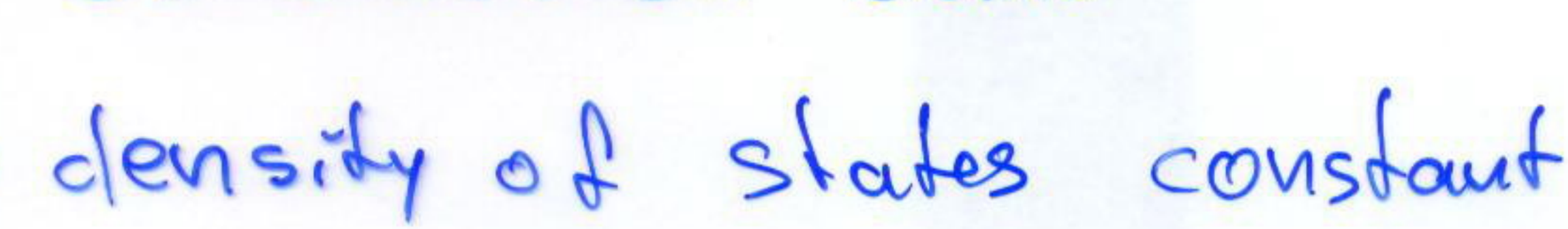
depend on ε_k and $\Delta(\omega)$

- they do not necessarily fall of with n (which is crucial for NRG)

- for convergence of NRG additional approximation must be made: logarithmic discretization of the conduction band

- density of states constant D
- conduction band $-D < \varepsilon_k < D$ division into intervals

$$D^+ = [\Lambda^{-n+1}, \Lambda^n], \quad D^- = [-\Lambda^n, -\Lambda^{-n+1}]$$



$$a^+_{np\sigma} \equiv \sum_{[k]_n} e^{i\omega_n p k} c^+_{k\sigma}; \quad [k_n]: \Lambda^{-(n+1)} < k < \Lambda^{-n},$$

p is an integer, $\omega_n = 2\pi \Lambda^{n+1} / \Lambda - 1$

for $-\Lambda^{-(n+1)} < k < -\Lambda^{-n} \Rightarrow b^+ \equiv$

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

- neglect all higher terms in Fourier series keeping one electron per logarithmic energy interval, i.e., $a_{n,0,\sigma}^{+}$ and $b_{n,0,\sigma}^{+}$ (error propodional with $(1-\Lambda^{-1})$)
- tricliagonalization procedure

(with $|0,\sigma\rangle$ generated by $f_{0,\sigma} = \sum_k c_{k\sigma}$ for the Kondo model with

$$H^{K} = J_K S_d \cdot s_0 + \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^{+} c_{k,\sigma}$$

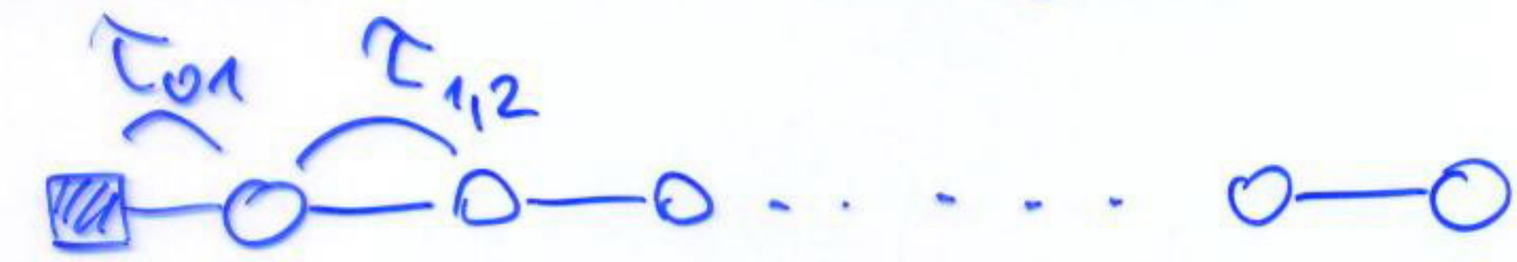
$$\tilde{\mathcal{H}} = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} f_{0\sigma}^{+} d_\sigma + d_\sigma^{+} f_{0,\sigma} + \sum_{\sigma, n=0}^{\infty} \epsilon_n f_{n\sigma}^{+} f_{n\sigma} + \Lambda^{-n/2} \left(f_{n,\sigma}^{+} f_{n+1,\sigma} + H.C. \right)$$

where ϵ_n "site energies", $\Lambda^{-n/2}$ hoppings

if $\Lambda \to 1$ NRG does not converges

if Λ too large → large error from logarithmic discretiz.

- semi infinite chain :



$\mathcal{H}_0$ $\mathcal{H}_1$ $\mathcal{H}_2$ ..... $\mathcal{H}_N$

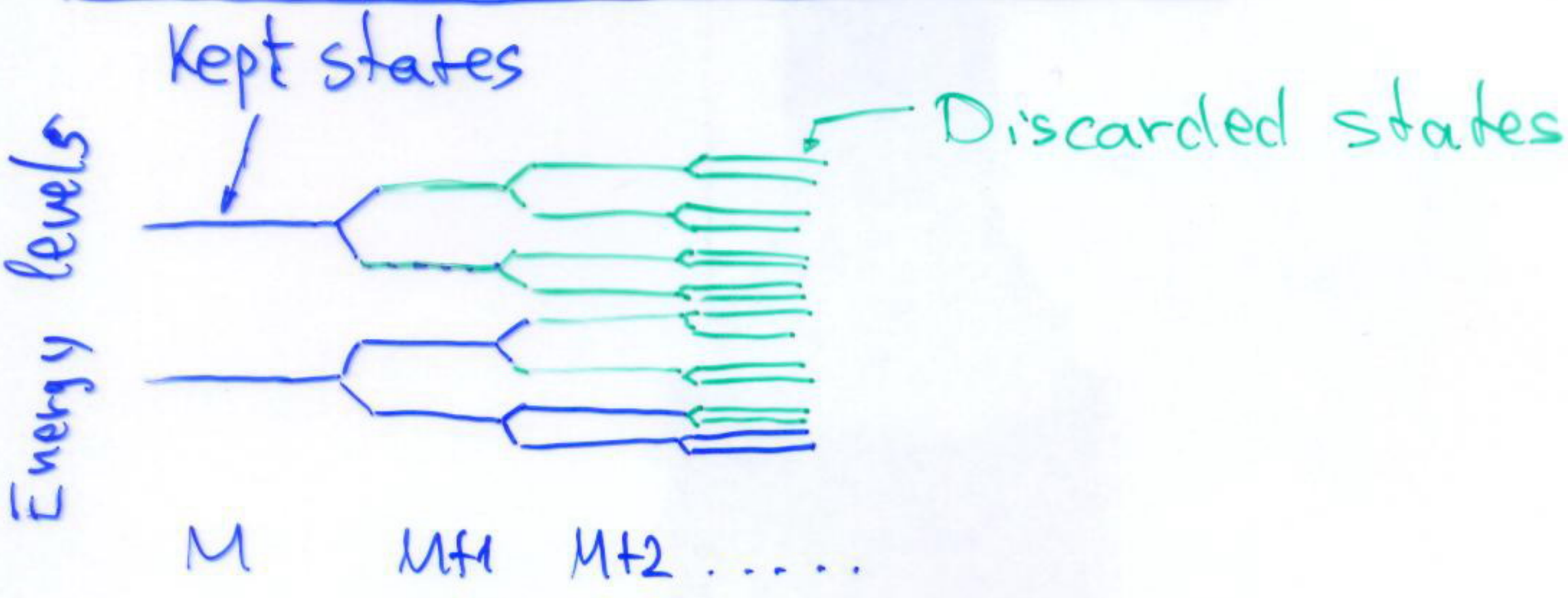
each "site" is a smaller energy scale

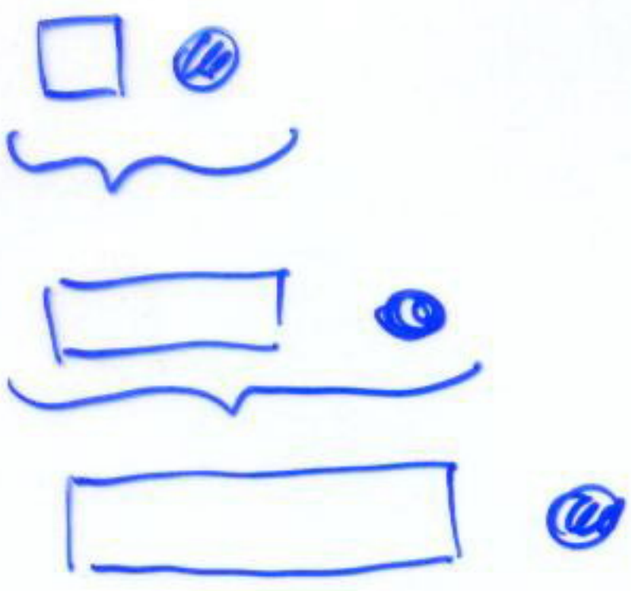
H_1

H_2

$$H_0 = \mathcal{H}_0$$

$$H_{n+1} = H_n + \tau_{n,n+1} + \mathcal{H}_{n+1}$$





~~1) diagonalize H_n~~

~~2) form O_n from eigen~~

1) Diagonalize $H_n \rightarrow |\psi_m\rangle$, E_m

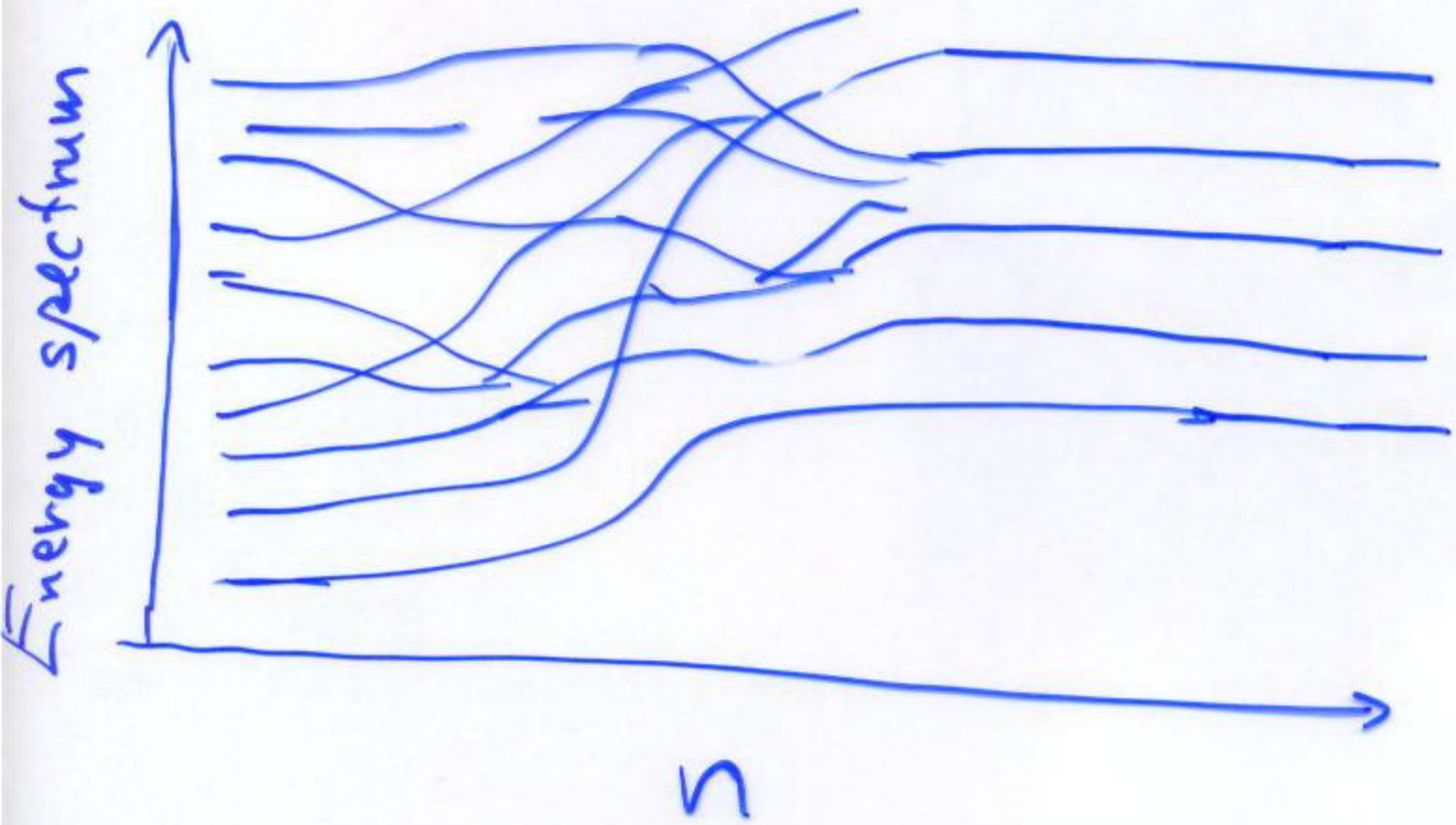
2) from m lowest states form transformation matrix

$$O = \left(\psi_m \; \vdots \; \psi_2 \; \psi_1 \right)$$

3) $\bar{H}_n = O^+ H_n O$, $\bar{A}_n = O^+ A_n O$

4) $H_{n+1} \Leftarrow \bar{H}_n$

5) go to step 1



$\mathcal{R}[H^*] = H^*$ fixed point if rescaled energy spectrum does not change