LECTURE

TIME-DEPENDENT DMRG

Literature:

1) DMRG – U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005)

2) time-dependent DMRG – Trotter-based, T=0, T>0

   - G. Vidal, PRL 93, 040502 (2004)
   - A.J. Daley, C. Kollath, U. Schollwöck, G. Vidal, J. Stat. Mech.: Theor. Exp. P04005 (2004)
   - A. Feiguin, S.R. White, PRL 93, 076401 (2004)
   - F. Verstraete, D. Porras, J.I. Cirac, PRL 93, 227204 (2004) (T>0)

3) time-dependent DMRG – Krylov-based

   - S.R. White, talk 2004, http://komet337.physik.uni-mainz.de/Jeckelmann/DMRG/workshop/%proceedings/white.pdf

(Krylov: S. Manmana et. al.)

calculate

- $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$
- $\langle \hat{O}_1(t)\hat{O}_2(0)\rangle = \langle\psi| e^{+i\hat{H}t}\hat{O}_1 e^{-i\hat{H}t}\hat{O}_2|\psi\rangle$

$= \langle\psi(t)|\hat{O}_1|\varphi(t)\rangle$ where $|\varphi(t)\rangle = e^{-iHt}|\varphi(0)\rangle$

$|\varphi(0)\rangle = \hat{O}_2|\psi\rangle$ $\Longrightarrow$ FT to structure function and other <u>frequency-dependent</u> quantities!

TIME-DEPENDENT DMRG

Problem: given $|\psi(t=0)\rangle$, $\hat{H}(t)$, what is $|\psi(t)\rangle$?

assume $\hat{H}\cancel{(t)}$ for simplicity

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle \qquad \hat{H}|n\rangle = E_n|n\rangle$$

$$= \sum_n e^{-iE_nt} c_n |n\rangle \qquad c_n = \langle n|\psi(0)\rangle$$

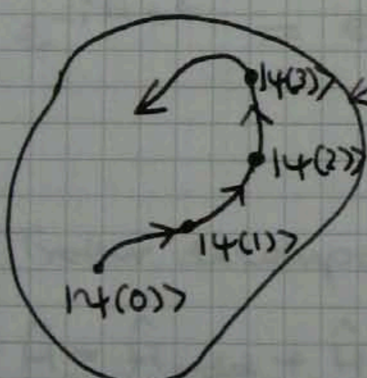
eigenbasis <u>unknown</u>

$$= \sum_{n\tilde{m}} e^{-iE_nt} c_n a_{n\tilde{m}} |\tilde{m}\rangle \qquad a_{n\tilde{m}} = \langle\tilde{m}|n\rangle$$

some other basis

$$= \sum_{\tilde{m}} \underbrace{\Big(\sum_n e^{-iE_nt} c_n a_{n\tilde{m}}\Big)}_{\text{changes in value}} |\tilde{m}\rangle$$

unknown



Hilbert space

time-evolving quantum state "explores" Hilbert space

$$|\psi(t)\rangle \longleftrightarrow \underbrace{\sum_{\{\sigma_i\}} A_1^{\sigma_1}(t) A_2^{\sigma_2}(t) \dots A_L^{\sigma_L}(t) |\sigma_1 \dots \sigma_L\rangle}$$

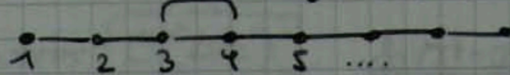
time-dependent matrix product state that – for given dimension D – has minimal distance

$$\| \, |\psi(t)\rangle - |\psi^D_{MPS}(t)\rangle \, \|_2 .$$

Strongly correlated quantum problems _often_ have short-ranged Hamiltonians

$\hat{h}_i$ e.g. $\underline{S}_i \cdot \underline{S}_{i+1}$

$$\hat{H} = \sum_i \hat{h}_i$$



① global _finite_-t evolution →
global _infinitesimal_-t evolution

$$e^{-i\hat{H}t} = \underbrace{e^{-i\hat{H}\Delta t}\, e^{-i\hat{H}\Delta t} \dots e^{-i\hat{H}\Delta t}}_{N = t/\Delta t}$$

② _global_ infinitesimal-t evolution →
local infinitesimal-t evolution

$$e^{-i\hat{H}\Delta t} = e^{-i\sum \hat{h}_i \Delta t} \neq \prod_i e^{-i\hat{h}_i \Delta t}$$

$$[\hat{h}_i, \hat{h}_{i+1}] \neq 0$$

Trotter decomposition:

$$\hat{H} = \hat{H}_{odd} + \hat{H}_{even}$$

$$\hat{H}_{odd} = \underbrace{\sum_{j=0} \hat{h}_{2j+1}}_{} \qquad \hat{H}_{even} = \sum_{j=1} \hat{h}_{2j}$$

these all commute, so the problem is separating odd from even in factorizing

Baker-Campbell-Hausdorff:

$$e^{\hat{X}} e^{\hat{Y}} = e^{\hat{Z}} \qquad \hat{Z} = \hat{X} + \hat{Y} + \frac{1}{2}[\hat{X}, \hat{Y}] + \frac{1}{12}([\hat{X}, [\hat{X}, \hat{Y}]] + [\hat{Y}, [\hat{Y}, \hat{X}]]) + \dots$$

assume $[\hat{X}, \hat{Y}]$ comm. with $\hat{X}, \hat{Y}$:

Glauber formula $e^{\hat{X}+\hat{Y}} = e^{\hat{X}} e^{\hat{Y}} \underbrace{e^{-\frac{1}{2}[\hat{X}, \hat{Y}]}}_{\text{neglected in naive factorization}}$

$$e^{-\frac{1}{2}[\hat{X},\hat{Y}]} \cong 1 - \frac{1}{2}\boxed{O(\Delta t)^2}$$

error of first order -Trotter decomp.: $O(\Delta t)^2$

$$e^{i\hat{H}\Delta t} = e^{i\hat{H}_0\Delta t} e^{i\hat{H}_e\Delta t}$$

over $\frac{T}{\Delta t}$ time steps : error $\boxed{O(\Delta t)}$ first-order in Δt.

generalizes to

$$e^{i\hat{H}\Delta t} = \underbrace{e^{a_{m+1}\hat{H}_0\Delta t}\left(\prod_{n=1}^{m} e^{b_n\hat{H}_e\Delta t} e^{a_n\hat{H}_0\Delta t}\right)}_{\text{approximate, decomposed time evol.}} + O(\Delta t^{p+1})$$

$$\sum a_n = \sum b_n = 1$$

huge variety, characterized by order of error Δt^p

Trotter second order: $e^{-i\hat{H}_0\Delta t/2} e^{-i\hat{H}_e\Delta t} e^{-i\hat{H}_0\Delta t/2}$

Trotter fourth order: $\hat{S}(w_1)\hat{S}(w_2)\hat{S}(w_3)$ ~~...~~ with

$$\hat{S}(w_i) = e^{-i\hat{H}_0 w_i\Delta t/2} e^{-i\hat{H}_e w_i\Delta t} e^{-i\hat{H}_0 w_i\Delta t/2}$$

and $w_1 = w_2 = \frac{1}{4-4^{1/3}}$, $w_3 = 1-2w_1-2w_2$. (Suzuki)

in any case, how do we implement

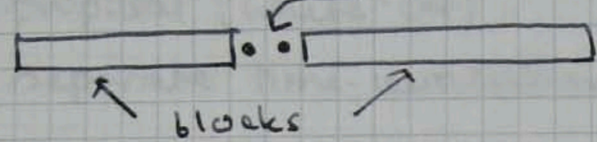
$$|\varphi\rangle = e^{-i\hat{h}_i\Delta t}|\psi\rangle,$$

i.e. find an optimal representation of $|\varphi\rangle$ given $|\psi\rangle$?

1)

answer (in "DMRG"-language):

- consider finite-system DMRG with sweeping (at position of bond)



- carry out infinitesimal local time evolution exactly:

$$|\psi\rangle = \sum_{m_L m_R} \sum_{\sigma_L \sigma_R} \psi_{m_L m_R \sigma_L \sigma_R} |m_L\rangle |\sigma_L \sigma_R\rangle |m_R\rangle$$

$$e^{-i\hat{h}\Delta t} = \sum_{\sigma_L \sigma_R \sigma_L' \sigma_R'} |\sigma_L \sigma_R\rangle\langle \sigma_L' \sigma_R'| \, U_{\sigma_L \sigma_R, \sigma_L' \sigma_R'}$$

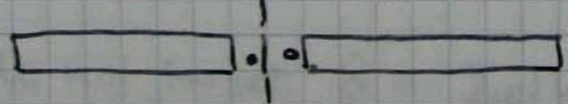
(diagonalize $\hat{h}$, exponentiate, transform back – 2 ~~st~~ site problem....)

$$|\varphi\rangle = \sum_{m_L m_R} \sum_{\sigma_L \sigma_R} \varphi_{m_L m_R \sigma_L \sigma_R} |m_L\rangle |\sigma_L \sigma_R\rangle |m_R\rangle$$

where

$$\varphi_{m_L m_R \sigma_L \sigma_R} = \sum_{\sigma_L' \sigma_R'} U_{\sigma_L \sigma_R \sigma_L' \sigma_R'} \psi_{m_L m_R \sigma_L' \sigma_R'} .$$

- continue sweeping to next bond in usual DMRG procedure: calculate new blocks by reduced density operator analysis:



$$|\varphi\rangle \to \hat{\rho}_S, \hat{\rho}_E$$

keep M highest-weight eigenstates!

- carry out Trotter steps while sweeping forth/back

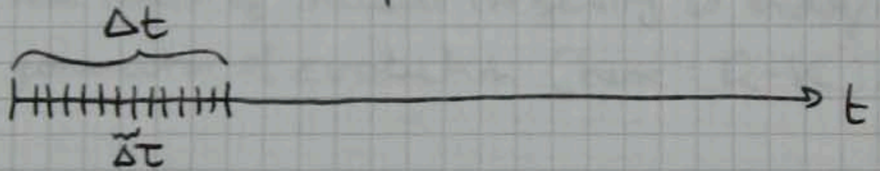
Krylov - time evolution

what can we do if $\hat{H}$ is <u>not</u> short-ranged?

proposal (White '04):
separate time-evolution and state selection

- from $|\psi(t)\rangle$, calculate approximately $|\psi(t+\Delta t)\rangle$ (and other states in near future) to obtain suitable ~~Hilbert~~ approximate state space (multiple targetting)

- carry out high-precision time evolution in this state space.



at time t, carry out standard finite-system sweeps ($\square \cdot\cdot \square$), generating and targetting at each step:

approx!

$$\left.\begin{aligned}
|k_1\rangle &= -i\Delta t\,\hat{H}\,|\psi(t)\rangle \\
|k_2\rangle &= -i\Delta t\,\hat{H}\left(|\psi(t)\rangle + \tfrac{1}{2}|k_1\rangle\right) \\
|k_3\rangle &= -i\Delta t\,\hat{H}\left(|\psi(t)\rangle + \tfrac{1}{2}|k_2\rangle\right) \\
|k_4\rangle &= -i\Delta t\,\hat{H}\left(|\psi(t)\rangle + |k_3\rangle\right)
\end{aligned}\right\}\ \text{Runge-Kutta vectors}$$

do not target $\hat{\rho} = \sum_i \alpha_i |k_i\rangle\langle k_i| + \beta|\psi(t)\rangle\langle\psi(t)|$ $\left(\sum\alpha_i + \beta = 1\right)$

but better

$$|\psi(t+\tfrac{1}{3}\Delta t)\rangle = |\psi(t)\rangle + \tfrac{1}{162}\left(31|k_1\rangle + 14(|k_2\rangle + |k_3\rangle) - 5|k_4\rangle\right)$$
$$|\psi(t+\tfrac{2}{3}\Delta t)\rangle = |\psi(t)\rangle + \tfrac{1}{81}\left(16|k_1\rangle + 20(|k_2\rangle + |k_3\rangle) - 2|k_4\rangle\right)$$
$$|\psi(t+\Delta t)\rangle = |\psi(t)\rangle + \tfrac{1}{6}|k_1\rangle + \tfrac{1}{3}|k_2\rangle + \tfrac{1}{3}|k_3\rangle + \tfrac{1}{6}|k_4\rangle$$

and target $\hat{\rho} = \sum_{i=1}^{4} |\psi(t_i)\rangle\langle\psi(t_i)|$

$(t_1 = t,\ t_2 = t + \tfrac{1}{3}\Delta t;\ t_3 = t + \tfrac{2}{3}\Delta t;\ t_4 = t + \Delta t)$

after some sweeps, basis adapted to these states.

Now high precision time-evolution e.g. Runge-Kutta

$\Delta\tau = \frac{\Delta t}{10}$ (R-K error $O(\Delta\tau^5)$)

The idea of multi-targetting is independent of generator of evolution (here: R-K).

Best: Krylov time-evolution

$e^{-i\hat{H}\Delta t}$

huge ⇝ exponential can't be calculated!

but $e^{-i\hat{H}\Delta t}|v\rangle$ is quite easy: Lanczos...

~~[illegible]~~

idea: Taylor expansion gives error $O(\Delta t^{n+1})$ if we calculate orders up to $\hat{H}^n|v\rangle$ – but does it give the best prefactor for the computational cost?

No, one can show that the answer is a Krylov sequence.

just consider $\hat{H}$ for simplicity.

unitary $V^{-1} = V^{\dagger}$

tridiagonalization: $T = V^{\dagger} H V$

free, we take $|v\rangle$

$$V = \begin{bmatrix} \underline{|v\rangle}, \dots \end{bmatrix}$$

krylov = Lanczos vectors formed iteratively

approximatively: $T_{n\times n} = V_n^{\dagger} H V_n$

the first n Lanczos vectors, starting from $|v\rangle$

$$e^{\hat{H}}|v\rangle = e^{VTV^{\dagger}}|v\rangle = V e^{T} V^{\dagger}|v\rangle$$

$$= V \underbrace{e^{T}\begin{bmatrix}1\\0\\0\\\vdots\end{bmatrix}}_{\text{first column of } e^{T}}$$

no proof:
≈ optimal

$$\approx V_n \underbrace{e^{T_{n\times n}}}\begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix}$$

n small, ... easily diagonalized and exponentiated.

result: $\boxed{\text{first n krylov vectors, weighted by first column entries of } e^{T_{n\times n}}.}$

construction of density operator:

How can we represent <u>density operators</u> as pure states? – finite-T DMRG.

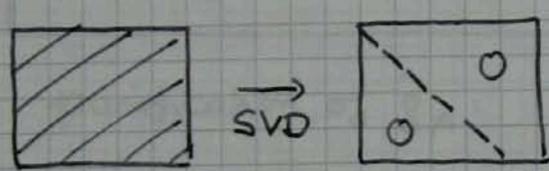
bipartite system AB

dimension state space A, B

$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B \longrightarrow |\psi\rangle_{AB} = \sum_{\alpha}^{\min(D_A, D_B)} \sqrt{w_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B \qquad \sqrt{w_\alpha} \geq 0$$

(Schmidt decomposition)

If normalized: $1 = \sum_\alpha (\sqrt{w_\alpha})^2 = \sum w_\alpha$



ψ_{ij} $\xrightarrow{\text{SVD}}$ $\tilde{\psi}_{\alpha\alpha} \equiv \sqrt{w_\alpha} \geq 0$

$$\hat{\rho}_{AB} = |\psi\rangle_{AB\,AB}\langle\psi| = \sum_\alpha w_\alpha |\alpha\rangle_A |\alpha\rangle_{B\,A}\langle\alpha|_B\langle\alpha| \qquad (\mathrm{tr}\,\hat{\rho}_{AB} = 1)$$

$$\hat{\rho}_A = \mathrm{tr}_B\, \hat{\rho}_{AB} = \sum_\beta {}_B\langle\beta| \left(\sum_\alpha w_\alpha |\alpha\rangle_A |\alpha\rangle_{B\,A}\langle\alpha|_B\langle\alpha| \right) |\beta\rangle_B$$

$$= \sum_\alpha w_\alpha |\alpha\rangle_{A\,A}\langle\alpha| \qquad w_\alpha \geq 0$$

pure state on AB $\longrightarrow$ mixed state on A

<u>purification</u>: invert this procedure!

A ≡ <u>physical system</u> (dimension D_A)

$$\hat{\rho} = \hat{\rho}_A = \sum_\alpha w_\alpha |\alpha\rangle_{(A)\,(A)}\langle\alpha| \qquad \text{(density op. in eigenbasis)}$$

introduce ficticious

B ≡ auxiliary system (dimension $D_B \geq D_A$) — focus on $D_B = D_A$

(arbitrary) basis $\{ |\alpha\rangle_B \}$

Then

$$\hat{\rho}_A = \mathrm{tr}_B\, \hat{\rho}_{AB} \quad \text{with}$$

$$\hat{\rho}_{AB} = \sum_\alpha w_\alpha |\alpha\rangle_A |\alpha\rangle_B \, {}_A\langle\alpha| \, {}_B\langle\alpha| = |\psi\rangle_{AB} \, {}_{AB}\langle\psi|$$

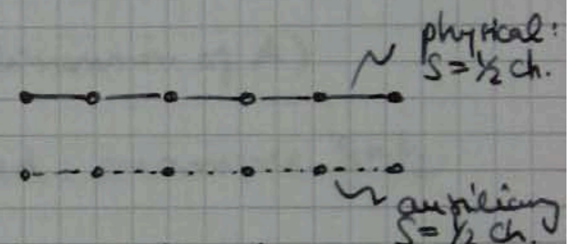
and

$$|\psi\rangle_{AB} = \sum_\alpha \sqrt{w_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B$$

$$\boxed{\hat{\rho}_A = \sum_\alpha w_\alpha |\alpha\rangle_A \, {}_A\langle\alpha| \Rightarrow |\psi\rangle_{AB} = \sum_\alpha \sqrt{w_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B}$$

purification of $\hat{\rho}_A$:

"double" physical system:



so, e.g., a density operator on a <u>spin chain</u>
can be mapped to a pure state on a <u>spin ladder</u>.

calculation of observables connects seamlessly
to pure state case:

$$\langle \hat{O} \rangle_{\hat{\rho}_A} = \mathrm{tr}_A (\hat{O}_A \hat{\rho}_A)$$

$$= \mathrm{tr}_A\, \hat{O}_A\, \mathrm{tr}_B\, \hat{\rho}_{AB}$$

$$= \mathrm{tr}_A \mathrm{tr}_B\, \hat{O}_A |\psi\rangle_{AB}\, {}_{AB}\langle\psi|$$

$$= {}_{AB}\langle\psi| \hat{O}_A |\psi\rangle_{AB} .$$

– no new routine needed!

problem: $\hat{\varrho}_A = \sum w_\alpha |\alpha\rangle_A \, {}_A\langle\alpha|$

unknown for general complex many-body problem $\Rightarrow$ naive purification fails

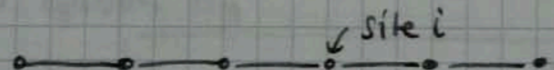
solution for thermal density operators:

① infinite-temperature ($\beta = 0$) density operator

$$\hat{\varrho}_A(0) = \frac{1}{Z(0)} e^{-0\cdot\hat{H}_A} = \frac{1}{Z(0)} \cdot \hat{\mathbb{1}}$$

$$Z(0) = \mathrm{tr}_A \hat{\mathbb{1}} = \cancel{\mathrm{dim}}\ D_A \qquad \text{(dimension of A)}$$

but $\hat{\varrho}_A(0)$ is easily constructed: example $S = 1/2$



$$\hat{\varrho}_A(0) = \bigotimes_i \hat{\varrho}_i(0) \qquad \text{(for } \beta = 0 \text{ only)}$$

$$\hat{\varrho}_i(0) = \cancel{\tfrac{1}{\sqrt{2}}}\ \underbrace{\frac{1}{2}}_{D_i \text{ local dimension}}\left(|\uparrow\rangle_i \, {}_i\langle\uparrow| + |\downarrow\rangle_i \, {}_i\langle\downarrow|\right)$$

properly normalized!

purification:

$$|\psi\rangle_{AB}(0) = \bigotimes_i |\psi\rangle_{AB,i}(0) \qquad \text{(for } \beta = 0 \text{ only)}$$

$$|\psi\rangle_{AB,i}(0) = \frac{1}{\sqrt{2}}\left(|\underset{A_i}{\uparrow}\underset{B_i}{\uparrow}\rangle + |\underset{A_i}{\downarrow}\underset{B_i}{\downarrow}\rangle\right)$$

A $\longrightarrow$ A physical

B auxiliary

not unique: also $\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right), \ldots$ feasible – advantageous if good quantum numbers used

② imaginary time-evolution

up to normalization:

$$\hat{\rho}_A(\beta) \propto e^{-\beta\hat{H}} = e^{-\beta\hat{H}/2}\,\hat{\mathbb{1}}\cdot e^{-\beta\hat{H}/2}$$

$$\propto e^{-\beta\hat{H}/2}\,\hat{\rho}_A(0)\,e^{-\beta\hat{H}/2}$$

$$= e^{-\beta\hat{H}/2}\,\mathrm{tr}_B\left(|\psi\rangle_{AB}(0)\,{}_{AB}\langle\psi|(0)\right)e^{-\beta\hat{H}/2}$$

$\hat{H}$ acts only on A $$= \mathrm{tr}_B\left(e^{-\beta\hat{H}/2}|\psi\rangle_{AB}(0)\,{}_{AB}\langle\psi|(0)\,e^{-\beta\hat{H}/2}\right)$$

$$= \mathrm{tr}_B\left(|\psi\rangle_{AB}(\beta)\,{}_{AB}\langle\psi|(\beta)\right)$$

So, up to normalization, the purification of $\hat{\rho}_A(\beta)$ is given by

$$\boxed{|\psi\rangle_{AB}(\beta) = \underbrace{e^{-\beta\hat{H}/2}}_{\text{by time-evolution}}\,\underbrace{|\psi\rangle_{AB}(0)}_{\text{by hand}}}$$

actually numerically <u>easier</u>: errors are damped out exponentially!

<u>normalization:</u>

$$1 \overset{!}{=} \mathrm{tr}_A\,\hat{\rho}_A(\beta) = \mathrm{tr}_A\mathrm{tr}_B\,|\psi\rangle_{AB}(\beta)\,{}_{AB}\langle\psi|(\beta)$$

$$= {}_{AB}\langle\psi(\beta)|\psi(\beta)\rangle_{AB}$$

simply by normalizing $|\psi(\beta)\rangle_{AB}$

monitoring normalization factors gives $\dfrac{Z(\beta)}{Z(0)}$.

③ dynamical quantities by real-time evolution:

$$\langle \hat{O}_1(t)\,\hat{O}_2(0)\rangle_{\hat{\rho}_A(\beta)}$$

$$= \mathrm{tr}_A\, \hat{O}_1(t)\,\hat{O}_2(0)\,\hat{\rho}_A(\beta)$$

$$= \mathrm{tr}_A \mathrm{tr}_B\, \hat{O}_1(t)\,\hat{O}_2(0)\,|\psi(\beta)\rangle_{AB}\,{}_{AB}\langle\psi(\beta)|$$

$$= {}_{AB}\langle\psi(\beta)|\,\hat{O}_1(t)\,\hat{O}_2(0)\,|\psi(\beta)\rangle_{AB}$$

$$= {}_{AB}\langle\psi(\beta)|\,e^{+i\hat{H}_A t}\,\hat{O}_1\,e^{-i\hat{H}_A t}\,\underbrace{\hat{O}_2|\psi(\beta)\rangle_{AB}}_{|\varphi(\beta;0)\rangle_{AB}}$$

$$= {}_{AB}\langle\psi(\beta;t)|\,\hat{O}_1\,|\varphi(\beta;t)\rangle_{AB}$$

again, no change with respect to old algorithm!

All so far holds independent of state representation (i.e. use of matrix product states)!

Last step: express $|\psi\rangle_{AB}(0)$ as MPS.

$|\psi\rangle_{AB}(0) = \bigotimes |\psi\rangle_{AB;i}(0) \Rightarrow$ "mean field" or "product state"

$\Rightarrow$ matrix dimension 1

phys. auxiliary

$$|\psi\rangle_{AB;i}(0) = \frac{1}{\sqrt{d}}\sum_{i=1}^{d} |\sigma_i \tau_i\rangle \equiv \sum_{\sigma_i\tau_i} A^{\sigma_i\tau_i}\,|\sigma_i\tau_i\rangle \Rightarrow$$

$$A_i^{\sigma_i\tau_i} = \frac{1}{\sqrt{d}}\,\delta_{\sigma_i,\tau_i}$$

— that's it! we can construct state by hand and start!

d^2 matrices