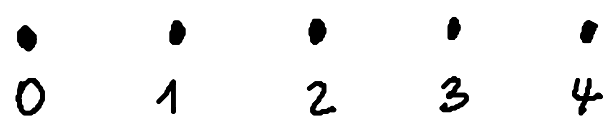
27.6.



size increases as 2^{3+2n}

$$H_{N+1} = \sqrt{\Lambda}\, H_N + \sum_{\sigma} \xi_N \left(f^{\dagger}_{N\sigma} f_{N+1\,\sigma} + f^{\dagger}_{N+1\,\sigma} f_{N\sigma} \right)$$

$$\mathcal{H}_1 = \begin{array}{c} |0\rangle_1 \\ |\uparrow\rangle_1 \\ |\downarrow\rangle_1 \\ |\uparrow\downarrow\rangle_1 \end{array} \begin{pmatrix} \sqrt{\Lambda}\,\mathcal{H}_0^d & \xi_0 (f_{0\uparrow}^d)^\dagger & \xi_0 (f_{0\downarrow}^d)^\dagger & 0 \\ & \cdots & & \\ & & & \\ & & & \end{pmatrix}$$

32 × 32 matrix

$$\mathcal{H}_0 \longrightarrow \mathcal{U}_0^T \mathcal{H}_0 \mathcal{U}_0 \equiv \mathcal{H}_0^d$$

8 × 8 matrix

$$f_{0\uparrow} \longrightarrow \mathcal{U}_0^T f_{0\uparrow} \mathcal{U}_0 \equiv f_{0\uparrow}^d$$

For example

$$f_{1\sigma}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \mathbb{1}\delta_{\sigma\uparrow} & 0 & 0 & 0 \\ \mathbb{1}\delta_{\sigma\downarrow} & 0 & 0 & 0 \\ 0 & -\mathbb{1}\delta_{\sigma\downarrow} & \mathbb{1}\delta_{\sigma\uparrow} & 0 \end{pmatrix}$$

In practice, this looks like (call $\mathcal{H}_0^d \equiv a_0(..)$ $n=8$)

$i = 1, n$
$j = 1, n$

f0up(i,j) = a0(2,i) a0(1,j) + a0(6,i) a0(5,j)
+ a0(4,i) a0(3,j) + a0(8,i) a0(7,j)

⋮

CONTINUE
CONTINUE

Next: Add $N=2$ to the Wilson Chain

$$f_{1\uparrow} \longrightarrow f_{1\uparrow}^d$$

Diagonalise $\mathcal{H}_2 = \mathcal{U}_2 \mathcal{H}_2^d \mathcal{U}_2^T$

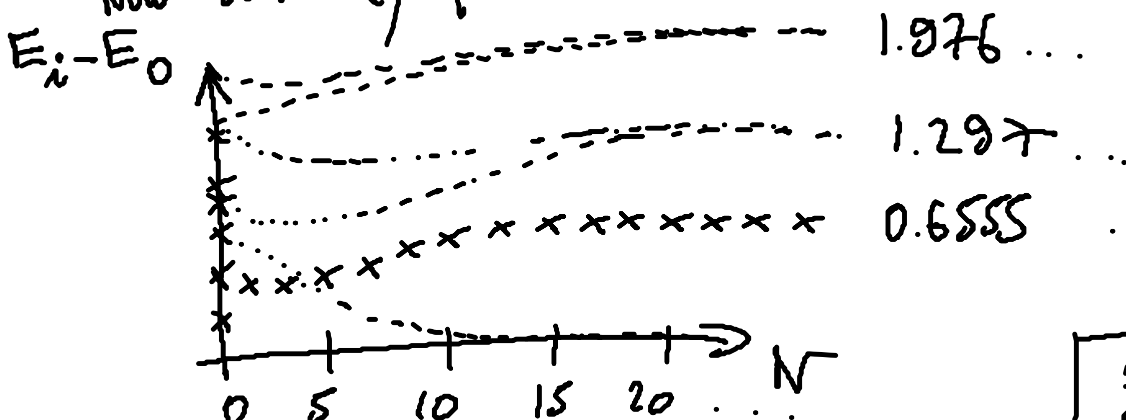
$N=3$, $\dim \mathcal{H}_3 = 512$

next step would be $\dim \mathcal{H}_4 = 2048$ too big!

Truncation leaves us with 128 eigenvalue + -vectors as diagonal input into $\mathcal{H}_4$

We need f_3-operator: transform with 512×512 matrix then truncate to 128×128.

Now similarly for $N \to N+1 \to N+2 \ldots$



$$\boxed{\begin{array}{l}\tilde{J} = 0.25 \\ \Lambda = 2\end{array}}$$

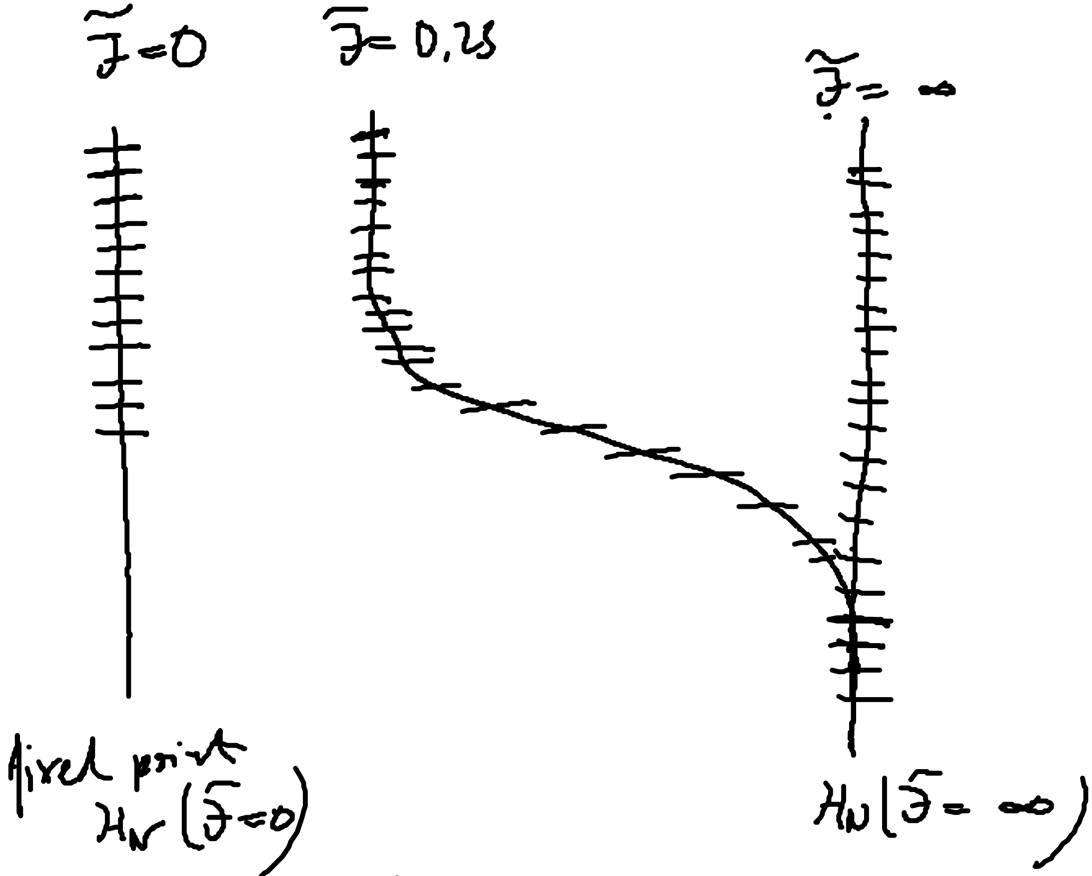
Wilson's „Railroad track" Analogy

$J = 0$ decoupled

$J = \infty$ infinitely strong

$\mathcal{H}_N^*(J=0)$ and $\mathcal{H}_N^*(J=\infty)$ are called fixed point Hamiltonians

Now small $J > 0$ (weak anti-ferrom. coupling)



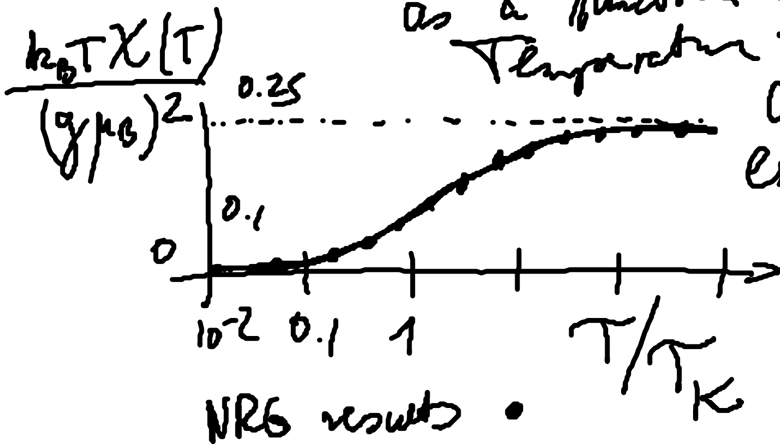
Moving Along the Chain

We construct a sequence of effective Hamiltonians $\mathcal{H}_N$ which describe the physical properties, derived from the (truncated spectrum), at an energy scale E or temperature scale $k_B T \sim \Lambda^{-(N-1)/2}$

If we fix $k_B T$ (fixed temperature), we need to terminate the iteration along the chain at that N with $k_B T \sim \Lambda^{-(N-1)/2}$

(usually, $\Lambda = 2$).

Example: χ_{imp} (susceptibility) of the impurity as a function of Temperature T



Curie-Weiss

exact Bethe Ansatz Solution.

NRG results •

textbook Hewson.

Outlook

- NRG is an important theoretical tool
- Quantum impurity problems
- Quantum Dots at low temperatures

Klassische Elektrolyte

Elektrostatik

Punktladungen in M Sorten $\alpha = 1, \dots, M$
(Ionen) position : $\underline{r}_{k_\alpha}$

$k_1 = 1 \dots N_1, \dots \qquad N_\alpha \gg 1$

Thermodynamik, stat. Beschreibung

großkan. Ensemble bei $k_B T \equiv \frac{1}{\beta}$

chem. Potentialen $\mu_1, \dots, \mu_M$

Systemladungsdichte $\qquad \underline{r}$ 3-dim. vector

$$\rho_S(\underline{r}) = \sum_{\alpha=1}^{M} \sum_{k_\alpha=1}^{N_\alpha} q_\alpha \, \delta(\underline{r} - \underline{r}_{k_\alpha})$$

$\uparrow$ Ladungen

Zusätzlich feste Ladungsdichte $\sigma(\underline{r})$

ges. Ladungsdichte $\rho(\underline{r}) = \rho_S(\underline{r}) + \sigma(\underline{r})$.

Elektrost. Ww energie E,

$$E = \frac{1}{2} \int d^3\underline{r} \, \rho(\underline{r}) \, \varphi(\underline{r})$$

$\varphi(\underline{r})$ Potential der Ladungsverteilung.

Annahme: $\quad \varepsilon = \varepsilon(\underline{r}) \quad$ Dielektrisch

$$\operatorname{div} \underline{D}(\underline{r}) = 4\pi \rho(\underline{r})$$ freie Ladungen, keine Polarisation

$$\underline{D}(\underline{r}) = \varepsilon(\underline{r}) \underline{E}(\underline{r}), \quad \underline{E} = -\underline{\nabla}\phi$$

$$\Vert \; -\underline{\nabla}\, \varepsilon(\underline{r}) \underline{\nabla}\, \phi(\underline{r}) = 4\pi \rho(\underline{r}) \quad \text{Poisson} \; \Vert$$

$$\left(\varepsilon = \text{const}: \quad -\frac{\varepsilon}{4\pi} \Delta \phi = \rho \right)$$

Green's function (Greensche Funktion)

$$-\frac{1}{4\pi} \underline{\nabla}\, \varepsilon(r) \underline{\nabla}\, G_0(\underline{r}, \underline{r}') = \delta(\underline{r} - \underline{r}')$$

$$\Rightarrow \quad \phi(\underline{r}) = \int d\underline{r}'\, G_0(\underline{r}, \underline{r}')\, \rho(\underline{r}') + \text{Randterme}$$

($\rightarrow$ weglassen)

$$E = \frac{1}{2} \int dr\, dr'\, \rho(r)\, G_0(r, r')\, \rho(r')$$

Beispiel $\frac{1}{2} \int dr\, dr'\, \rho(r) \frac{1}{|r - r'|} \rho(r')$

Hiervon Selbstwechselwirkung abziehen

$$E' = \frac{1}{2} \int dr\, dr'\, \rho(r)\, G_0(r, r')\, \rho(r') - \frac{1}{2} \sum_{k\alpha} q_\alpha^2\, G_0(r_{k\alpha}, r_{k\alpha})$$

Jetzt externe Potentiale $u_\alpha(\underline{r})$
(1-Teilchen)

Damit Hamilton-Funktion

$$\mathcal{H} = \sum_{\alpha=1}^{M} \sum_{k_\alpha=1}^{N_\alpha} \left[\frac{p_{k\alpha}^2}{2 m_\alpha} + u_\alpha(\underline{r}_{k\alpha}) + E'\{r_{k\alpha}\} \right]$$

keine Dynamik

Thermodynamik:

großkan. Zustandssumme (grand partition sum)

$$Z_G = \sum_{N_1=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \prod_{\alpha=1}^{n} e^{\beta \mu_\alpha N_\alpha} \underbrace{Z(N_1, \ldots, N_n)}_{\text{kan. Zust. Summe}}$$

Hier $[p_{k\alpha}, r_{k\beta}] = 0$.

Impuls-Integrationen liefern

$$Z_G = \sum_{N_1=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \prod_{\alpha=1}^{n} \frac{e^{\beta \mu_\alpha N_\alpha}}{\Lambda_\alpha^{3 \cdot N_\alpha} \, N_\alpha!} \times$$

therm. Wellenlänge — Gibbsche Korrektur

$$\times \int \prod_{\alpha=1}^{n} \prod_{k_\alpha=1}^{N_\alpha} d^3 r_{k\alpha} \, e^{-\beta \left\{ \sum_{\alpha k} u_\alpha(r_{k\alpha}) + E'\{r_{k\alpha}\} \right\}}$$