Computational physics

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Contents

- Quantum Monte Carlo

Introduction

- When quantum effects become important?
- Near absolute zero temperature, where quantum fluctuations, arising from Heisenberg's uncertainty principle, dominate the systems behavior, i.e., if

$$\hbar\omega > k_B T, \tag{1}$$

where ω is the characteristic frequency of quantum oscillations, $\hbar$ is the Plank constant and $k_B T$ is the thermal energy.

- When the interparticle distance (N particles in volume V) is less than the thermal de Broglie wavelength, i.e.,

$$\left(\frac{V}{N}\right)^{1/3} \leq \lambda_{th} = \frac{\hbar}{\sqrt{2\pi m k_B T}} \tag{2}$$

in the case of a nonrelativistic free particles with mass m. In this case the gas will obey Bose-Einstein statistics or Fermi-Dirac statistics, whichever is appropriate.

Introduction

- Connection between statistical mechanics and quantum mechanics.
- Boltzmann weight: $\rho = \exp\left(-\beta\mathcal{H}\right)$
- Formal solution of the Schrödinger equation $i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{\mathcal{H}}\left|\psi(t)\right\rangle$ is time evolution operator, or propagator, $\hat{U}(t) = \exp\left(\frac{-i\hat{\mathcal{H}}t}{\hbar}\right)$.
- Isomorphism:

$$\begin{aligned} \rho &\leftrightarrow \hat{U} \\ \beta &\leftrightarrow \frac{it}{\hbar} \end{aligned} \tag{3}$$

Introduction

- In quantum statistical mechanics the the partition function is

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta\hat{\mathcal{H}}}\right] \tag{4}$$

  with inverse temperature $\beta = 1/k_B T$.
- Trace can be computed using a complete orthonormal set of basis states $\{|\chi_i\rangle\}$ such that

$$\langle\chi_i \,|\, \chi_j\rangle = \delta_{ij} \quad \text{and} \quad \sum_i |\chi_i\rangle \langle\chi_i| = \hat{\mathbb{1}} \tag{5}$$

  and partition function becomes

$$\mathcal{Z} = \sum_i \left\langle \chi_i \left| e^{-\beta\hat{\mathcal{H}}} \right| \chi_i \right\rangle \tag{6}$$

- If $|\chi_i\rangle$ is are also the eigenstates of $\hat{\mathcal{H}}$, i.e., $\hat{\mathcal{H}}\,|\chi_i\rangle = E_i\,|\chi_i\rangle$, it follows that

$$\mathcal{Z} = \sum_i e^{-\beta E_i} \tag{7}$$

Introduction

- The thermal expectation value of an observable X is

$$\langle X \rangle = \frac{1}{\mathcal{Z}} \operatorname{Tr}\left[\hat{X} e^{-\beta \hat{\mathcal{H}}}\right] \tag{8}$$

- If $\{|\chi_i\rangle\}$ are orthonormal eigenstates of $\hat{\mathcal{H}}$

$$\langle X \rangle = \frac{1}{\mathcal{Z}} \sum_i \left\langle \chi_i \middle| \hat{X} \middle| \chi_i \right\rangle e^{-\beta E_i}, \tag{9}$$

  which is reminiscent of an classical expectation value.
- If the eigenenergies and eigenstates of $\hat{\mathcal{H}}$ are known the problem of sampling the partition function $\mathcal{Z}$ is identical to the classical problem.
- In most cases, $\hat{\mathcal{H}}$ is not explicitly diagonalizable and the challenge is to construct a numerical method to calculate $e^{-\beta \hat{\mathcal{H}}}$.

Trotter-Suzuki approximation

- If $\hat{\mathcal{H}}$ is not explicitly diagonalizable it is yet often possible to break $\hat{\mathcal{H}}$ in to a sum of two trivaly diagonalizable pieces, for example, kinetic $\frac{\hat{\mathbf{p}}^2}{2m}$ and potential energy $V(\hat{\mathbf{x}})$.
- Trotter-Suzuki method is based on this assumption and uses the following identity

$$e^{\lambda(A+B)} = \lim_{m\to\infty}\left(e^{\lambda\frac{A}{m}}e^{\lambda\frac{B}{m}}\right)^m, \tag{10}$$

  where A and B are operators.
- Eq.(10) can be verified using Taylor expansion:

$$e^{\lambda\frac{(A+B)}{m}} = 1+\frac{\lambda}{m}(A+B)+\frac{1}{2}\frac{\lambda^2}{m^2}(A^2+AB+BA+B^2) + \mathcal{O}\left(\frac{\lambda^3}{m^3}\right)$$

  and

$$e^{\lambda\frac{A}{m}}e^{\lambda\frac{B}{m}} = 1+\frac{\lambda}{m}(A+B)+\frac{1}{2}\frac{\lambda^2}{m^2}(A^2+2AB+B^2)+\mathcal{O}\left(\frac{\lambda^3}{m^3}\right).$$

Trotter-Suzuki approximation

- Both expressions match up to terms of order $\mathcal{O}\left(\frac{\lambda^2}{m^2}\|[A,B]\|\right)$ and for large m

$$e^{\lambda(A+B)} \approx \left(e^{\lambda\frac{A}{m}}e^{\lambda\frac{B}{m}}\right)^m \tag{11}$$

- More precisely,

$$\left\|e^{\lambda(A+B)} - \left(e^{\lambda\frac{A}{m}}e^{\lambda\frac{B}{m}}\right)^m\right\| \leq \frac{\lambda^2}{2m}\|[A,B]\|\exp\left[|\lambda|\left(\|A\|+\|B\|\right)\right] \tag{12}$$

  and for commuting A and B, i.e., $[A,B]=0$, Eq.(11) becomes exact.

- More generally holds

$$\left\|\exp\left[\lambda\sum_{i=1}^{p}A_i\right] - \left(\prod_{i=1}^{p}e^{\lambda\frac{A_i}{m}}\right)^m\right\| \leq \frac{\lambda^2}{2m}\left(\sum_{i>j}\|[A_i,A_j]\|\right)\exp\left[|\lambda|\sum_{i=1}^{p}\|A_i\|\right]. \tag{13}$$

Trotter-Suzuki approximation

- Any additive decomposition of the $\mathcal{H}$ can be used as a candidate for the Trotter-Suzuki method
- Consider a mth approximation of the partition function

$$\mathcal{Z}_m = \mathrm{Tr}\left[\left(e^{-\beta\frac{A}{m}}e^{-\beta\frac{B}{m}}\right)^m\right] \quad \text{such that} \quad \mathcal{Z} = \lim_{m\to\infty}\mathcal{Z}_m \quad (14)$$

- Using the definition $\Delta\tau = \beta/m$ the mth approximation of $\mathcal{Z}_m$ can be written as

$$\begin{aligned}
\mathcal{Z}_m &= \mathrm{Tr}\left[\left(e^{-\Delta\tau A}e^{-\Delta\tau B}\right)^m\right] \\
&= \mathrm{Tr}\left[\underbrace{e^{-\Delta\tau A}e^{-\Delta\tau B}}_{1}\cdot\ldots\cdot\underbrace{e^{-\Delta\tau A}e^{-\Delta\tau B}}_{m}\right] \\
&= \sum_{\chi}\langle\chi|\underbrace{e^{-\Delta\tau A}e^{-\Delta\tau B}}_{1}\cdot\ldots\cdot\underbrace{e^{-\Delta\tau A}e^{-\Delta\tau B}}_{m}|\chi\rangle\,,
\end{aligned}$$

where the sum runs over an d-dimensional orthonormal basis set of the Hibert space (the dimension of $e^{-\beta\hat{\mathcal{H}}}$ is the number of energy eigenstates of the system).

Trotter-Suzuki approximation

- We insert $2m-1$ unity operators

$$\mathcal{Z}_m = \sum_{\chi^{(1)}} \langle \chi^{(1)} | e^{-\Delta\tau A} \left(\sum_{\chi^{(2)}} |\chi^{(2)}\rangle \langle \chi^{(2)}| \right) e^{-\Delta\tau B} \cdot \ldots |\chi^{(1)}\rangle$$
$$= \sum_{\{\chi^{(i)}\}} \langle \chi^{(1)} | e^{-\Delta\tau A} |\chi^{(2)}\rangle \langle \chi^{(2)} | e^{-\Delta\tau B} |\chi^{(3)}\rangle \cdot \ldots$$
$$\ldots \cdot \langle \chi^{(2m)} | e^{-\Delta\tau B} |\chi^{(1)}\rangle ,$$

  where $\sum_{\{\chi^{(i)}\}} \ldots = \sum_{\{\chi^{(1)},\ldots,\chi^{(2m)}\}} \ldots$ is a sum over $2m$ different d-dimensional states.

- Formally, the above procedure can be considered as an expansion of the system by an extra dimension (τ-direction), which is called Trotter dimension.

Trotter-Suzuki approximation

- From the path-integral representation, it follows that the τ-direction is actually an imaginary-time direction. The trace contains the required periodicity.
- The expectation value is given by

$$\langle X \rangle = \frac{1}{\mathcal{Z}} \sum_{\chi} \left\langle \chi \left| \hat{X} e^{-\beta \hat{\mathcal{H}}} \right| \chi \right\rangle \tag{15}$$

and if $\hat{X}$ is diagonal in the basis $\{|\chi\rangle\}$, i.e., $\langle \chi | \hat{X} | \chi' \rangle = X(\chi)\delta(\chi, \chi')$, then

$$\langle X \rangle = \sum_{\{\chi^{(i)}\}} X(\chi^{(1)}) P(\chi^{(1)}, \ldots, \chi^{(2m)}) \tag{16}$$

with weights

$$P(\chi^{(1)}, \ldots, \chi^{(2m)}) = \frac{1}{\mathcal{Z}_m} \langle \chi^{(1)} | e^{-\Delta\tau A} | \chi^{(2)} \rangle \cdot \langle \chi^{(2)} | e^{-\Delta\tau B} | \chi^{(3)} \rangle \cdot \ldots \cdot \langle \chi^{(2m)} | e^{-\Delta\tau B} | \chi^{(1)} \rangle \tag{17}$$

Trotter-Suzuki approximation

- In numerical simulations we do not calculate the exact sum over all configurations, rather we sum over states, which we generate according to the distribution $P(\{\chi^{(i)}\})$.
- This method correspond to classical Monte-Carlo simulation, if $P(\{\chi^{(i)}\})$ is nonnegative. Note that, only in the diagonal representation the matrix corresponding to $e^{-\beta\hat{\mathcal{H}}}$ is nonnegative.

Example: single quantum spin in external fields

- In the following we exemplify the path integral formulation of quantum models.
- We consider a single spin $\frac{1}{2}$ particle exposed to a longitudinal h_z and transverse field h_x. The Hamiltonoan is given by

$$\hat{\mathcal{H}} = -h_z\sigma_z - h_x\sigma_x = A + B, \tag{18}$$

with Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{19}$$

- Since $[\sigma_z, \sigma_x] = 2i\sigma_y$, the Trotter-Suzuki approximation is not trivial.
- For the representation we choose the eigenstates of σ_z and label them by Ising spin variables $S = \pm 1$, i.e., $\sigma_z |S\rangle = S |S\rangle$.

Example: single quantum spin in external fields

- Using $\sigma_x^2 = \mathbb{1}$, we obtain

$$\langle S|e^{\Delta\tau h_z\sigma_z}|S'\rangle = \delta_{SS'}e^{\Delta\tau h_z S'} \tag{20}$$

and

$$\begin{aligned}\langle S|e^{\Delta\tau h_x\sigma_x}|S'\rangle &= \begin{cases}\cosh(\Delta\tau h_x) & \text{for } S = S' \\ \sinh(\Delta\tau h_x) & \text{for } S \neq S'\end{cases} &(21)\\ &= \sqrt{\frac{1}{2}\sinh(2\Delta\tau h_x)}e^{kSS'}, &(22)\end{aligned}$$

where $k = -\frac{1}{2}\ln(\tanh[\Delta\tau h_x])$.

- The mth approximation of the partition function reads as

$$\begin{aligned}\mathcal{Z}_m = &\left(\frac{1}{2}\sinh(2\Delta\tau h_x)\right)^{m/2} \cdot \\ &\sum_{S_1,\ldots,S_{2m}} e^{\Delta\tau h_z S_2}\delta_{S_1S_2}e^{kS_2S_3}e^{\Delta\tau h_z S_4}\delta_{S_3S_4}e^{kS_4S_5}\cdot\ldots \\ &\qquad \ldots\cdot e^{\Delta\tau h_z S_{2m}}\delta_{S_{2m-1}S_{2m}}e^{kS_{2m}S_1}\end{aligned} \tag{23}$$

Example: single quantum spin in external fields

- Or in a more familiar form

$$\mathcal{Z}_m = \left(\frac{1}{2}\sinh\left(2\Delta\tau h_x\right)\right)^{m/2} \cdot \sum_{S_1,\ldots,S_m} \exp\left(\Delta\tau h_z \sum_{n=1}^{m} S_n + k\sum_{n=1}^{m} S_n S_{n+1}\right), \quad (24)$$

  with periodic boundary condition $S_{m+1} = S_1$.

- The mth approximation of the partition function of a single quantum spin in a longitudinal and transverse field is similar to a partition function of a classical one-dimensional chain of m coupled Ising spin in an external field b at temperature T_{cl}.

$$\mathcal{H} = -J\sum_{n=1}^{m} S_n S_{n+1} - b\sum_{n=1}^{m} S_n, \quad (25)$$

  with

$$\frac{J}{k_B T_{cl}} = k \quad \text{and} \quad \frac{b}{k_B T_{cl}} = \Delta\tau h_z \quad (26)$$

Example: single quantum spin in external fields

- The general feature of the Trotter-Suzuki method is that in addition to physical dimensions an imaginary dimension, called Trotter dimension, appear as a consequence of the discretization of the trace.
- Analog: A one-dimensional spin-$\frac{1}{2}$ chain in transverse field with Hamiltonian

$$\hat{\mathcal{H}} = -J_z \sum_{i=1}^{N} \sigma_{z,i}\sigma_{z,i+1} - h_x \sum_{i=1}^{N} \sigma_{x,i} \tag{27}$$

is equivalent to a classical, two-dimensional, Ising-model with anisotropic coupling

$$\mathcal{H} = -\sum_{i=1}^{N}\sum_{n=1}^{m} (J_x S_{i,n} S_{i+1,n} + J_\tau S_{i,n} S_{i,n+1}) \tag{28}$$

Off-lattice path integral formulation

- Next we consider as an example an off-lattice model of N interacting particles with a Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N}\frac{\hat{\mathbf{p}}_i^2}{m} + V\left(\hat{\mathbf{r}}_1, \ldots, \hat{\mathbf{r}}_N\right) = \mathcal{H}_1 + \mathcal{H}_2, \tag{29}$$

  where $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ and $\hat{\mathbf{r}} = (\hat{r}_x, \hat{r}_y, \hat{r}_z)$.
- $\mathcal{H}_1$ and $\mathcal{H}_2$ do not commutate because

$$[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta} \quad \text{for } \alpha, \beta \in \{x, y, z\} \tag{30}$$

- In the following we set $\hbar = 1$ and mass $m = 1$.
- In oder to calculate the partition function we use again the Trotter-Suzuki formula and alternately the eigenbasis of $\hat{\mathbf{P}} = (\hat{\mathbf{p}}_1, \ldots, \hat{\mathbf{p}}_N)$ and $\hat{\mathbf{R}} = (\hat{\mathbf{r}}_1, \ldots, \hat{\mathbf{r}}_N)$.

Off-lattice path integral formulation

- The Mth approximation of the partition function reads as

$$\mathcal{Z}_M = \sum_{\{\mathbf{P}^{(s)}\},\{\mathbf{R}^{(s)}\}} \langle \mathbf{P}^{(1)}|e^{-\Delta\tau\mathcal{H}_1}|\mathbf{R}^{(1)}\rangle \langle \mathbf{R}^{(1)}|e^{-\Delta\tau\mathcal{H}_2}|\mathbf{P}^{(2)}\rangle \cdot \ldots$$
$$\ldots \cdot \langle \mathbf{P}^{(M)}|e^{-\Delta\tau\mathcal{H}_1}|\mathbf{R}^{(M)}\rangle \langle \mathbf{R}^{(M)}|e^{-\Delta\tau\mathcal{H}_2}|\mathbf{P}^{(1)}\rangle ,$$

  with $\Delta\tau = \beta/M$ and where $\{\mathbf{P}^{(s)}\} = \{\mathbf{P}^{(1)}, \ldots, \mathbf{P}^{(M)}\}$

- The individual terms in $\mathcal{Z}_M$ can be calculated as

$$\langle \mathbf{P}^{(s)}|e^{-\Delta\tau\mathcal{H}_1}|\mathbf{R}^{(s)}\rangle = \exp\left(-\frac{\Delta\tau}{2}(\mathbf{P}^{(s)})^2\right) \langle \mathbf{P}^{(s)}|\mathbf{R}^{(s)}\rangle$$
$$= \exp\left(-\frac{\Delta\tau}{2}(\mathbf{P}^{(s)})^2\right) \frac{e^{i\left(\mathbf{P}^{(s)}\cdot\mathbf{R}^{(s)}\right)}}{(2\pi)^{3N/2}},$$

$$\langle \mathbf{R}^{(s)}|e^{-\Delta\tau\mathcal{H}_2}|\mathbf{P}^{(s+1)}\rangle = \exp\left(-\Delta\tau V(\mathbf{R}^{(s)})\right) \langle \mathbf{R}^{(s)}|\mathbf{P}^{(s+1)}\rangle$$
$$= \exp\left(-\Delta\tau V(\mathbf{R}^{(s)})\right) \frac{e^{-i\left(\mathbf{P}^{(s+1)}\cdot\mathbf{R}^{(s)}\right)}}{(2\pi)^{3N/2}}$$

Off-lattice path integral formulation

- For a continuous spectrum the sum becomes an integral over the phase space and

$$\mathcal{Z}_M = (2\pi)^{-3NM} \int \prod_{s=1}^{M} d\mathbf{R}^{(s)} d\mathbf{P}^{(s)}$$

$$\exp\left[-\Delta\tau \sum_{s=1}^{M} \left\{ \frac{(\mathbf{P}^{(s)})^2}{2} - i\mathbf{P}^{(s)} \cdot \frac{\mathbf{R}^{(s+1)} - \mathbf{R}^{(s)}}{\Delta\tau} + V(\mathbf{R}^{(s)}) \right\}\right],$$

  with periodic boundary condition $\mathbf{R}^{(M+1)} = \mathbf{R}^{(1)}$.
- The integral over the momentum space is reminiscent of the propagator of N free particles if $\tau \to \frac{it}{\hbar}$.
- The integral over the momentum space can be solved analytically completing the square in the exponent, which results in Gaussian-like integrals.

Off-lattice path integral formulation

- The result is a discrete version of Feynman's path integral in imaginary time, i.e., after Wick rotation $\tau \rightarrow \frac{it}{\hbar}$,

$$\mathcal{Z}_M = (2\pi\Delta\tau)^{-3NM/2} \int \prod_{s=1}^{M} d\mathbf{R}^{(s)}$$
$$\exp\left[-\sum_{s=1}^{M}\left\{\frac{1}{2}\left(\frac{\mathbf{R}^{(s+1)}-\mathbf{R}^{(s)}}{\Delta\tau}\right)^2 + V(\mathbf{R}^{(s)})\right\}\Delta\tau\right] \quad (31)$$

- An alternative interpretation is that the effective Hamiltonian

$$\mathcal{H}_{eff} = \frac{\kappa}{2}\sum_{i=1}^{N}\sum_{s=1}^{M}\left(\mathbf{r}_i^{(s+1)}-\mathbf{r}_i^{(s)}\right)^2 + \frac{1}{M}\sum_{i<j}\sum_{s=1}^{M} V(|\mathbf{r}_i^{(s)}-\mathbf{r}_j^{(s)}|) \quad (32)$$

in Eq.(31) describes a 'melt' of ring polymers with effective spring constant $\kappa = \frac{mM}{\beta^2\hbar^2}$. The melt has unusual properties, since monomer-monomer interactions occur only if the 'Trotter-index' is the same.

Off-lattice path integral formulation

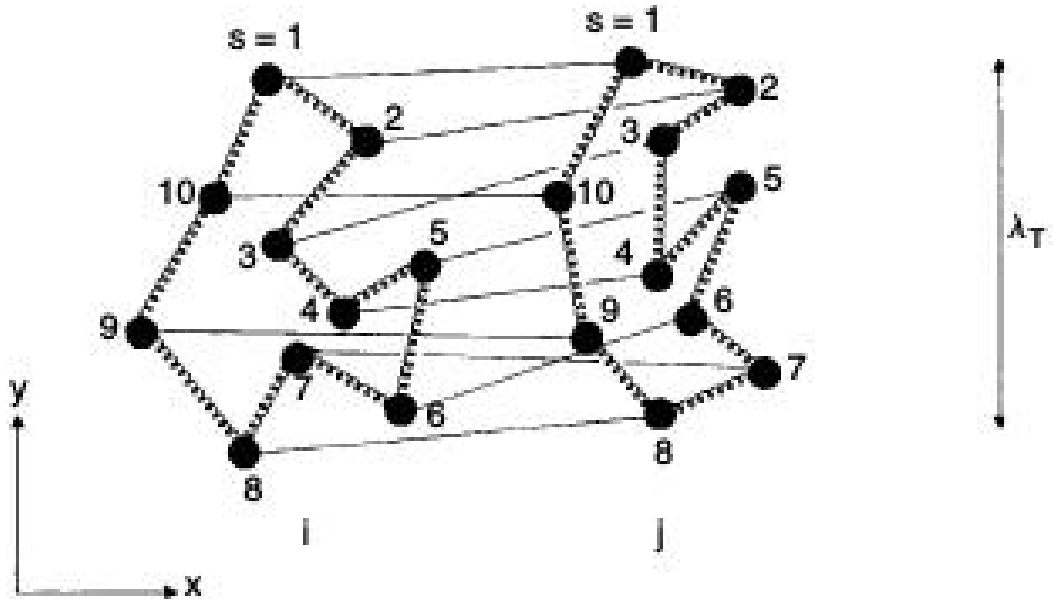


Figure 1: Schematic representation of two interacting quantum particles i, j in 2D: each particle is represented by a 'ring polymer' composed of $M = 10$ effective monomers $\mathbf{r}_i^{(s)}$, with $s = 1, \ldots, M$. Harmonic springs (of strength κ) only connect 'monomers' in the same 'polymer', while interatomic forces join different monomers with the same Trotter index s, indicated by the thin straight lines. In the absence of such interactions, the size of such a ring polymer coil would be given by the thermal de Broglie wavelength λ_T.

Off-lattice path integral formulation

- If potential V could be neglected, the equipartition theorem implies, that the potential energy carried by each spring is

$$\frac{d}{2}k_B T = \frac{\kappa}{2}\left\langle \left(\mathbf{r}_i^{(s+1)} - \mathbf{r}_i^{(s)}\right)^2 \right\rangle \tag{33}$$

  and the mean-square distance of two neighboring particles is

$$l^2 = \left\langle \left(\mathbf{r}_i^{(s+1)} - \mathbf{r}_i^{(s)}\right)^2 \right\rangle = \frac{d\hbar^2}{mk_B TM}. \tag{34}$$

- The radius of gyration $R_g^2 = \frac{1}{2M^2}\sum_{s,q}\left(\mathbf{r}^{(s)} - \mathbf{r}^{(q)}\right)^2$ of a polymer with M monomers is $\left\langle R_g^2 \right\rangle = \frac{l^2 M}{12} = \frac{d\hbar^2}{12mk_b T}$.
- The diameter of the polymer

$$2\sqrt{\left\langle R_g^2 \right\rangle} = \frac{\sqrt{d}\hbar}{\sqrt{3mk_B T}} \tag{35}$$

  is of the same order as the thermal de Broglie wavelength

$$\lambda_T = \frac{\hbar}{\sqrt{3\pi mk_B T}}. \tag{36}$$

Further example

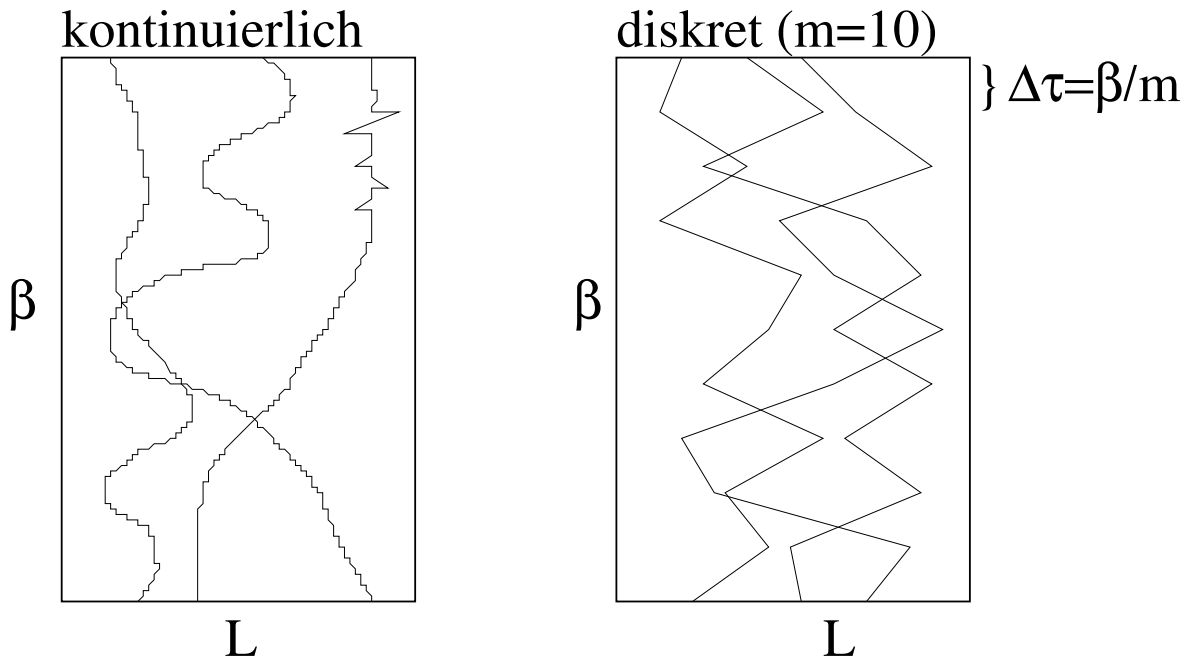


Figure 2: Path integrals along the Trotter dimension for 3 bosons with Coulomb interaction. Starting from world-lines $\{x_i(\tau)\}_{i=1,\ldots,N}^{\tau=1,\ldots,m}$ one tries to move the nodes along the spatial direction. The MC moves are accepted with probability $e^{-\Delta E}$.

Boson Hubbard model

- The Hamiltonian of the boson Hubbard model, which describes bosons on a 1D lattice with N sites, reads as

$$\mathcal{H} = -t \sum_{i=1}^{N} \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) + V \sum_{i=1}^{N} n_i \left(n_i - 1 \right), \qquad (37)$$

  where $b_i^\dagger$ and b_i are creation and annihilation operators for bosons at ith lattice site and $n_i = b_i^\dagger b_i$ is the corresponding particle number operator.
- For bosons the occupation number is $n_i \in \{0, 1, 2, \ldots\}$.
- The first term describes hopping of particles between neighboring lattice sites.
- The second term 'penalize' or 'reward' occupation of ith lattice site by multiple particles depending on the sign of V.
- The ratio of the hopping parameter t to the interaction parameter V determines the phase behaviour of the system.

Spinless Fermion model with nearest-neighbor interactions

- The Hamiltonian of the spinless Fermion model with nearest-neighbor interactions:

$$\mathcal{H} = -t \sum_{i=1}^{N} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + V \sum_{i=1}^{N} \left(n_i - \tfrac{1}{2} \right) \left(n_{i+1} - \tfrac{1}{2} \right), \quad (38)$$

  where $c_i^\dagger$ and c_i are creation and annihilation operators for fermions and $n_i = c_i^\dagger c_i$ is the particle number operator.
- For fermions the occupation number is $n_i \in \{0, 1\}$.
- In the following, we assume an even number of lattice sites N.
- The Hamiltonian can be written as

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_{i,i+1} \quad (39)$$

  and we choose the following splitting of $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$ with

$$\mathcal{H}_1 = \sum_{i \text{ odd}} \mathcal{H}_{i,i+1} \quad \text{and} \quad \mathcal{H}_2 = \sum_{i \text{ even}} \mathcal{H}_{i,i+1}. \quad (40)$$

Spinless Fermion model

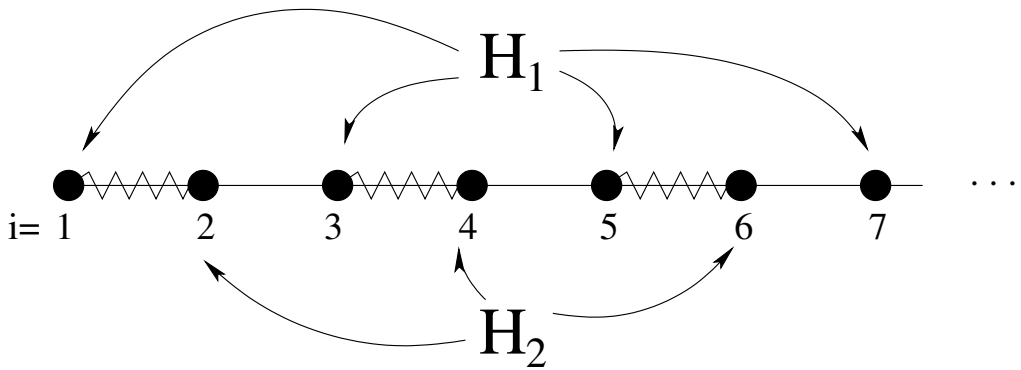
- $[\mathcal{H}_1, \mathcal{H}_2] \neq 0$, however, $\mathcal{H}_1$ and $\mathcal{H}_2$ are each composed of a sum of $N/2$ mutually commuting terms, due to fermionic anticommutator relations

$$\{c_i, c_j^\dagger\} = \delta_{ij} \quad \text{and} \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0. \tag{41}$$

- Because of that it exact factorization is possible:

$$U_1 = e^{-\Delta\tau\mathcal{H}_1} = \prod_{i \text{ odd}} e^{-\Delta\tau\mathcal{H}_{i,i+1}} \tag{42}$$

$$U_2 = e^{-\Delta\tau\mathcal{H}_2} = \prod_{i \text{ even}} e^{-\Delta\tau\mathcal{H}_{i,i+1}} \tag{43}$$



Spinless Fermion model

- Use Trotter-Suzuki approximation and occupation number basis $|\mathbf{n}\rangle = |n_1, n_2, \ldots, n_N\rangle$ with $n_i \in \{0, 1\}$.
- The mth approximation of the partition function reads as

$$\mathcal{Z}_m = \sum_{\{\mathbf{n}_j\}} \langle \mathbf{n}_1 | U_1 | \mathbf{n}_2 \rangle \langle \mathbf{n}_2 | U_2 | \mathbf{n}_3 \rangle \cdot \ldots \cdot \ldots \cdot \langle \mathbf{n}_{2m-1} | U_1 | \mathbf{n}_{2m} \rangle \langle \mathbf{n}_{2m} | U_2 | \mathbf{n}_1 \rangle , \quad (44)$$

- For further calculation we write the basis vectors as

$$|\mathbf{n}\rangle = |n_1, n_2\rangle \otimes |n_3, n_4\rangle \otimes \ldots \otimes |n_{N-1}, n_N\rangle \quad (45)$$

$$|\mathbf{n}\rangle = |n_2, n_3\rangle \otimes |n_4, n_5\rangle \otimes \ldots \otimes |n_N, n_1\rangle \quad (46)$$

such that

$$e^{-\Delta\tau \mathcal{H}_1} |\mathbf{n}\rangle = e^{-\Delta\tau \mathcal{H}_{1,2}} |n_1, n_2\rangle \otimes e^{-\Delta\tau \mathcal{H}_{3,4}} |n_3, n_4\rangle \otimes \ldots \otimes e^{-\Delta\tau \mathcal{H}_{N-1,N}} |n_{N-1}, n_N\rangle \quad (47)$$

and in analogous way $e^{-\Delta\tau \mathcal{H}_2} |\mathbf{n}\rangle$ using basis vectors (46).

Spinless Fermion model

- Thus the calculation of matrices $\langle \mathbf{n}_j | U_1 | \mathbf{n}_{j+1} \rangle$ and $\langle \mathbf{n}_{j+1} | U_2 | \mathbf{n}_{j+2} \rangle$ reduced to an effective problem of two lattice sites.
- The basis matrix elements we need to evaluate are

$$w \begin{pmatrix} n_{i,j+1} & n_{i+1,j+1} \\ n_{i,j} & n_{i+1,j} \end{pmatrix} =$$

$$\langle n_{i,j}, n_{i+1,j} | e^{-\Delta\tau \mathcal{H}_{i,i+1}} | n_{i,j+1}, n_{i+1,j+1} \rangle =$$

$$\langle n_{i,j}, n_{i+1,j} | e^{\Delta\tau t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) - \Delta\tau V \left(n_i - \frac{1}{2} \right) \left(n_{i+1} - \frac{1}{2} \right)} | n_{i,j+1}, n_{i+1,j+1} \rangle \tag{48}$$

- We obtain

$$\begin{aligned}
e^{-\Delta\tau \mathcal{H}_{i,i+1}} |0,0\rangle &= |0,0\rangle \, e^{-\Delta\tau \frac{V}{4}} \\
e^{-\Delta\tau \mathcal{H}_{i,i+1}} |1,1\rangle &= |1,1\rangle \, e^{-\Delta\tau \frac{V}{4}} \\
e^{-\Delta\tau \mathcal{H}_{i,i+1}} |1,0\rangle &= \left[\cosh(\Delta\tau t) |1,0\rangle + \sinh(\Delta\tau t) |0,1\rangle \right] e^{\Delta\tau \frac{V}{4}} \\
e^{-\Delta\tau \mathcal{H}_{i,i+1}} |0,1\rangle &= \left[\cosh(\Delta\tau t) |0,1\rangle + \sinh(\Delta\tau t) |1,0\rangle \right] e^{\Delta\tau \frac{V}{4}}
\end{aligned}$$

Spinless Fermion model

- The explizit form of possible matrix elements is

$$\begin{pmatrix} w\begin{pmatrix}0&0\\0&0\end{pmatrix} & w\begin{pmatrix}0&1\\0&0\end{pmatrix} & w\begin{pmatrix}1&0\\0&0\end{pmatrix} & w\begin{pmatrix}1&1\\0&0\end{pmatrix} \\ w\begin{pmatrix}0&0\\0&1\end{pmatrix} & w\begin{pmatrix}0&1\\0&1\end{pmatrix} & w\begin{pmatrix}1&0\\0&1\end{pmatrix} & w\begin{pmatrix}1&1\\0&1\end{pmatrix} \\ w\begin{pmatrix}0&0\\1&0\end{pmatrix} & w\begin{pmatrix}0&1\\1&0\end{pmatrix} & w\begin{pmatrix}1&0\\1&0\end{pmatrix} & w\begin{pmatrix}1&1\\1&0\end{pmatrix} \\ w\begin{pmatrix}0&0\\1&1\end{pmatrix} & w\begin{pmatrix}0&1\\1&1\end{pmatrix} & w\begin{pmatrix}1&0\\1&1\end{pmatrix} & w\begin{pmatrix}1&1\\1&1\end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} e^{-\Delta\tau\frac{V}{2}} & 0 & 0 & 0 \\ 0 & \cosh(\Delta\tau t) & \sinh(\Delta\tau t) & 0 \\ 0 & \sinh(\Delta\tau t) & \cosh(\Delta\tau t) & 0 \\ 0 & 0 & 0 & e^{-\Delta\tau\frac{V}{2}} \end{pmatrix} e^{\Delta\tau\frac{V}{4}} \quad (49)$$

Spinless Fermion model

- The odd-even site breakup of $\mathcal{H}$ and the Trotter decomposition created a structure of $2m$ layers in the imaginary-time direction.
- Thus, single fermion hops one site to the left or right with matrix element $\sinh(\Delta\tau t)$ and moves forward along the Trotter dimension with matrix element $\cosh(\Delta\tau t)$.
- Pairs of creation and annihilation operators starting at odd sites, U_1, act on layers $j = 2, 4, \ldots$, while pairs of operators starting at even sites, U_2, act on layers $j = 1, 3, \ldots$
- Within each Trotter time interval $\Delta\tau$ there is one application of the operator U_1 and one of the operator U_2.
- The transition matrix depends on the state of four sites, namely, $n_{i,j}, n_{i+1,j}, n_{i,j+1}, n_{i+1,j+1}$, which define a plaquette.
- Plaquettes naturally decompose space-time into a checkerboard pattern, see Fig.(3), and the shaded plaquettes correspond to the areas in which fermions can hop and interact.

Spinless Fermion model

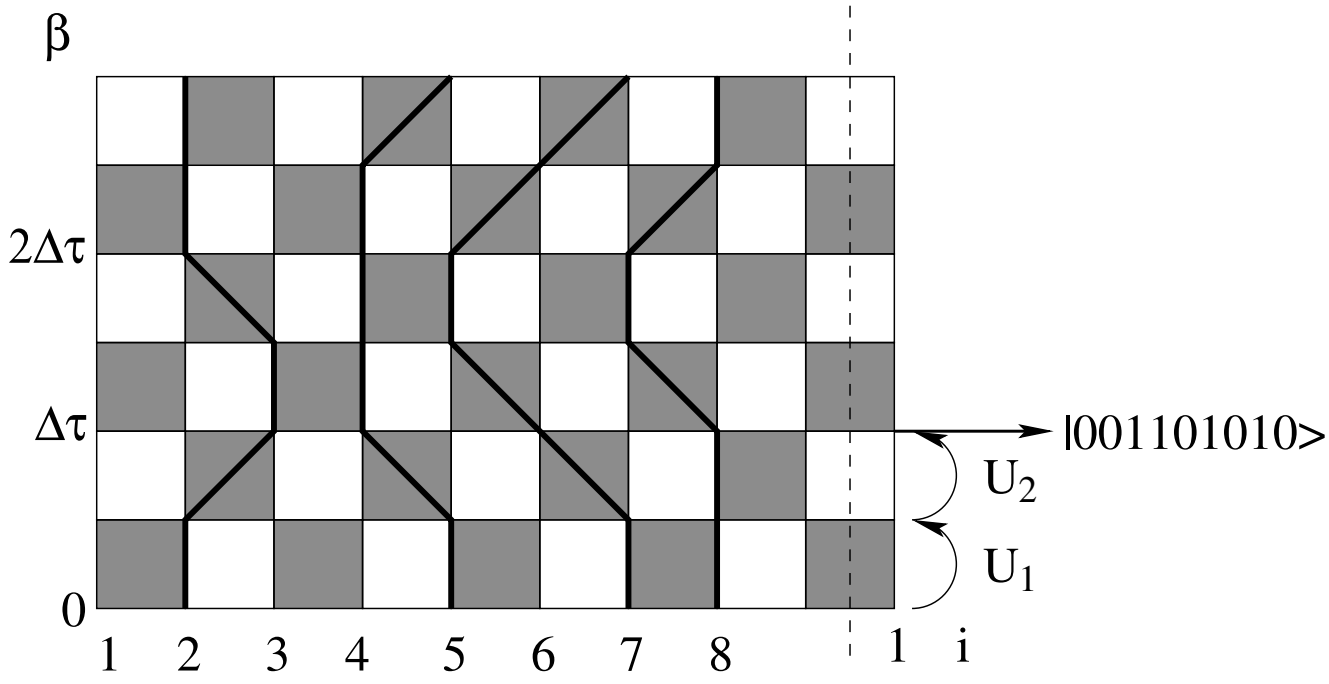


Figure 3: Breakup of the time-evolution into U_1 and U_2 leads to the checkerboard pattern. Here the periodic spatial lattice of sites is labeled by i and the imaginary-time axis τ has been sliced into $2\beta/\Delta\tau = 2m$ segments. Fermions can hop and interact in the shaded square but not in the unshaded ones. Heavy lines are examples of allowed fermion world lines. The occupation on each τ slice corresponds to one of the states $|\mathbf{n}\rangle = |n_1, n_2, \ldots, n_N\rangle$ in the sum for $\mathcal{Z}_m$.

Spinless Fermion model

- The lattice is periodic in space and imaginary-time.
- To each plaquette correspond 16 possible occupation configuration, however, only 6 are allowed and the nonzero matrix element express a conservation law:

$$n_{i,j} + n_{i+1,j} = n_{i,j+1} + n_{i+1,j+1} \tag{50}$$

- Number of fermions is conserved at every imaginary-time step.
- If we connect the occupied sites at each τ slice by lines we obtain continuous paths looping in the Trotter direction and we call them world lines of the fermions.
- The sum over intermediate states that satisfy fermion-number conservation is equivalent to the sum over all allowed configurations of the world lines.
- Notice that world lines can be drawn along the vertical edge of a shaded box or diagonally across a shaded box, but they cannot be drawn diagonally across an unshaded box.

Spinless Fermion model

- Monte Carlo sampling becomes a matter of deforming the world lines.
- Deformations are accepted according to a probability which satisfies detailed-balance. This is possible because matrix elements needed to construct the transition probability are nonnegative.
- A single fermion move is not allowed due to the conservation law.
- The minimum change we can make is to move two fermions from one vertical edge of an unshaded box to the other.

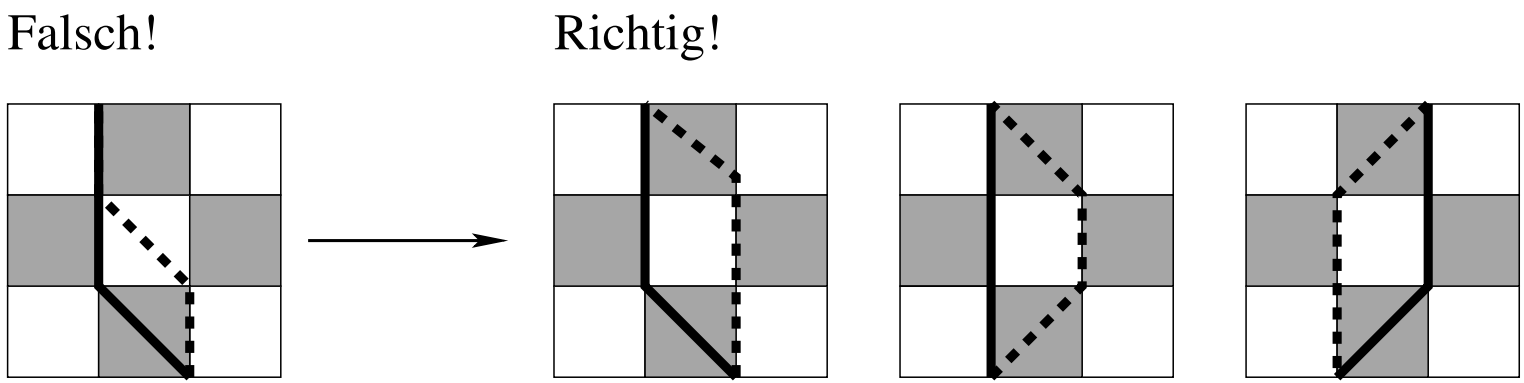


Figure 4: (1) An example of an illegal move. (2-4) Basic world line updates. World lines may move from the heavy solid line to the dashed one and vice versa.

Monte Carlo algorithm

- We designate each lattice point by (i, j) with $i = 1, \ldots, N$ (space) and $j = 1, \ldots, 2m$ (time).
- At each lattice site, we define an occupation number $n_{i,j} \in \{0, 1\}$.
- In sweeping through the lattice, we must check whether it is possible to move a world line across each unshaded square.
- Focus on the unshaded square whose lower left-hand corner is at the site (i, j).
- A move from left to right is possible if $s = +2$, from right to left if $s = -2$ and otherwise no move is possible, where

$$s = n_{i,j} + n_{i,j+1} - n_{i+1,j} - n_{i+1,j+1} \tag{51}$$

- If a move is possible, we must calculate the ratio R of the product of matrix elements in Eq.(44) after and before the move.

Monte Carlo algorithm

- R depends on $n_{i+1,j-1}$ and $n_{i+1,j+2}$, because they determine whether the world line we are moving is vertical or diagonal in the shaded boxes above and below our unshaded one.
- R depends on $n_{i-1,j}$ and $n_{i+2,j}$, because they determine whether there is an additional world line running through the shaded boxes to the left and right of our unshaded one.

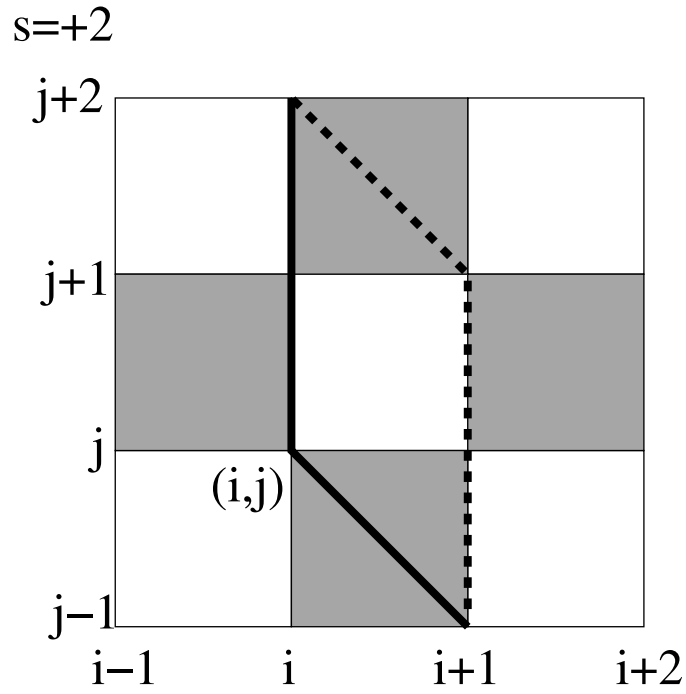


Figure 5: Move across the unshaded plaquette. The acceptance probability is governed by the weights of the north, south, east and west plaquettes.

Monte Carlo algorithm

- Using matrix in Eq.(49) one obtains

$$R = \tanh\left(\Delta\tau t\right)^{su} \cosh\left(\Delta\tau t\right)^{sv} e^{\Delta\tau \frac{V}{2} sv}, \tag{52}$$

with

$$\begin{aligned} u &= 1 - n_{i+1,j-1} - n_{i+1,j+2}, && (53)\\ v &= n_{i-1,j} - n_{i+2,j}. && (54)\\ s &= n_{i,k} + n_{i,k+1} - n_{i+1,k} - n_{i+1,k+1} && (55) \end{aligned}$$

- We accept the proposed new configuration with probability

$$P_{accept} = \frac{R}{1-R} \tag{56}$$

Monte Carlo algorithm

- For the move shown in Fig.(6) it is $s = 2$, $u = -1$, $v = 1$ and $R = \sinh(\Delta\tau t)^{-2} \cosh(\Delta\tau t)^4 \, e^{\Delta\tau V}$

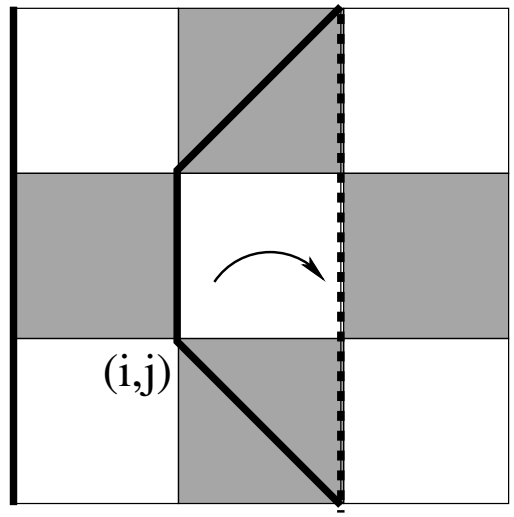


Figure 6: Example world-line update.

- Exact calculation gives:

$$
\begin{aligned}
R &= \frac{\langle X01X|U_2|1010\rangle \langle 1010|U_1|1010\rangle \langle 1010|U_2|X01X\rangle}{\langle X01X|U_2|1100\rangle \langle 1100|U_1|1100\rangle \langle 1100|U_2|X01X\rangle} \\
&= \frac{\cosh(\Delta\tau t)\, e^{\Delta\tau \frac{V}{4}} \cdot \cosh(\Delta\tau t)^2 \, e^{\Delta\tau \frac{V}{2}} \cdot \cosh(\Delta\tau t)\, e^{\Delta\tau \frac{V}{4}}}{\sinh(\Delta\tau t)\, e^{\Delta\tau \frac{V}{4}} \cdot e^{-\Delta\tau \frac{V}{2}} \cdot \sinh(\Delta\tau t)\, e^{\Delta\tau \frac{V}{4}}} \\
&= \sinh(\Delta\tau t)^{-2} \cosh(\Delta\tau t)^4 \, e^{\Delta\tau V}
\end{aligned}
$$

Monte Carlo algorithm

- Alternative formulation of the Monte Carlo algorithm.
- Visit every unshaded plaquette, which is located at

$$\begin{pmatrix} n_{i,j+1} & n_{i+1,j+1} \\ n_{i,j} & n_{i+1,j} \end{pmatrix}. \tag{57}$$

- If $n_{i,j} = n_{i,j+1}$ and $n_{i+1,j} = n_{i+1,j+1}$ and $n_{i,j} = 1 - n_{i+1,j}$, we attempt to move the segment from one edge to the other.
- The move is accepted via a Metropolis algorithm

$$P_{accept} = \min\left[1, R_{north} R_{south} R_{east} R_{west}\right], \tag{58}$$

with ratios of the local weights before and after the proposed move.

- Ratio for north plaquette

$$R_{north} = w \begin{pmatrix} n_{i,j+2} & n_{i+1,j+2} \\ 1 - n_{i,j+1} & 1 - n_{i+1,j+1} \end{pmatrix} \Big/ w \begin{pmatrix} n_{i,j+2} & n_{i+1,j+2} \\ n_{i,j+1} & n_{i+1,j+1} \end{pmatrix}$$

Monte Carlo algorithm

- Ratio for south plaquette

$$R_{south} = w \begin{pmatrix} 1 - n_{i,j} & 1 - n_{i+1,j} \\ n_{i,j-1} & n_{i+1,j-1} \end{pmatrix} \Big/ w \begin{pmatrix} n_{i,j} & n_{i+1,j} \\ n_{i,j-1} & n_{i+1,j-1} \end{pmatrix}$$

- Ratio for east plaquette

$$R_{east} = w \begin{pmatrix} 1 - n_{i+1,j+1} & n_{i+2,j+1} \\ 1 - n_{i+1,j} & n_{i+2,j} \end{pmatrix} \Big/ w \begin{pmatrix} n_{i+1,j+1} & n_{i+2,j+1} \\ n_{i+1,j} & n_{i+2,j} \end{pmatrix}$$

- Ratio for west plaquette

$$R_{west} = w \begin{pmatrix} n_{i-1,j+1} & 1 - n_{i,j+1} \\ n_{i-1,j} & 1 - n_{i,j} \end{pmatrix} \Big/ w \begin{pmatrix} n_{i-1,j+1} & n_{i,j+1} \\ n_{i-1,j} & n_{i,j} \end{pmatrix}$$

Jordan–Wigner transformation

- Using the Jordan–Wigner transformation it is possible to map the spinless Fermion model with nearest-neighbor interactions onto the one-dimensional quantum Heisenberg model.
- The spin creation and annihilation operators acting on a site i anti-commute

$$\{S_i^+, S_i^-\} = 1, \quad \{S_i^+, S_i^+\} = \{S_i^-, S_i^-\} = 0 \tag{59}$$

  as fermions do.
- However, on different sites i and j, we have the relation

$$[S_i^+, S_j^-] = 0, \quad [S_i^+, S_j^+] = [S_i^-, S_j^-] = 0, \tag{60}$$

  so spins on different sites commute unlike fermions which anti-commute.
- Introduction of a phase operator (kink operator) $K_i = e^{i\pi \sum_{j=1}^{i-1} S_j^+ S_j^-}$, which counts the number of down-to-up spin flips that appear to the left of i, restores the anticommutator relation of fermions.

Jordan–Wigner transformation

- The operators $c_i = K_i S_i^+$ and $c_i^\dagger = S_i^- K_i^\dagger$ satisfy anticommutator relation

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0 \tag{61}$$

- Thus, the Hamiltonian of the 1D Heisenberg model can be writen as

$$\begin{aligned}
\mathcal{H}_{Heisenberg} &= -J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\
&= -J \sum_{i=1}^{N} \left[\frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \right] \\
&= -\frac{J}{2} \sum_{i=1}^{N} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) \\
&\quad -J \sum_{i=1}^{N} \left(c_i^\dagger c_i - \frac{1}{2} \right) \left(c_{i+1}^\dagger c_{i+1} - \frac{1}{2} \right)
\end{aligned}$$

Measurements

- Measurements
- Phase behaviour
- Winding number
- Negative sign problem

Introduction to exact diagonalization

- A common challenge in quantum mechanics is to identify the eigenstates $|\phi_n\rangle$ and eigenenergies E_n of the Hamiltonian $\hat{H}$, i.e., we have to solve the stationary Schrödinger equation

$$\hat{H}\,|\phi_n\rangle = E_n\,|\phi_n\rangle\,, \tag{62}$$

  where $E_0 < E_1 < E_2 < \ldots$ with ground state energy E_0.

- Consider, for example, an anharmonic oscillator with Hamiltonian ($m = 1$ and $\hbar = 1$):

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right), \quad \hat{H}_1 = \lambda \hat{x}^4, \tag{63}$$

  where $\hat{x}$ is the position and $\hat{p} = -i\frac{\partial}{\partial x}$ the momentum operator.

Introduction to exact diagonalization

- We introduce a creation $\hat{a}^\dagger = (\hat{x} - i\hat{p})/\sqrt{2}$ and annihilation operator $\hat{a} = (\hat{x} + i\hat{p})/\sqrt{2}$ with commutator $[\hat{a}, \hat{a}^\dagger] = 1$ and obtain the eigenenergies of $\hat{H}_0 = \left(\hat{n} + \frac{1}{2}\right)$, where $\hat{n} = \hat{a}^\dagger \hat{a}$ is the number operator, as $\hat{H}_0 |n\rangle = E_n |n\rangle$ with $E_n = n + \frac{1}{2}$.
- Using the ladder operator representation of $\hat{x} = \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right)$ and $\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$ we are able to calculate the matrix

$$\left\langle n \left| \hat{H} \right| m \right\rangle = E_n \delta_{nm} + \lambda \left\langle n \left| \hat{x}^4 \right| m \right\rangle . \tag{64}$$

- Only for $|n - m| \leq 4$ we get nonzero matrix elements, i.e.,

$$\left\langle n \left| \hat{x}^4 \right| m \right\rangle = \frac{1}{4} \left\langle n \left| \left(\hat{a}^\dagger + \hat{a}\right)^4 \right| m \right\rangle \neq 0. \tag{65}$$

Introduction to exact diagonalization

- For example,

$$\begin{aligned}\langle n|(\hat{a}^\dagger + \hat{a})^4|n+4\rangle &= \langle n|\hat{a}^4|n+4\rangle \\ &= \langle n+4|(\hat{a}^\dagger + \hat{a})^4|n\rangle = \langle n+4|\hat{a}^{\dagger 4}|n\rangle \\ &= \sqrt{(n+1)(n+2)(n+3)(n+4)} \quad (66)\end{aligned}$$

- The introduction of the occupation number representation with basis $|n\rangle$ converted the task to estimate the stationary states of the Schrödinger equation to an eigenvalue problem of linear algebra.
- A very common approximation is to truncate Hilbert space $\mathcal{H}$ to finite dimension, for example, consider only $n < N$ states, such that the infinite dimensional matrix reduced to a $N \times N$-matrix.

Introduction to exact diagonalization

- In order to diagonalize the resulting matrix it is necessary to consider $\hat{H}$ on a subspace $\mathcal{U}$ of the full Hilbert space $\mathcal{H}$. Let be $\{|\varphi_1\rangle, \ldots, |\varphi_N\rangle\}$ an orthonormal basis of the N-dimensional subspace $\mathcal{U} \subset \mathcal{H}$. The projection of $\hat{H}$ on $\mathcal{U}$ is given by the hermitian matrix

$$H_{nm} = \langle \varphi_n | \hat{H} | \varphi_m \rangle \,. \tag{67}$$

  The matrix can be diagonalized numerically and we obtain N real eigenvalues $\varepsilon_0 < \varepsilon_0 < \ldots < \varepsilon_{N-1}$.
- Hylleraas-Undheim-Theorem:
  - $\varepsilon_i \geq E_i$ for $i = 0, \ldots, N-1$, i.e., ε_i is an upper limit.
  - If $\mathcal{U} \subset \mathcal{U}' \subset \mathcal{H}$ it is $\varepsilon_i \geq \varepsilon'_i \geq \varepsilon_{i-1}$, i.e., ε_i decrease with increasing subspace $\mathcal{U}$.
- The larger the dimension of $\mathcal{U}$ the better ε_i approximates E_i.

Introduction to exact diagonalization

- The full spectrum of not to large matrices ($N \approx 10^3 - 10^4$) can be estimated using common iterative methods, which are based on unitary transformations $H \to U^\dagger H U$ that makes the Hamiltonian diagonal, here we have assumed that $H = H^\dagger$ is Hermitian and thus $U^\dagger U = \mathbb{1}$ is an unitary matrix.
- If all matrix elements of the Hamiltonian are real an orthogonal transformations $H \to U^T H U$ diagonalize H, where $H = H^T$ is a symmetric and thus $U^T U = \mathbb{1}$ is an orthogonal matrix.
- The iteration $H \to U_1^\dagger H U_1 \to U_2^\dagger U_1^\dagger H U_1 U_2 \to \ldots$ is carried out until H becomes diagonal. The diagonal of H contains its eigenvalues and the columns of $U_1 U_2 \ldots$ contains the corresponding eigenvectors.

Introduction to exact diagonalization

- Examples are: Jacobi-rotation of a symmetric matrix, Householder reduction of a symmetric matrix to a tridiagonal matrix combined with QR or QL algorithm, etc.
- For large matrices (large N) only the ground state (largest eigenvalue and the corresponding eigenvector) can be calculated and fast methods, like, power iteration or Lanczos method, must be used.

Ground state

- Once the eigenstates are known, the density operator, which represents the canonical ensamble in quantum mechanics, can be obtained as

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}} = \frac{\sum_n e^{-\beta E_n} |\phi_n\rangle \langle \phi_n|}{\sum_n e^{-\beta E_n}}, \tag{68}$$

  with $\beta = 1/k_B T$

- Close to zero temperature, $T \to 0$ (or $\beta \to \infty$), only the ground state $|\phi_0\rangle$ of $\hat{H}$ with energy $E_0 = \min_n\{E_n\}$ will provide the dominant contribution to $\hat{\rho}$.
- Nevertheless, the system can still undergo phase transitions if the ground state energy E_0 itself exhibits non-analytic behavior.

Example: Single quantum spin in external fields

-

Power iteration

- Power iteration will produce the greatest eigenvalue together with the corresponding eigenvector of matrix H_{mn}.
- However, in quantum mechanical problems the smallest eigenvalue is of interest. The solution is to consider the largest eigenvalue of $\hat{H}' = -\hat{H} + c$ with some constant c.
- Since $\hat{H}'$ is a Hermitian operator there is an orthonormal basis $|\psi_1\rangle, \ldots, |\psi_N\rangle$, such that

$$\hat{H}' |\psi_n\rangle = E_n |\psi_n\rangle \quad \text{with} \quad E_1 > E_2 > \ldots > E_N. \tag{69}$$

- For simplicity, we assume that the ground state of $\hat{H}$ is not degenerate.
- Without loss of generality $E_N > 0$, otherwise $H_{mn} \to H_{mn} + (|E_N| + \epsilon)\delta_{mn}$ with $\epsilon > 0$.

Power iteration

- Pick at random an initial state $|\phi_0\rangle = \sum_{n=1}^{N} a_n |\psi_n\rangle$.
- Repeatedly apply $\hat{H}'$ on $|\phi_0\rangle$:

$$
\begin{aligned}
|\phi_1\rangle &= \hat{H}' |\phi_0\rangle = \sum_{n=1}^{N} a_n E_n |\psi_n\rangle \\
|\phi_2\rangle &= \hat{H}' |\phi_1\rangle = \hat{H}'^2 |\phi_0\rangle = \sum_{n=1}^{N} a_n E_n^2 |\psi_n\rangle \\
&\cdots \\
|\phi_k\rangle &= \hat{H}'^k |\phi_0\rangle = E_1^k \left\{ a_1 |\psi_1\rangle + \sum_{n=2}^{N} a_n \left(\frac{E_n}{E_1} \right)^k |\psi_n\rangle \right\}
\end{aligned}
$$

- Beacuse $E_1 > E_n$ for $n > 1 \Rightarrow \lim_{k\to\infty} \left(\frac{E_n}{E_1}\right)^k = 0$ and

$$
\Rightarrow \lim_{k\to\infty} |\phi_k\rangle = a_1 E_1^k |\psi_1\rangle \tag{70}
$$

Power iteration

- Successive application of $\hat{H}'$ on $|\phi_0\rangle$ amplifies the component $|\psi_1\rangle$, which is the eigenvector corresponding to the largest eigenvalue E_1.
- Normalize $|\phi_k\rangle$ after each iteration $|\phi_k\rangle \rightarrow |\phi_k\rangle / \sqrt{\langle\phi_k|\phi_k\rangle}$, such that $\lim_{k\rightarrow\infty} |\phi_k\rangle = |\psi_1\rangle$ and $\lim_{k\rightarrow\infty} \langle\phi_k|\hat{H}'\phi_k\rangle = E_1$
- Once we found E_1 it is possible to obtain E_2 if we apply the power method on

$$\hat{H}' - E_1 |\psi_1\rangle \langle\psi_1| . \tag{71}$$

Because $\left(\hat{H}' - E_1 |\psi_1\rangle \langle\psi_1|\right) |\psi_1\rangle = 0$ the eigenvalue corresponding to $|\psi_1\rangle$ is $E_1 = 0$ and the largest eigenvalue of the new Hamiltonian is E_2.

Power iteration

- How to estimate $|\psi_2\rangle$ and E_2.
  - Estimate $|\psi_1\rangle$.
  - Pick at random an initial state $|\phi_0\rangle$, orthogonalize with respect to $|\psi_1\rangle$: $|\phi_0\rangle \to |\phi_0\rangle - \langle\phi_0|\psi_1\rangle\,|\psi_1\rangle$ and normalize: $|\phi_0\rangle \to |\phi_0\rangle \,/\sqrt{\langle\phi_0|\phi_0\rangle}$.
  - Iterate $|\phi_{k+1}\rangle = \hat{H}'\,|\phi_k\rangle$, orthogonalize: $|\phi_{k+1}\rangle \to |\phi_{k+1}\rangle - \langle\phi_{k+1}|\psi_1\rangle\,|\psi_1\rangle$ and normalize: $|\phi_{k+1}\rangle \to |\phi_{k+1}\rangle \,/\sqrt{\langle\phi_{k+1}|\phi_{k+1}\rangle}$.
- Comments:
  - Convergence of the method is slow if $\frac{E_2}{E_1} \approx 1$.
  - If the largest energy is degenerated, $E_1 = E_2$, still $\lim_{k\to\infty} \langle\phi_k|\hat{H}'\phi_k\rangle = E_1 = E_2$, however, $\lim_{k\to\infty} |\phi_k\rangle = \frac{a_1|\psi_1\rangle + a_2|\psi_2\rangle}{\|a_1|\psi_1\rangle + a_2|\psi_2\rangle\|}$

Excursus: Google PageRank

- PageRank is an algorithm used by Google Search to rank websites in their search engine results.
- PageRank is a way of measuring the importance of website pages.
- The PageRank algorithm assign to every web pages i an relative importance r_i, called PageRank, and the dimension of $\mathbf{r} = (r_i, \ldots, r_N)$ is the number of World Wide Web pages $N \approx 47 \cdot 10^9$.
- The PageRank algorithm interprets WWW as a directed graph: web pages (vertices) are connected by links (edges), which point from one to another page.
- Every page is characterized by the number of incoming I_i and outgoing links O_i.

Excursus: Google PageRank

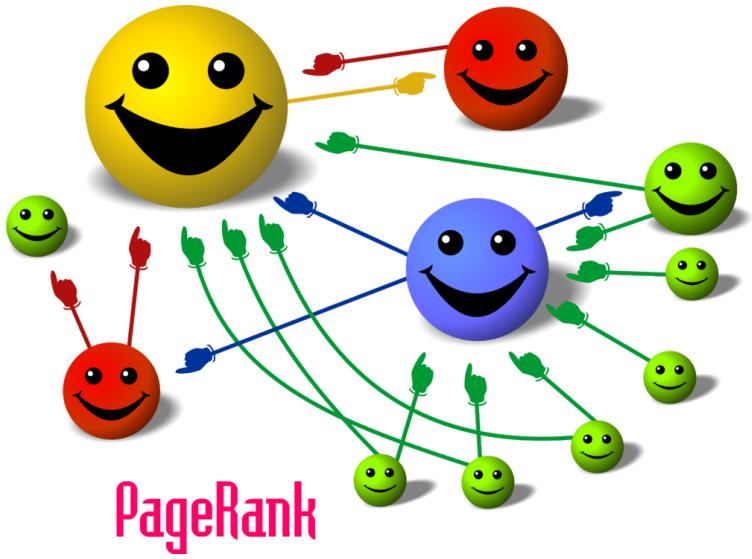


Figure 7: Cartoon illustrating the basic principle of PageRank. The size of each face is proportional to the total size of the other faces which are pointing to it.

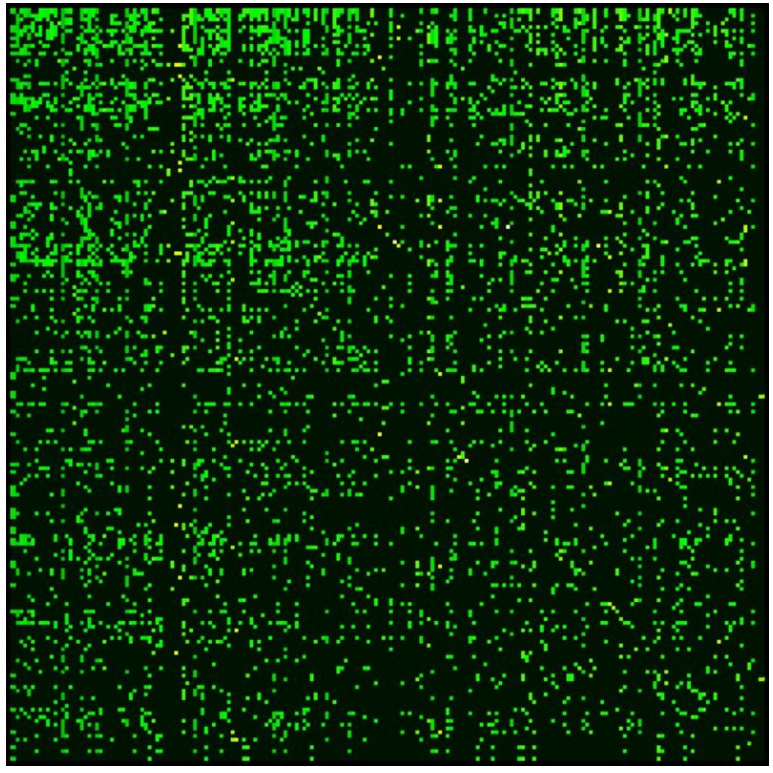


Figure 8: Google matrix of Wikipedia articles network, written in the bases of PageRank index; fragment of top 200×200 matrix elements is shown, total size $N = 3282257$.

Excursus: Google PageRank

- The equation for the PageRank is based on two assumptions:
  - Every page i evenly distribute its PageRank r_i on all O_i outgoing links.
  - The PageRank of page i is the sum of all incoming PageRank's.
- So, the equation is as follows:

$$r_i = \sum_{j \in M_i} \frac{r_j}{O_j}, \tag{72}$$

  where M_i is the set of pages that points to i.
- The adjacency matrix (or connection matrix) is defined as

$$C_{ij} = \begin{cases} 1 & \text{if } j \text{ points to } i \\ 0 & \text{else} \end{cases} \tag{73}$$

  and the number of outgoing links is $O_j = \sum_{i=1}^{N} C_{ij}$.

Excursus: Google PageRank

- The equation for the PageRank can be rewritten as

$$r_i = \sum_{j=1}^{N} \frac{C_{ij}}{O_j} r_j = \sum_{j=1}^{N} \frac{C_{ij}}{\sum_{k=1}^{N} C_{kj}} r_j = \sum_{j=1}^{N} G_{ij} r_j \tag{74}$$

- It means that PageRank vector $\mathbf{r}$ is the eigenvector of the Google matrix $\mathbf{G}$ corresponding to the eigenvalue 1:

$$\mathbf{G} \cdot \mathbf{r} = 1 \cdot \mathbf{r}. \tag{75}$$

- Google matrix $\mathbf{G}$ is high-dimensional ($N^2 \approx 2.2 \cdot 10^{21}$) and $\mathbf{r}$ can be found effectively with the power method, i.e., we iterate

$$\mathbf{r}_{n+1} = \frac{\mathbf{G} \cdot \mathbf{r}_n}{\|\mathbf{G} \cdot \mathbf{r}_n\|} \tag{76}$$

  till convergence.

Excursus: Google PageRank

- The Perron–Frobenius theorem resolves the issue of convergence (or existence of a solution):
  - If all $G_{ij} > 0$, then the largest eigenvalue λ_1 is real, positive and not degenerated. The entries of the corresponding eigenvector $\mathbf{r}$ are all positiv, i.e., $r_i > 0$.
  - If $\mathbf{G}$ is a stochastic matrix ($G_{ij} > 0$ and $\sum_{i=1}^{N} G_{ij} = 1$), then $\lambda_1 = 1$.
- If $\mathbf{G}$ is a stochastic matrix:
  - Power method converges to the eigenvector $\mathbf{r}$ corresponding to eigenvalue $\lambda = 1$.
  - The entries of $\mathbf{r}$ are all positiv and $\mathbf{r}$ can be normalized such that $\sum_i r_i = 1$.
  - r_i can be viewed as a probability distribution that a random surfer arrives at page i.
  - $\mathbf{r}$ can be interpreted as a stationary probability distribution of a Markov chain with transition probabilities G_{ij} from state i to state j.

Excursus: Google PageRank

- It is $\sum_{i=1}^{N} G_{ij} = 1$, however, $\mathbf{G}$ is not a stochastic matrix so far, because $G_{ij} > 0$ is not fulfilled, which means that every page is linked to every other page in the web.
- Power iteration may not converge if dangling nodes ($O_i = 0$) and loops exists.
- The problem can be fixed if we allow the surfer to jump randomly on any page with probability $1 - p$ and to follow the transition matix $\frac{C_{ij}}{\sum_{k=1}^{N} C_{kj}}$ with probability p.
- The modified Google matrix

$$G_{ij} = p\frac{C_{ij}}{\sum_{k=1}^{N} C_{kj}} + \frac{(1-p)}{N} \tag{77}$$

  is a stochastic matrix, because $G_{ij} > 0$ for all links (i, j). Google uses $p = 0.85$.

Lanczos algorithm

- The Lanczos method is an iterative algorithm that transforms the eigendecomposition problem for a symmetric matrix $\mathbf{H} \in \mathbb{R}^{N \times N}$ into the eigendecomposition problem for a smaller tridiagonal symmetric matrix $\mathbf{T} \in \mathbb{R}^{m \times m}$, where $m \ll N$.
- Lanczos method is based on invariant subspace.
- Consider a subspace $\mathcal{Q} = \text{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_m\}$ spanned by $m \leq N$ linearly independent vectors $\mathbf{q}_i \in \mathbb{R}^N$.
- Assume that $\{\mathbf{q}_1, \ldots, \mathbf{q}_m\}$ is an orthonormal basis of $\mathcal{Q}$ and define a matrix

$$\mathbf{Q} = (\mathbf{q}_1, \ldots, \mathbf{q}_m) \in \mathbb{R}^{m \times N}. \tag{78}$$

- Assume that the subspace $\mathcal{Q}$ is invariant under $\mathbf{H}$, i.e.,

$$\forall \mathbf{q} \in \mathcal{Q} : \mathbf{H}\mathbf{q} \in \mathcal{Q}. \tag{79}$$

Lanczos algorithm

- Because $\mathcal{Q}$ is an invariant subspace, $\mathbf{H}\mathbf{q}_i$ can be writen as a linear combination of $\{\mathbf{q}_1, \ldots, \mathbf{q}_m\}$ or in other words, for $i = 1, \ldots, m$ it is

$$\mathbf{H}\mathbf{q}_i = \sum_{j=1}^{m} \mathbf{q}_j T_{ji} \tag{80}$$

- Or in matrix form: for matrix $\mathbf{HQ} \in \mathbb{R}^{m \times N}$ there is a matrix $\mathbf{T} \in \mathbb{R}^{m \times m}$ such that

$$\mathbf{HQ} = \mathbf{QT} \quad \text{or} \quad \mathbf{T} = \mathbf{Q}^{-1}\mathbf{HQ}, \tag{81}$$

- Because $\mathbf{Q}$ is a matrix with orthonormal columns, i.e., $\mathbf{Q}^T\mathbf{Q} = \mathbb{1}$, it is

$$\mathbf{T} = \mathbf{Q}^T\mathbf{HQ}, \tag{82}$$

Lanczos algorithm

- $\mathbf{H}$ is a symmetric matrix, hence $\mathbf{T}$ is symmetric, too, and there exist eigenpairs, $\lambda_1, \ldots, \lambda_m$ and $\mathbf{y}_1, \ldots, \mathbf{y}_m$, such that

$$\lambda_i \mathbf{y}_i = \mathbf{T}\mathbf{y}_i \tag{83}$$

- If λ_i is an eigenvalue of $\mathbf{T}$ then it is also an eigenvalue of $\mathbf{H}$, because

$$\lambda_i \left(\mathbf{Q}\mathbf{y}_i\right) = \mathbf{Q}\mathbf{T}\mathbf{y}_i = \mathbf{H}\left(\mathbf{Q}\mathbf{y}_i\right), \tag{84}$$

  and $\mathbf{Q}\mathbf{y}_i$ is the corresponding eigenvector of $\mathbf{H}$.

Résumé: Eigenpairs of large matrix $\mathbf{H}$ can be estimated from a smaller matrix $\mathbf{T}$, if the space spanned by $\mathcal{Q}$ is invariant under $\mathbf{H}$.

Lanczos algorithm

- The Lanczos method generates an invariant subspace approximately. It uses the Krylov subspace defined as

$$\begin{aligned} \mathcal{K}^m(\mathbf{b}, \mathbf{H}) &= \text{span}\left\{\mathbf{b}, \mathbf{H}\mathbf{b}, \ldots, \mathbf{H}^{m-1}\mathbf{b}\right\} \\ &= \text{span}\left\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_m\right\}, \end{aligned}$$

  where $\mathbf{b}$ is some random vector.
- The subspace $\mathcal{K}^m$ consists of a sequence of vectors generated by the power method.
- $\mathbf{H}^i\mathbf{b}$ converge to the direction of the eigenvector corresponding to the largest eigenvalue of $\mathbf{H}$.
- The vectors $\mathbf{H}\mathbf{b}_1, \mathbf{H}\mathbf{b}_2, \ldots, \mathbf{H}\mathbf{b}_{m-1}, \mathbf{H}\mathbf{b}_m$ are in $\mathcal{K}^m$, except for the last vector $\mathbf{H}\mathbf{b}_m = \mathbf{H}^m\mathbf{b}$.
- For sufficiently large m, $\mathbf{H}^m\mathbf{b}$ is approximately proportional to $\mathbf{H}^{m-1}\mathbf{b}$ and $\mathbf{H}^m\mathbf{b}$ is almost in $\mathcal{K}^m$.
- The Krylov space $\mathcal{K}^m$ for $m < N$ is almost an invariant subspace of $\mathbf{H}$, which contains the ground-state of $\mathbf{H}$.

Lanczos algorithm

- Ground-state of $\mathbf{H}$ can be estimated from the diagonalisation of the smaller matrix $\mathbf{T}$.
- It follows from the selection of $\mathcal{K}^m$ that:
  - The matrix $\mathbf{T} = \mathbf{Q}^T\mathbf{H}\mathbf{Q}$ is symmetric tridiagonal (easy to diagonalize).
  - A three term recursion relation exists for the calculation of $\mathbf{Q}$.
  - $\mathbf{H}$ is needed only to compute matrix-vector multiplication.
  - The convergence is fast. Typically, we need only $m = 10^2$ even for a matrix with $N \approx 10^7$.
- How does this properties lead to a practical algorithm?
- Consider a symmetric tridiagonal matrix

$$\mathbf{T} = \begin{pmatrix} a_1 & b_1 & \cdots & 0 \\ b_1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & b_{m-1} \\ 0 & \cdots & b_{m-1} & a_m \end{pmatrix}, \tag{85}$$

with entries a_i and b_i.

Lanczos algorithm

- If we equate the columns of $\mathbf{HQ} = \mathbf{QT}$, we obtain a three term recursion relation

$$\mathbf{H}\mathbf{q}_j = b_{j-1}\mathbf{q}_{j-1} + a_j\mathbf{q}_j + b_j\mathbf{q}_{j+1} \tag{86}$$

  for $j = 1, \ldots, m-1$, where $\mathbf{q}_j$ is the jth column of $\mathbf{Q}$.
- It is convenient to rearrange the recursion relation as

$$\mathbf{r}_j := b_j\mathbf{q}_{j+1} = \mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1} - a_j\mathbf{q}_j, \tag{87}$$

  and to define a new unknown vector $\mathbf{r}_j$.
- The aim of Lanczos algorithm is to generate orthonormal basis $\{\mathbf{q}_1, \ldots, \mathbf{q}_m\}$ of $\mathcal{K}^m$.
- We postulate orthogonality of $\mathbf{q}_{j+1} \perp \mathbf{q}_j, \mathbf{q}_{j-1}$, as a results we obtain that

$$a_j = \mathbf{q}_j^T\mathbf{H}\mathbf{q}_j \tag{88}$$

  and

$$b_{j-1} = \mathbf{q}_{j-1}^T\mathbf{H}\mathbf{q}_j = \mathbf{q}_j^T\mathbf{H}\mathbf{q}_{j-1}, \tag{89}$$

  where the last identity follows from the fact that $\mathbf{H} = \mathbf{H}^T$.

Lanczos algorithm

- From the normalization condition $\|\mathbf{q}_{j+1}\| = 1$ it follows that

$$b_j = \|\mathbf{r}_j\| = \|\mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1} - a_j\mathbf{q}_j\| \tag{90}$$

- Proof of $\mathbf{q}_{j+1} \perp \mathbf{q}_j, \mathbf{q}_{j-1}$:
  - Assume $\{\mathbf{q}_1, \ldots \mathbf{q}_j\}$ is an orthonormal basis.
  - It is $\mathbf{q}_{j+1} \perp \mathbf{q}_j$ due to

$$\begin{aligned} b_j\mathbf{q}_j^T\mathbf{q}_{j+1} &= \mathbf{q}_j^T\mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_j^T\mathbf{q}_{j-1} - a_j\mathbf{q}_j^T\mathbf{q}_j \\ &= a_j - 0 - a_j = 0 \end{aligned}$$

  - It is $\mathbf{q}_{j+1} \perp \mathbf{q}_{j-1}$ due to

$$\begin{aligned} b_j\mathbf{q}_{j-1}^T\mathbf{q}_{j+1} &= \mathbf{q}_{j-1}^T\mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1}^T\mathbf{q}_{j-1} - a_j\mathbf{q}_{j-1}^T\mathbf{q}_j \\ &= b_{j-1} - b_{j-1} - 0 = 0 \end{aligned}$$

- Proof of $\|\mathbf{q}_{j+1}\| = 1$:
  - It is $\|\mathbf{q}_{j+1}\| = 1$ due to

$$\mathbf{q}_{j+1} = \frac{\mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1} - a_j\mathbf{q}_j}{\|\mathbf{H}\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1} - a_j\mathbf{q}_j\|} \tag{91}$$

Lanczos algorithm

- Lanczos algorithm is based on successive Gram-Schmidt orthogonalization of $\mathbf{H}\mathbf{q}_j$ against $\mathbf{q}_j$ and $\mathbf{q}_{j-1}$.
- Choose a random vector $\mathbf{q}_1$ such that $\|\mathbf{q}_1\| = 1$.
- $\mathbf{r}_1 = \mathbf{H}\mathbf{q}_1 - (\mathbf{q}_1^T \mathbf{H}\mathbf{q}_1)\mathbf{q}_1 = \mathbf{H}\mathbf{q}_1 - a_1\mathbf{q}_1$
  and $\mathbf{q}_2 = \mathbf{r}_1/\|\mathbf{r}_1\| = \mathbf{r}_1/b_1$
  $\Rightarrow \mathbf{q}_2 \perp \mathbf{q}_1$
- $\mathbf{r}_2 = \mathbf{H}\mathbf{q}_2 - (\mathbf{q}_2^T \mathbf{H}\mathbf{q}_2)\mathbf{q}_2 - (\mathbf{q}_1^T \mathbf{H}\mathbf{q}_2)\mathbf{q}_1 = \mathbf{H}\mathbf{q}_2 - a_2\mathbf{q}_2 - b_1\mathbf{q}_1$
  and $\mathbf{q}_3 = \mathbf{r}_2/\|\mathbf{r}_2\| = \mathbf{r}_2/b_2$
  $\Rightarrow \mathbf{q}_3 \perp \mathbf{q}_2, \mathbf{q}_1$
- $\vdots$
- $\mathbf{r}_j = \mathbf{H}\mathbf{q}_j - (\mathbf{q}_j^T \mathbf{H}\mathbf{q}_j)\mathbf{q}_j - (\mathbf{q}_{j-1}^T \mathbf{H}\mathbf{q}_j)\mathbf{q}_{j-1} = \mathbf{H}\mathbf{q}_j - a_j\mathbf{q}_j - b_{j-1}\mathbf{q}_{j-1}$
  and $\mathbf{q}_{j+1} = \mathbf{r}_j/\|\mathbf{r}_j\| = \mathbf{r}_j/b_j$
  $\Rightarrow \mathbf{q}_{j+1} \perp \mathbf{q}_j, \mathbf{q}_{j-1}$

Lanczos algorithm

- Furthermore, $\mathbf{q}_{j+1} \perp \mathbf{q}_i$ for $i < j-1$, because

$$\begin{aligned} \mathbf{q}_i \mathbf{q}_{j+1} &= \mathbf{q}_i^T \mathbf{H} \mathbf{q}_j - a_j \mathbf{q}_i^T \mathbf{q}_j - b_{j-1} \mathbf{q}_i^T \mathbf{q}_{j-1} \\ &= \mathbf{q}_i^T \mathbf{H} \mathbf{q}_j - 0 - 0 \\ &= \mathbf{q}_j^T \mathbf{H} \mathbf{q}_i = 0, \end{aligned}$$

  where in the last step we used $\mathbf{H} = \mathbf{H}^T$ and

$$\mathbf{H}\mathbf{q}_i \in \text{span}\left\{\mathbf{q}, \ldots, \mathbf{H}^{j-2}\mathbf{q}\right\} = \text{span}\left\{\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}\right\} \qquad (92)$$

  for $i < j-1$, such that $\mathbf{q}_j \perp \text{span}\left\{\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}\right\}$.
- It is $\mathbf{T} = \mathbf{Q}^T \mathbf{H} \mathbf{Q}$ or $T_{ij} = \mathbf{q}_i^T \mathbf{H} \mathbf{q}_j$. Since $\mathbf{H}$ is symmetic, $\mathbf{T}$ is symmetic. From the above argumentation it follows that $T_{ij} = 0$ for $i < j-1$, and similar arguments lead to $T_{ij} = 0$ for $i > j+1$. Therefore, $\mathbf{T}$ is tridiagonal.

Lanczos algorithm

- Basic Lanczos algorithm for the computation of an orthonormal basis for of the Krylov space $\mathcal{K}^m$.
- Let $\mathbf{H} \in \mathbb{R}^{N \times N}$ be a symmetic (or Hermitan) matrix. This algorithm computes the tridiagonal matrix $\mathbf{T}$ and an orthonormal basis $\mathbf{Q}_m = (\mathbf{q}_1, \ldots, \mathbf{q}_m)$ for $\mathcal{K}^m$, where m is the smallest index such that $\mathcal{K}^m = \mathcal{K}^{m+1}$.
- Pseudocode:
  - Pick a random $\mathbf{q}$ such that $\|\mathbf{q}\| = 1$;
  - $\mathbf{Q}_1 = (\mathbf{q})$;
  - $\mathbf{r} = \mathbf{H}\mathbf{q}$; $a_1 = \mathbf{q}^T\mathbf{r}$; $\mathbf{r} = \mathbf{r} - a_1\mathbf{q}$; $b_1 = \|\mathbf{r}\|$;
  - for $j = 2, 3, \ldots$ do
  - $\mathbf{w} = \mathbf{q}$; $\mathbf{q} = \mathbf{r}/b_{j-1}$; $\mathbf{Q}_j = (\mathbf{Q}_{j-1}, \mathbf{q})$;
  - $\mathbf{r} = \mathbf{H}\mathbf{q} - b_{j-1}\mathbf{w}$; $a_j = \mathbf{q}^T\mathbf{r}$;
  - $\mathbf{r} = \mathbf{r} - a_j\mathbf{q}$; $b_j = \|\mathbf{r}\|$;
  - if $b_j = 0$ then
  - return $\mathbf{Q}_j$; $a_1, \ldots, a_j$; $b_1, \ldots, b_{j-1}$;
  - end if
  - end for

Lanczos algorithm

- The termination condition $b_j = 0$ (or $\mathbf{r}_j = 0$) for some $j < N$ implies that,

$$\mathbf{H}\mathbf{q}_j = (\mathbf{q}_j^T \mathbf{H}\mathbf{q}_j)\mathbf{q}_j + (\mathbf{q}_{j-1}^T \mathbf{H}\mathbf{q}_j)\mathbf{q}_{j-1} = a_j \mathbf{q}_j + b_{j-1}\mathbf{q}_{j-1}, \quad (93)$$

  thus $\mathbf{H}\mathbf{q}_j$ is a linear combination of $\{\mathbf{q}_1, \ldots, \mathbf{q}_j\}$ and $\mathbf{H}\mathbf{q}_j$ is within an invariant subspace

$$\begin{aligned} \mathcal{K}^j &= \text{span}\,\{\mathbf{q}_1, \mathbf{H}\mathbf{q}_1, \ldots, \mathbf{H}^{j-1}\mathbf{q}_1\} && (94) \\ &= \text{span}\,\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_j\}. && (95) \end{aligned}$$

- The termination condition $b_j = 0$ for some j implies the loss of orthogonality, i.e., it is not possible to orthogonalize $\mathbf{H}\mathbf{q}_j$ against $\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_j\}$.

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