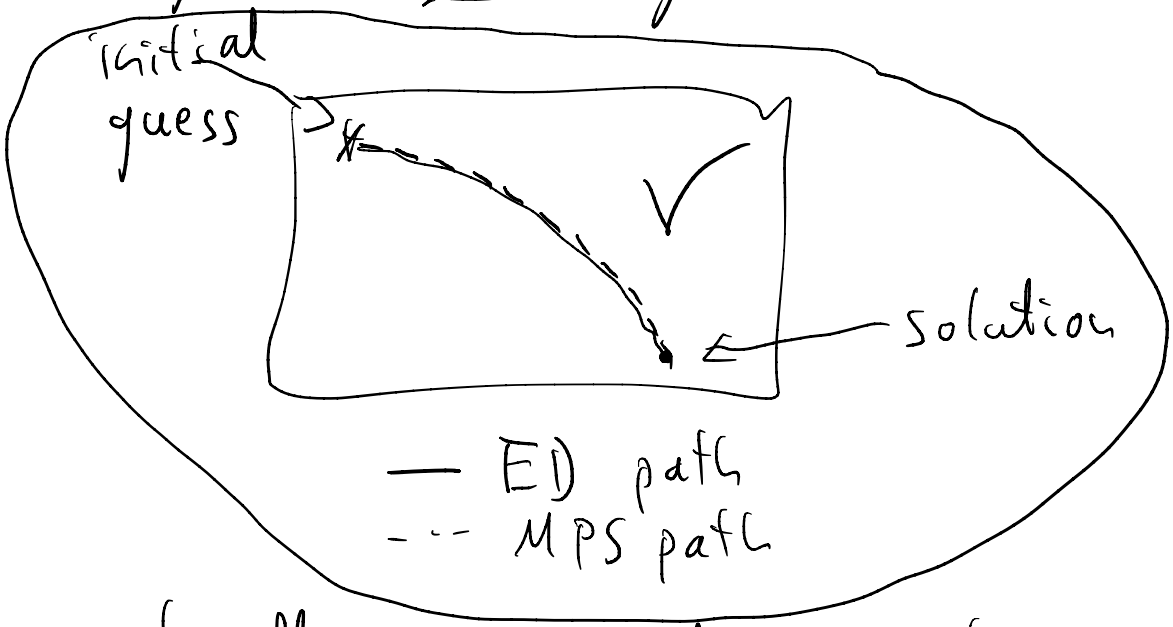
- How reliably do TNS algorithms find the optimal solution within the TNS manifold

  ↳ For local 1D Hamiltonian with constant (as a function of system size N) gap, MPS algorithms guaranteed to find a globally optimal MPS in polynomial time are known (Zeph Landau et al., Nature Physics 2015).

  ↳ Heuristically, for gapped (and even critical) local 1D Hamiltonians, finding a very good MPS approximation works well with DMRG and MPS-algorithms (e.g. imaginary time propagation).

↳ Conjecture (for more general settings):

If the entire path in Hilbert space from your initial MPS to the final (approximation to the) solution can be well approximated by MPS (low entanglement), MPS-algorithms (specifically imaginary time propagation) will not get stuck in local minima.



- Works for heuristically confirmed case above.
  (no phase transitions at finite T in 1D)
- Counter-example: 1D gapped non-local Hamiltonians encoding

hard combinatorial problems.

D.1: Basics of Monte Carlo Integration

- Goal: Compute physical properties of QMB systems, such as expectation values of observables in spin systems

$$\langle O \rangle_\psi = \frac{\langle \psi | O | \psi \rangle}{\langle \psi | \psi \rangle} \overset{\left[\langle \sigma | \psi \rangle = \psi(\sigma)\right]}{=} \frac{\sum_{\{\sigma\}} \psi^*(\sigma) \langle \sigma | O | \psi \rangle}{\sum_{\{\sigma\}} |\psi(\sigma)|^2}$$

$$\left[\mathbb{1} = \sum_{\{\sigma\}} |\sigma\rangle\langle\sigma|\right]$$

$$= \frac{\sum_{\{\sigma\}} |\psi(\sigma)|^2 \frac{\langle \sigma | O | \psi \rangle}{\langle \sigma | \psi \rangle}}{\sum_{\{\sigma\}} |\psi(\sigma)|^2} \qquad \left(\frac{\langle \sigma | O | \psi \rangle}{\langle \sigma | \psi \rangle} = O^L_\sigma\right)$$

$$= \frac{\sum_{\{\sigma\}} |\psi(\sigma)|^2 O^L_\sigma}{\sum_{\{\sigma\}} |\psi(\sigma)|^2}$$

- Key issue: $\sum_{\{\sigma\}} \dots$ contains exponentially many terms.

- Remedy from stochastic analysis: Monte-Carlo "integration" (here discrete sum)

  ↳ Interpret $P_\psi(\sigma) = \frac{|\psi(\sigma)|^2}{\sum_\sigma |\psi(\sigma)|^2}$ as a probability density and compute $\langle O \rangle_\psi$ by stochastic sampling of spin configurations $\overline{O} = \frac{1}{M} \sum_{k=1}^{M} O_{\sigma_k}$.

- Statistical uncertainty of Monte-Carlo integration
  - The central limit theorem applied to $\bar{O}$ (interpreted as a random variable with varying configurations) tells us that generically

uncertainty → $$\Delta[\bar{O}] = \frac{\Delta[O^L]}{\sqrt{M}} \sim \frac{1}{\sqrt{M}}$$ (sample size M)

  - Crucial advantage over other (deterministic) methods: Uncertainty of results scales as $\frac{1}{\sqrt{M}}$, independently of the physical system size (dimension of integration volume).
- Challenges: L> Distribution of O^L might not be

"well behaved" such that central limit theorem is not applicable (fat tails).

↳ In many Quantum Monte Carlo methods, $P_\psi(G)$ is replaced by a function that may become non-positive definite (negative sign problem).

- Basics of stochastic sampling:
  - Sampling amounts to designing a stochastic process ("time-evolution" of a random variable) $G_1 \to G_2 \to G_3 \cdots$ that generates an unbiased (representative) sample.

- Markov chains are stochastic processes characterized by having no memory:

$$P(\sigma_k \mid \sigma_{k-1}, \sigma_{k-2}, \dots \sigma_1) \overset{!}{=} P(\sigma_k \mid \sigma_{k-1}), \quad \sigma_k = (\sigma_k^{(1)}, \dots, \sigma_k^{(N)})$$

(N: # sites)

Conditional probability

Transition matrix (non-negative) fully characterizes the Markov chain.

$\rightsquigarrow$ Step $\sigma_{k-1} \to \sigma_k$ only depends on σ_{k-1}, but not on further history.

$\rightsquigarrow$ $P(\sigma_k, \sigma_{k-1}, \dots, \sigma_1) = P(\sigma_k \mid \sigma_{k-1}) P(\sigma_{k-1} \mid \sigma_{k-2}) \dots P(\sigma_1)$

joint probability

- Sample distributed according to given distribution $\rho(\sigma)$ is ensured by detailed balance stationarity

Condition:

Cancellation of opposite probability currents

$$P(\sigma_j|\sigma_i)\,\rho(\sigma_i) = P(\sigma_i|\sigma_j)\,\rho(\sigma_j) \quad \forall_{\sigma_i,\sigma_j}$$

which is a sufficient condition if $P(\sigma_j|\sigma_i)$ is ergodic, i.e. if every σ_j can be reached from any σ_i in a finite number of steps (P^n strictly positive (no zero modes) for some $n \geq 1$).

$\rightsquigarrow$ Stationary distribution is eigenstate associated with the largest eigenvalue of P.