27.6.

0 1 2 3 4

size increases as 2^{3+2n}

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

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

32×32 matrix

$$
\mathcal{H}_0 \longrightarrow U_0^T \mathcal{H}_0 U_0 = \mathcal{H}_0^d \qquad 8\times 8 \text{ matrix}
$$

$$
f_{0\uparrow} \longrightarrow U_0^T f_{0\uparrow} U_0 = f^d_{0\uparrow}
$$

For example

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

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

$i = 1, n$ $\quad j = 1, n$ $\quad n = 8$

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

CONTINUE
CONTINUE

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

$$
f_{1\uparrow} \longrightarrow f^d_{1\uparrow}
$$

Diagonalise $\quad \mathcal{H}_2 = U_2 \mathcal{H}_2^d U_2^T$

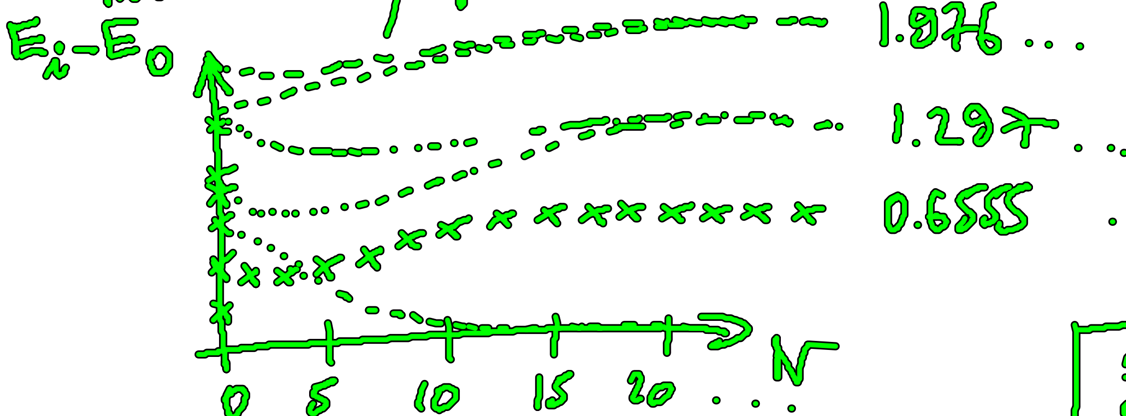
$N = 3$, $\dim \mathcal{H}_3 = 512$

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 $N \to N+1 \to N+2 \ldots$



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

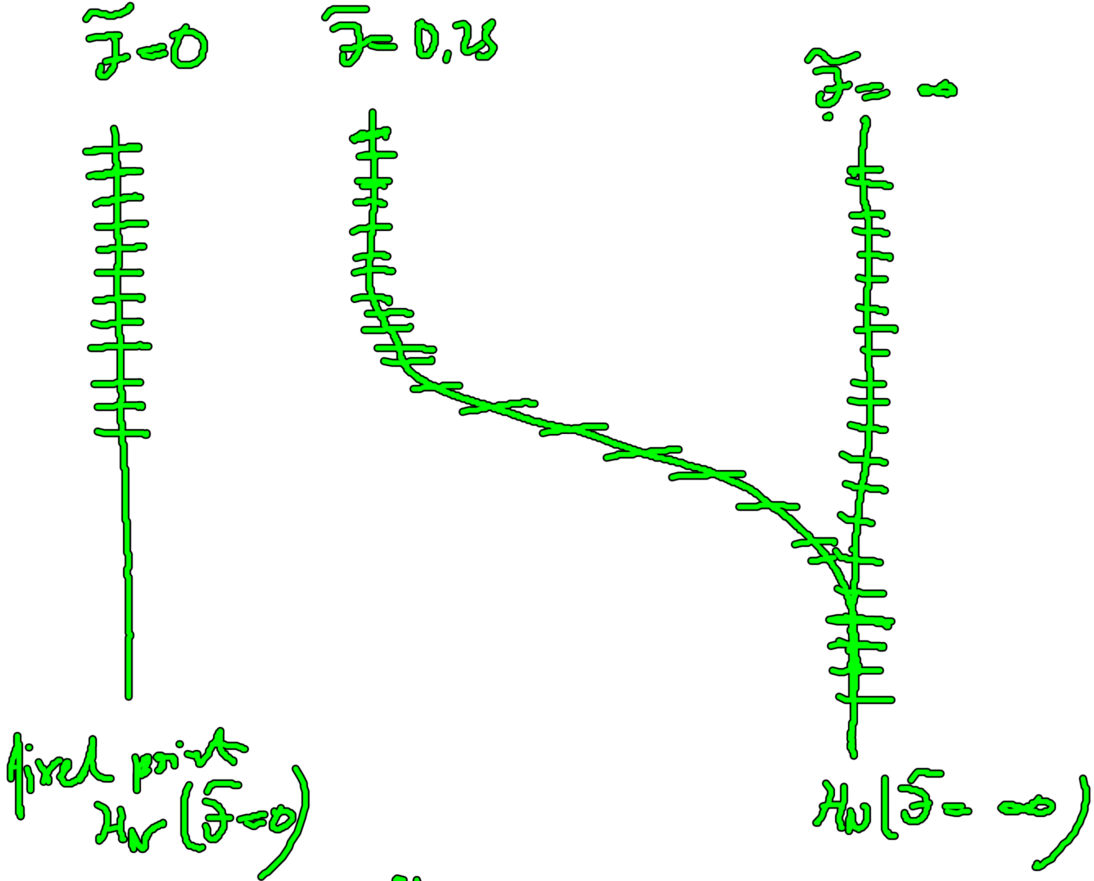
Wilson's „Railroad track" Analogy

$J = 0$ 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)



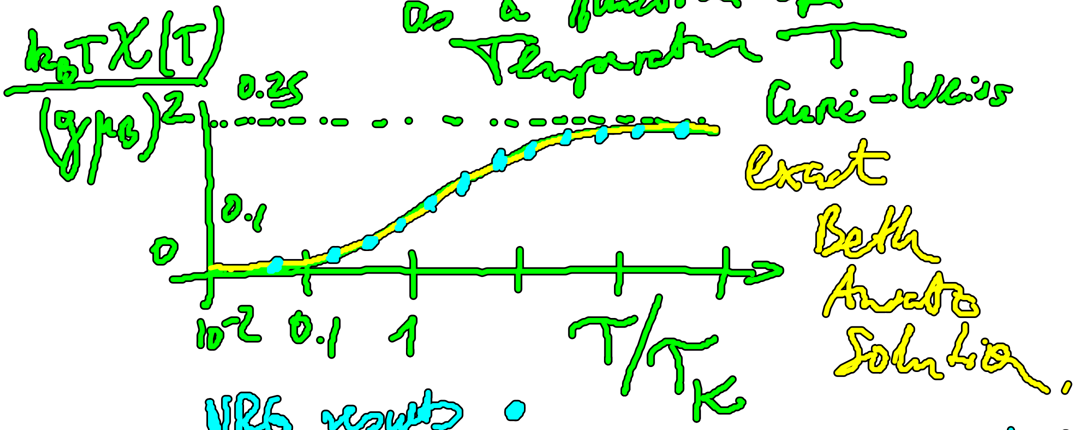
Moving Along the Chain

We construct a sequence of effective Hamiltonians $\mathcal{H}_N$ which describe the physical properties (truncated spectrum) derived from the 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



NRG results •

textbook Hewson.

Outlook

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

$\hbar$ $\boxed{\text{Klassische Elektrolyte}}$

Elektrostatik

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

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

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

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

q_α: Ladungen

Zusätzlich fixe 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

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

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

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

Green's function (Greensche Funktion)

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

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

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

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)

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

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

Impuls-Integrationen liefern

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

therm. Wellenlänge

Gibbsche Korrektur

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