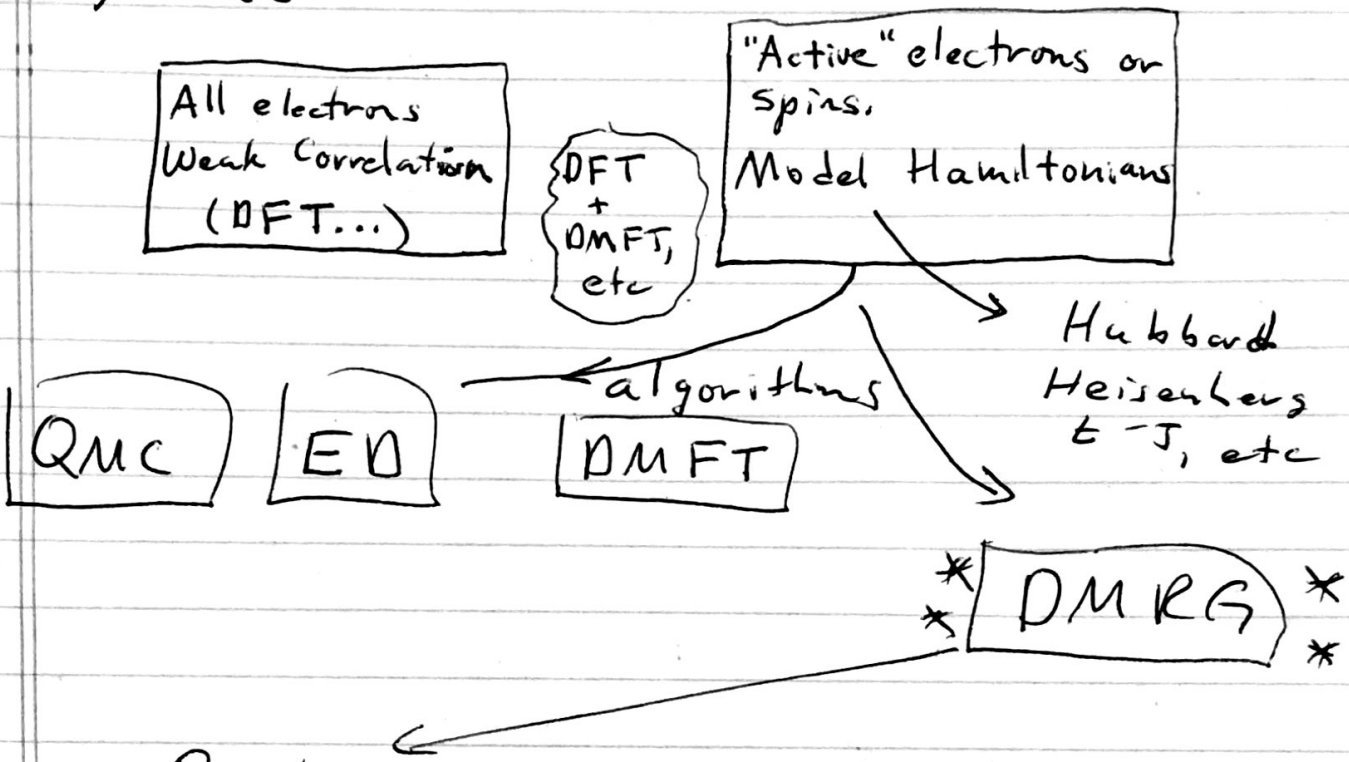
Density Matrix Renormalization Group

Steven R. White, UC Irvine

Spin systems
Exact diagonalization
Entanglement
Area Law
Matrix Product States
DMRG

Julia for fast development
C++/ITensor for state of the art efficiency

Overview: QM of many electron systems



Background: ED, Model Systems,

New Connection: Quantum Information + Entanglement

Todays Topics

Spin-$\frac{1}{2}$ systems
ED / Lanczos
Entanglement

julia programming language
Simple exercises

Tomorrow: Matrix Product States, DMRG, ITensor library (C++)

Exact Diagonalization of small clusters of spin-1/2's.

Review: $S=\frac{1}{2}$, Pauli matrices

Spin operator $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

Spin basis: $\begin{matrix}\uparrow\\\downarrow\end{matrix}\begin{pmatrix} a \\ b \end{pmatrix} = a|\uparrow\rangle + b|\downarrow\rangle$ (z-basis)

$$\sigma_x = \begin{matrix}\uparrow & \downarrow \\ \end{matrix}\begin{matrix}\uparrow\\\downarrow\end{matrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

σ_z is diagonal in this z-basis,

e.g. $\sigma_z|\uparrow\rangle = |\uparrow\rangle$

But $\sigma_x|\uparrow\rangle = |\downarrow\rangle$ not diagonal

Two $S=\frac{1}{2}$'s: Suppose $H = \vec{S}_1 \cdot \vec{S}_2$. What are the energy levels?

Algebraic Trick

$\vec{S}_{total} = \vec{S}_1 + \vec{S}_2$ spins 1 and 2

$\vec{S}_1 + \vec{S}_2$ commute, e.g. $[S_{1z}, S_{2z}] = 0$

$$S^2_{total} = \vec{S}_{total} \cdot \vec{S}_{total} = (\vec{S}_1 + \vec{S}_2)\cdot(\vec{S}_1 + \vec{S}_2)$$

$$= \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

Now $\vec{S}^2 = \hbar^2 S(S+1)$ any total spin S

$S = \frac{1}{2}$: $\vec{S}^2 = \frac{3}{4}$ [now set $\hbar = 1$]

$S = 0$: $\vec{S}^2 = 0$

$S = 1$: $\vec{S}^2 = 2$

} Two possible states for two spins with definite $\vec{S}^2$

Thus

$$S(S+1) = \frac{3}{4} + \frac{3}{4} + 2\,\vec{S}_1 \cdot \vec{S}_2$$

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left[S(S+1) - \frac{3}{2}\right] = \begin{cases} -\frac{3}{4} & S=0 \\ \frac{1}{4} & S=1 \end{cases}$$

— — — $S=1$ Triplet

— $S=0$ singlet

More general approach: Write H as a matrix in a basis

2 spins: $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$

A wavefunction is a vector, length $= 4\ (=2^N)$

An operator is a matrix, 4×4 $(2^N \times 2^N)$

Let $\vec{S} = \frac{1}{2}\vec{\sigma}$, $S^{\pm} = S_x \pm i S_y$, etc

$$S_z = \begin{matrix}\uparrow \\ \downarrow\end{matrix}\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \qquad S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

So $S^+|\downarrow\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle$

$S^+|\uparrow\rangle = 0$, $S^-|\downarrow\rangle = 0$, $S^-|\uparrow\rangle = |\downarrow\rangle$

A little algebra gives

$$\vec{S}_1 \cdot \vec{S}_2 = S_{1z} S_{2z} + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right)$$

When applied to several spins, each op acts on only its spin

$$S_1^+ S_2^- |\underset{1}{\downarrow}\underset{2}{\uparrow}\underset{3}{\uparrow}\rangle = \left(S_1^+|\downarrow\rangle\right)\left(S_2^-|\uparrow\rangle\right) \times (|\uparrow\rangle)$$

$$= |\uparrow\downarrow\uparrow\rangle$$

Heisenberg Model $\boxed{H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j}$

Exercise 1

Show for 2 spins: $H = J$

$$H = \begin{matrix} \\ \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix}\begin{matrix} \begin{matrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \end{matrix} \\ \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & -a & b & 0 \\ 0 & b & -a & 0 \\ 0 & 0 & 0 & a \end{pmatrix} \end{matrix}$$

Find a & b.

[Note sparseness]

Solution $H = J \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -1/4 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$

Diagonalize:

Singlet: $\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ +1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

$E = -\frac{3}{4}$

Triplet: $E = \frac{1}{4}$ $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$

Julia: `H=[1/4 0 0 0; 0 -1/4 1/2 0; 0 1/2 -1/4 0; 0 0 0 1/4]`

`eig fact(H)`

Many spins: Hilbert Space = $\{|s_1 s_2 \ldots s_N\rangle\}$ spanned by

* The key difficulty of many ptle QM is the exponentially large size of the Hilbert space

$|\Psi\rangle$ = 2^N-long vector = $\begin{pmatrix} a \\ b \\ c \\ d \\ \vdots \end{pmatrix} \begin{matrix} \uparrow\uparrow\uparrow \\ \uparrow\uparrow\downarrow \\ \uparrow\downarrow\uparrow \\ \uparrow\downarrow\downarrow \\ \vdots \end{matrix}$

$H = 2^N \times 2^N$ matrix (Find lowest E eigenvector)

Directly treating $N=100$ this way is hopeless. But lets see how to do a cluster of 3 or 4 or 10 spins.

$N=2$ case: algebra already done

$$H = \begin{array}{c} \\ \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{array} \begin{array}{c} \begin{array}{cccc} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \end{array} \\ \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -1/4 & \frac{1}{2} & 0 \\ 0 & 1/2 & -1/4 & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \end{array} \cdot J$$

note substantial sparseness

The elements are $\langle s_1' s_2' | H | s_1 s_2 \rangle$ w.th $s_1 = \uparrow$ or $\downarrow$, etc.

$N=3$ $\quad H = (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3) J$

$\vec{S}_1 \cdot \vec{S}_2$ only operates on 1 & 2 — It leaves spin 3 alone. Thus

$$\langle S_1' S_2' S_3' \mid \vec{S}_1 \cdot \vec{S}_2 \mid S_1 S_2 S_3 \rangle \propto \delta_{S_3 S_3'}$$

The z-z part of $\vec{S}_1 \cdot \vec{S}_2$ doesn't change S_1 or S_2. It gives a factor of $\pm \frac{1}{4}$ for parallel or opp. spins.

The $\frac{1}{2}(S^+S^- + S^-S^+)$ flips the spins and puts in $+\frac{1}{2}$.

These observations turn into simple rules for the elements of H

1) Diagonal elements are $\frac{J}{4} \cdot \left(\#\text{ parallel} - \#\text{ opposite neighbors} \right)$

2) Off diag are zero if more than two spins differ. If two n.n. spins are flipped, get $+\frac{1}{2}$. Otherwise, zero. $\rightarrow (\uparrow\downarrow) \leftrightarrow (\downarrow\uparrow)$ not $|\uparrow\uparrow\rangle \leftrightarrow |\downarrow\downarrow\rangle$

Example $N=3$

Let $0 \equiv \uparrow$, $1 \equiv \downarrow$

$$H = \begin{array}{c|cccccccc} & 000 & 001 & 010 & 011 & 100 & 101 & 110 & 111 \\ \hline 000 & 2\cdot\frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 001 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 010 & 0 & 1/2 & -2\cdot\frac{1}{4} & 0 & 1/2 & 0 & 0 & 0 \\ 011 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 100 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 101 & 0 & 0 & 0 & 1/2 & 0 & -2\cdot\frac{1}{4} & 1/2 & 0 \\ 110 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 111 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\cdot\frac{1}{4} \end{array} \cdot J$$

We can call our eigensolver on this to get the energies + eigenvectors

Conservation of S^z_{total}

H does not change the number of up and down spins.

$$[H, S^z_{total}] = 0$$

This makes H Block diagonal.

For example the $\uparrow\uparrow\downarrow$ block for $N=3$

$$H_{block} = J \begin{array}{c} \\ \uparrow\uparrow\downarrow \\ \uparrow\downarrow\uparrow \\ \downarrow\uparrow\uparrow \end{array} \begin{array}{c} \begin{array}{ccc} \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \downarrow\uparrow\uparrow \end{array} \\ \begin{pmatrix} 0 & 1/2 & 0 \\ 1/2 & -1/2 & 1/2 \\ 0 & 1/2 & 0 \end{pmatrix} \end{array}$$

$S^z_{tot} = \frac{1}{2}$

Get $E_{gr.} = -J$

$$|2\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

This is a big help, but the block sizes are still $O\left(\frac{2^N}{N}\right)$

Exercise: $N=4$

open chain, so no J_{14} term

For $S^z_{total}=0$, there are 6 basis states, 0011, 0101, etc.

$= \uparrow\uparrow\downarrow\downarrow \quad \uparrow\downarrow\uparrow\downarrow$

Find the 6×6 H_{block}, diagonalize it with julia, get the ground state energy & vector.

Hard

Exercise: For a chain of N spins (say up to $N=10$) write a julia function to give H and find the ground state energy.

Memory & Calculation Time

For an $M \times M$ matrix, storage is M^2

A desktop has $\sim 10^{10}$ bytes

1 double prec $\sim$ 10 bytes (actually 8)

Can store $\sim 10^9$ reals, or $10^{4.5} \times 10^{4.5}$ matrix

or ~30K x 30K

Thus $2^N = 30\text{K} \rightarrow \underline{N \sim 15}$ storage

Calculation time: Full diagonalization, $M \times M$

$\sim M^3 \equiv$ CPU-time $\quad M^3 \sim 10^{4.5 \cdot 3} \sim 10^{13.5}$

calc time $\sim \dfrac{10^{13.5}}{10^{10}}$ $\quad 10^{10} \sim$ # of floating pt. o/s per second

10 GFLOPS

$\sim 10^{3.5} \sim 3000$ sec $\sim$ 1 hr. OK

How can we do better?

1) Sparseness: Each row of H has only $O(N)$ non zero els, say $N \sim 20$

Storage $\rightarrow N 2^N \sim 2^{N+4}$

say up to $N \sim 25$ much better!

But can't use full diag: millions of hours, storage also

Power Method

Let $\tilde{H} = (I - \varepsilon H)$. For ε small enough, the largest magnitude eigenvalue is $1 - \varepsilon E_{gr}$, with same "ground" state

Then $|G.S\rangle = \lim_{k \to \infty} \tilde{H}^k |\xi\rangle$

where $|\xi\rangle$ is any vector not $\perp$ to $|GS\rangle$. The power method only stores (sparse) H and one or two $|V\rangle$ $|V'\rangle = \tilde{H}|V\rangle$ iterate. But it is slow: large k needed.

Lanczos Method

Given $|\xi\rangle = \vec{\xi}$, the Krylov space is

$\{\xi, H\xi, H^2\xi, H^3\xi, \ldots\}$ + all linear combinations (vector space)

Note $(1 - \varepsilon H)^k \xi$ is in the Krylov space.

Lanczos is an efficient way of finding the lowest energy vector in a truncate Krylov space (up to $H^k \xi$ for some k)

Lanczos rarely needs k bigger than $k \sim 100$–200 for the ground state, much better than the power method

Lanczos basis:

$\vec{x}_1 = \vec{\xi}$

$\vec{x}_2 = \eta_2 (H\vec{x}_1 - \alpha_2 \vec{x}_1)$ α chosen so $\vec{x}_1 \perp \vec{x}_2$

↑ normalization factor

$\vec{x}_3 = \eta_3 (H\vec{x}_2 - \alpha_3 \vec{x}_2 - \beta_3 \vec{x}_1)$

$\vec{x}_4 = \eta_4 (H\vec{x}_3 - \alpha_4 \vec{x}_3 - \beta_4 \vec{x}_2 - \gamma_4 \vec{x}_1)$

etc.

This makes an orthonormal basis $\langle x_i | x_j \rangle = \delta_{ij}$. It turns out that γ, etc are all zero: only α + β. Also, $\tilde{H}_{ij} = \langle x_i | H | x_j \rangle$ is tridiagonal.

Calc time $\sim M \cdot (\sim 30)_{\text{sparseness}} \cdot (\sim 100)_{k = \#\text{ of steps}}$

$M \sim 10^9$ OK!

Exercise: Look up the julia Lanczos method. Modify your general diag method for S=1/2 chains to 1) use sparse matrices (julia- built-in) and the julia Lanczos method.

How big a system can you do?

Product States

The simplest type of states are product states

Examples: $|\uparrow_1 \downarrow_2\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2 = |\uparrow\rangle \otimes |\downarrow\rangle$

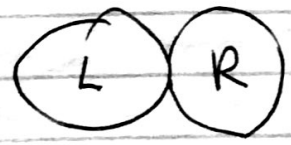
or

$\frac{1}{\sqrt{2}}(|\uparrow\rangle_1 - |\downarrow\rangle_1)\left(|\uparrow\rangle_2 + |\downarrow\rangle_2\right)\cdot\frac{1}{\sqrt{2}}$

In general, if you can write $|\psi\rangle$ as $|\psi\rangle = |\phi\rangle_1 |\eta\rangle_2 |\xi\rangle_3 \ldots$ it is a product state

Entanglement If $|\psi\rangle$ is not a product state, the system is **entangled.**

Usually we consider a system divided into two parts, L (left) and R (right)



L + R disjoint spaces

Then $|\psi\rangle \stackrel{?}{=} |\phi_L\rangle |\phi_R\rangle$

Suppose $\hat{O}$ is an op. acting only on L

$\langle\psi|\hat{O}|\psi\rangle = \langle\phi_R|\langle\phi_L|\hat{O}|\phi_L\rangle|\phi_R\rangle$

$= \langle\phi_R|\phi_R\rangle\langle\phi_L|\hat{O}|\phi_L\rangle = \langle\phi_L|\hat{O}|\phi_L\rangle$

Conclusion: Product states describe independent systems.

Entangled states – how do you tell if a state is entangled?

Example: 2 spins

Let $|A\rangle = \frac{1}{\sqrt{2}}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\downarrow\rangle$

and

$|B\rangle = \frac{1}{2}|\uparrow\uparrow\rangle + \frac{1}{2}|\uparrow\downarrow\rangle + \frac{1}{2}|\downarrow\uparrow\rangle + \frac{1}{2}|\downarrow\downarrow\rangle$

Which is entangled?

$|B\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \quad \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

so $|B\rangle$ is a product state, an unentangled.

It is easy to see $|A\rangle$ is entangled (exercise).

Show there is no $\alpha, \beta, \gamma, \delta$ so

$|A\rangle = (\alpha|\uparrow\rangle + \beta|\downarrow\rangle)(\gamma|\uparrow\rangle + \delta|\downarrow\rangle)$

To know in general if a state is entangled you need to do a singular value decomposition.

Singular Value Decomposition (SVD)

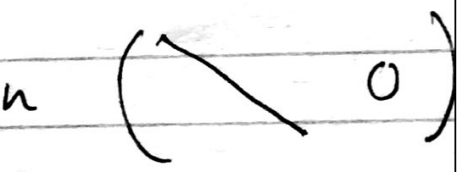
Let M be any complex $m \times n$ matrix with $n \geq m$. (If $n < m$, SVD on M^T)

Then there exists $U = m \times m$, $D = m \times m$ with D diagonal, $V = m \times n$ with

$$\boxed{M = UDV}$$

with $D_{ii} \geq 0$, U = unitary, V = row-unitary ($VV^\dagger = 1$) (rows of V orthonormed)

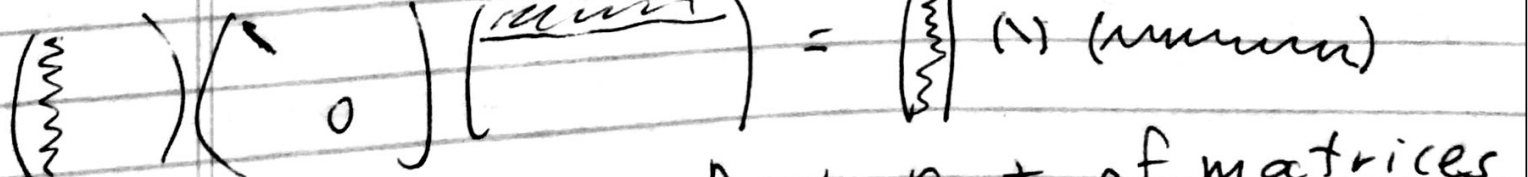
This is the SVD. The D_{ii} are the singular values, unique. $D_{ii} = \lambda_i$

Another form: $\tilde{D} = m \times n$ 

then $\tilde{V}$ is unitary, $n \times n$

$$M = U \tilde{D} \tilde{V}$$

SVD's have many uses. One is matrix compression. Suppose only a few D_{ii} are nonnegligible

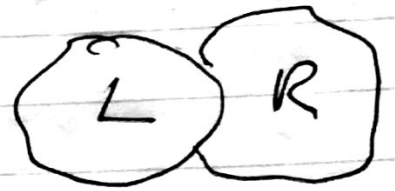


Drop rest of matrices

Schmidt Decomposition

Let $|\psi\rangle = \sum_{lr} \psi_{lr} |l\rangle |r\rangle$

$|l\rangle$ in L, $|r\rangle$ in R



ψ_{lr} is a wavefunction, but treat it as a matrix, do SVD

$$\psi_{lr} = [U \tilde{D} \tilde{V}]_{lr}$$

Normalization $\sum_{lr} |\psi_{lr}|^2 = 1 = tr\{\psi^\dagger \psi\}$ ← matrix

Let

$$|i\rangle_L \equiv \sum_l U_{li} |l\rangle$$

$$|i\rangle_R \equiv \sum_r \tilde{V}_{ir} |r\rangle$$

$$|\psi\rangle = \sum_{lr} \sum_i U_{li} \tilde{D}_{ii} \tilde{V}_{ir} |l\rangle |r\rangle$$

$$= \sum_i \tilde{D}_{ii} |i\rangle_L |i\rangle_R = \boxed{\sum_i \lambda_i |i\rangle_L |i\rangle_R = |\psi\rangle}$$

this is the Schmidt decomposition

Normalization:

$$1 = \mathrm{tr}\{\psi^\dagger \psi\} = \mathrm{tr}\{\tilde{V}^\dagger \tilde{D}^\dagger \underbrace{U^\dagger U}_{1} \tilde{D} \tilde{V}\}$$

$$= \mathrm{tr}\{\tilde{D}^\dagger \tilde{D}\} \Rightarrow \boxed{\sum_i \lambda_i^2 = 1}$$

λ_i^2 is the probability of the Schmidt-state pair $|i\rangle_L |i\rangle_R$

If $|\psi\rangle = |\phi\rangle |\xi\rangle$, it is already in Schmidt decomp form, w. th $\lambda_1 = 1$, $\lambda_{i>1} = 0$. So this tells us if $|\psi\rangle$ is entangled.

Von Neumann Entanglement Entropy

$$\boxed{S \equiv -\sum_i \lambda_i^2 \ln \lambda_i^2}$$ VN ent. entropy

This is the stat mech formula for entropy using λ_i^2 = prob of $|i\rangle$

S measures entanglement. $S=0 \Rightarrow$ product state

Example Two $S=\frac{1}{2}$'s

Is $|\psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\uparrow\rangle - \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle$

entangled?

$$\psi = \begin{array}{c} \\ \uparrow_1 \\ \downarrow_1 \end{array}\begin{array}{c} \begin{array}{cc} \uparrow_2 & \downarrow_2 \end{array} \\ \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \end{array}$$

Need to do SVD (by hand)

Trick $\psi = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$

unitary since rows orthonormal

$$= \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{U}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{D}\underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}}_{V}$$

So $\lambda_1 = 1 \quad \lambda_2 = 0 \qquad S = -|\lambda_1|\ln|\lambda_1| - 0\ln 0$

$= 0$

Unentangled

Product form: $|\psi\rangle = |\uparrow\rangle\left(\frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle\right)$