The Monte Carlo method in/and statistical physics

Lattice simulations of quantum fields, Orsay–Bielefeld

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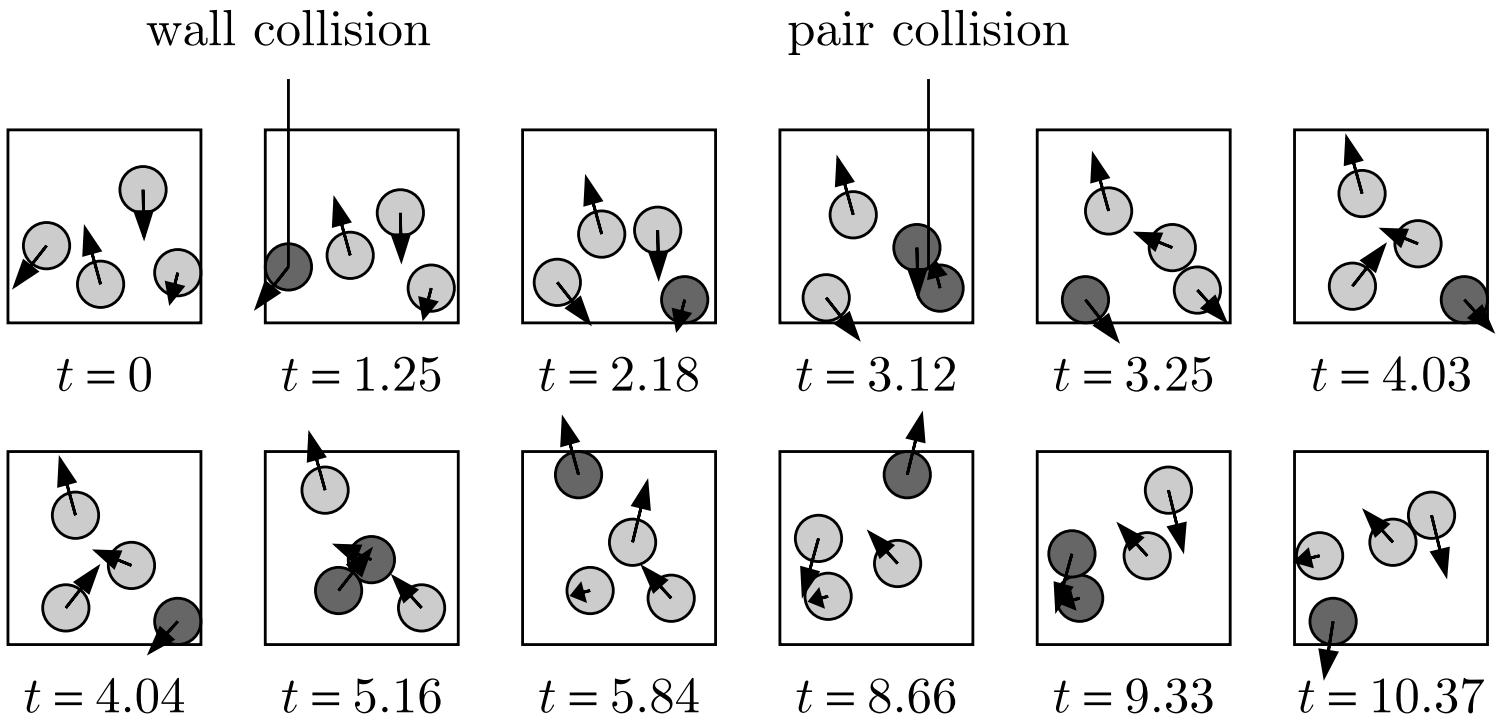
Molecular dynamics ('Newton')

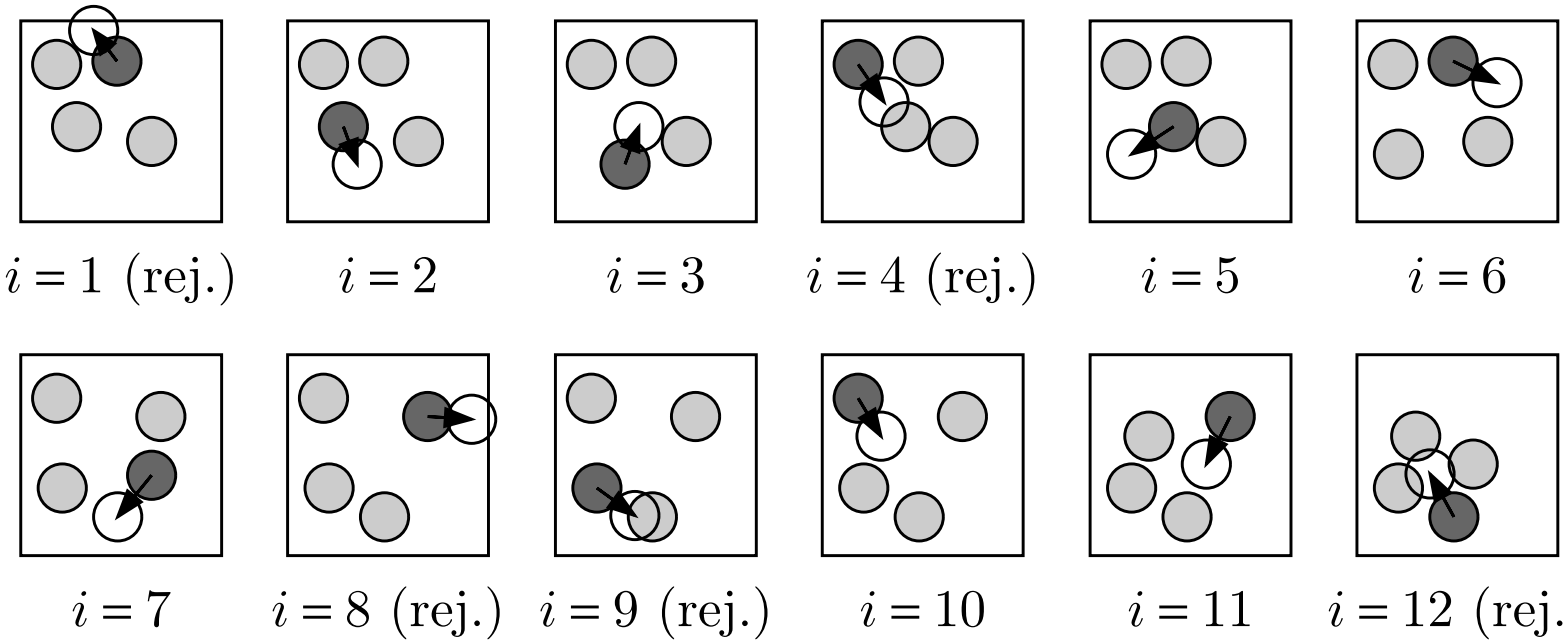
- A molecular dynamics algorithm for hard spheres (billiard):



- . . . starting point of Molecular dynamics, in 1957 . . .
- . . . treats positions and velocities . . .
- . . . useful for $N \gg 4$ . . .
- . . . converges towards thermal equilibrium.

Markov-chain Monte Carlo ('Boltzmann')

- A local Markov-chain Monte Carlo algorithm for hard spheres (billiard):

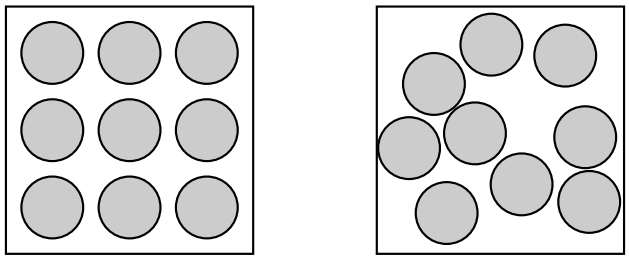


- . . . starting point of Markov chain Monte Carlo, in 1953 . . .
- . . . treats only positions . . .
- . . . useful for $N \gg 4$ . . .
- . . . converges towards thermal equilibrium.

‘Equilibrium’ means for hard spheres . . . I

1. For $t \to \infty$, the equiprobability principle holds:

$$\pi(\mathbf{x}_1, , \ldots, \mathbf{x}_N) = \begin{cases} 1 & \text{if configuration legal} \\ 0 & \text{otherwise} \end{cases} .$$



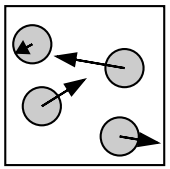
a b

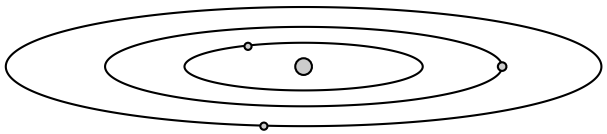
2. Applies to molecular dynamics and to Monte Carlo.
3. For $t \to \infty$, configurations $\mathbf{x}_t$ independent of initial condition.

‘Equilibrium’ means for hard spheres . . . II

1. The equiprobability principle is the # 1 axiom of statistical physics.
2. Trivially OK for Monte Carlo (detailed balance, ergodicity).
3. It rigorously holds for molecular dynamics of hard disks, but proof is non-trivial and very recent:
   - Sinai (1970) (52 pages, two disks),
   - Simanyi (2003) (55 pages, *N* disks),

   (Boltzmann–Sinai ergodicity).
4. OK for 4 disks, but not for small planets + sun (KAM):





Exercises I

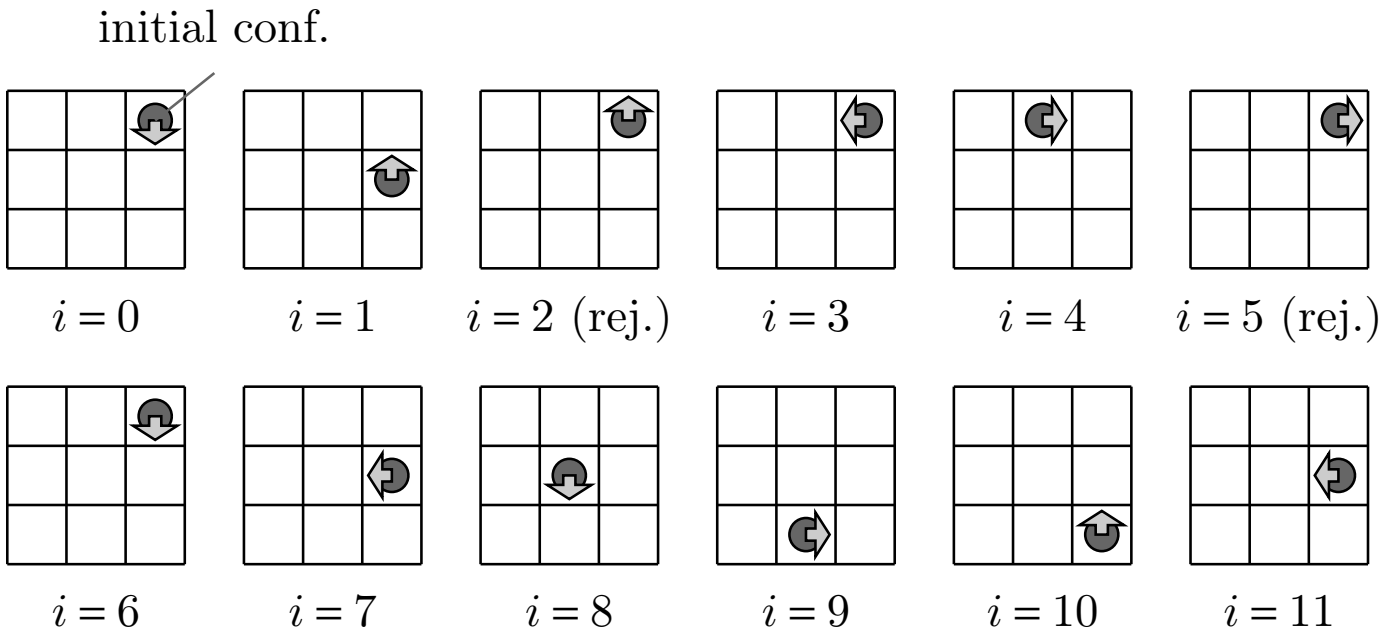
- Hard-sphere direct sampling (Alg. `direct-disks`)
- Hard-sphere Markov-chain sampling (Alg. `markov-disks`)
- miscellaneous questions on ergodicity, detailed balance, sampling . . .

Approach to ‘Equilibrium’

We must better understand convergence issues and the approach towards equilibrium...

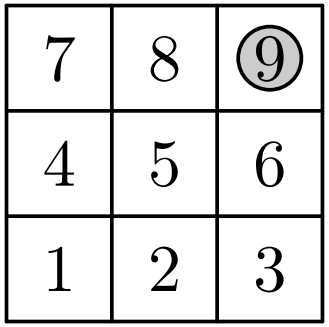
Single discrete hard sphere ('3 $\times$ 3 pebble game')

- Monte Carlo algorithm for one hard disk on a lattice:



- Move 'up', 'down', 'left', 'right', each with probability $1/4$.
- Reject moves if necessary ($i = 2$, $i = 5$).

Approach of equilibrium in the 3×3 pebble game



(numbering scheme on a lattice)

- A Monte Carlo simulation that starts in the upper right corner (site 9) at iteration $i = 0$ approaches thermal equilibrium for $t \to \infty$ (all sites equally probable).
- The transfer matrix allows us to understand this much better.

Transfer matrix of 3×3 pebble game

- Transfer matrix of algorithmic probabilities $p(a \to b)$:

$$\{p(a \to b)\} = \begin{bmatrix}
\boxed{\frac{1}{2}} & \frac{1}{4} & . & \frac{1}{4} & . & . & . & . & . \\
\frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} & . & \frac{1}{4} & . & . & . & . \\
. & \frac{1}{4} & \boxed{\frac{1}{2}} & . & . & \frac{1}{4} & . & . & . \\
\frac{1}{4} & . & . & \boxed{\frac{1}{4}} & \frac{1}{4} & . & \frac{1}{4} & . & . \\
. & \frac{1}{4} & . & \frac{1}{4} & \boxed{0} & \frac{1}{4} & . & \frac{1}{4} & . \\
. & . & \frac{1}{4} & . & \frac{1}{4} & \boxed{\frac{1}{4}} & . & . & \frac{1}{4} \\
. & . & . & \frac{1}{4} & . & . & \boxed{\frac{1}{2}} & \frac{1}{4} & \\
. & . & . & . & \frac{1}{4} & . & \frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} \\
. & . & . & . & . & \frac{1}{4} & . & \frac{1}{4} & \boxed{\frac{1}{2}}
\end{bmatrix}.$$

- $\{\pi(1), \ldots, \pi(9)\} = \{\frac{1}{9}, \ldots, \frac{1}{9}\}$ is eigenvector.

Transfer matrix of 3×3 pebble game (cont...)

- Probability vector for initial state (iteration $i = 0$):

$$\{\pi^0(1), \ldots, \pi^0(9)\} = \{0, \ldots, 0, 1\}.$$

- Probability at iteration $i + 1$ from probability at iteration i:

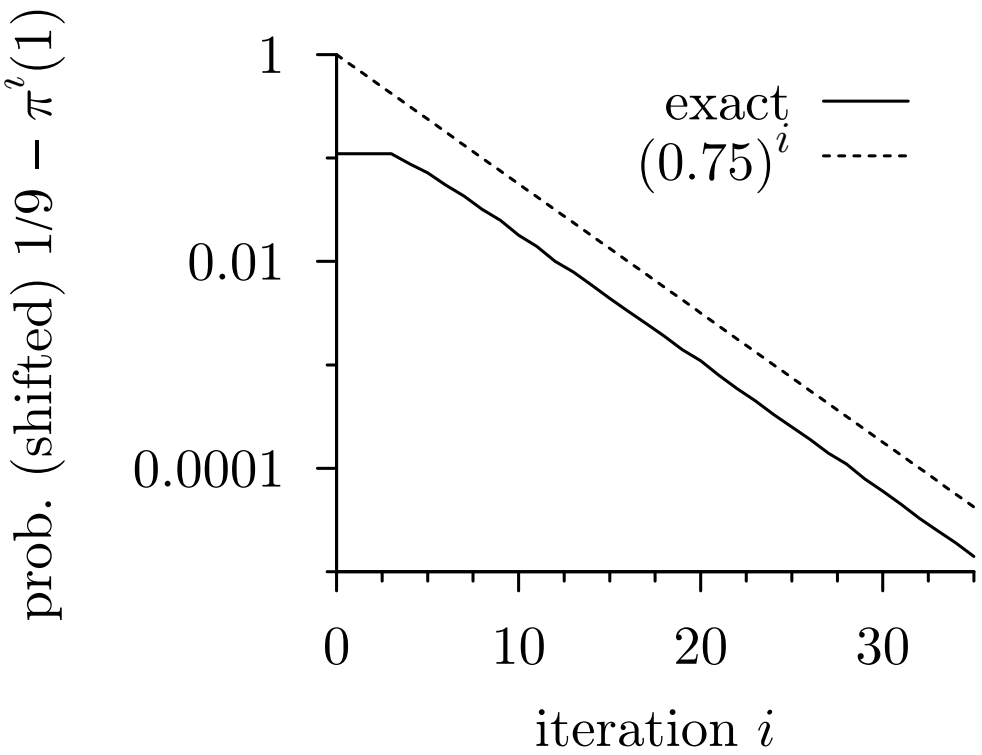
$$\pi^{i+1}(a) = \sum_{b=1}^{9} p(b \to a)\pi^i(b).$$

- Eigenvectors and eigenvalues:

$$\{\pi^i(1), \ldots, \pi^i(9)\} = \underbrace{\{\tfrac{1}{9}, \ldots, \tfrac{1}{9}\}}_{\substack{\text{first eigenvector} \\ \text{eigenvalue } \lambda_1 = 1}} + \alpha_2 (0.75)^i \underbrace{\{-0.21, \ldots, 0.21\}}_{\substack{\text{second eigenvector} \\ \text{eigenvalue } \lambda_2 = 0.75}} + \ldots.$$

Exponential convergence in the 3×3 pebble game

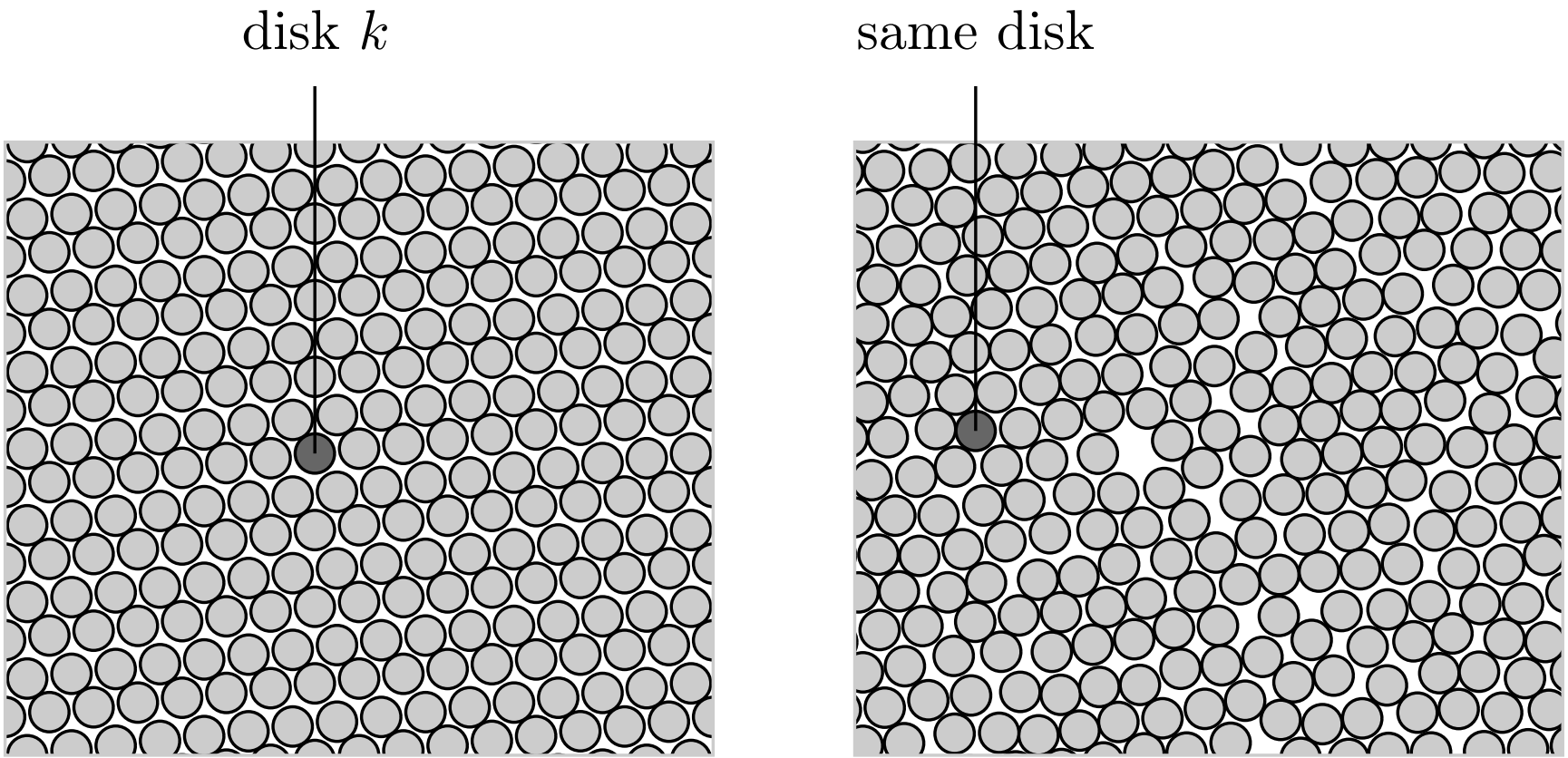
- π^i(site 1) for game started in the right upper corner (site 9):



- Exponential convergence $\equiv$ scale:

$$(0.75)^i = \exp\left[i \cdot \log\ 0.75\right] = \exp\left[-\frac{i}{3.476}\right].$$

Correlation time in larger simulations



- τ exists, but it is large ($\tau \gg 25\,600\,000\,000$).

Minimum running time of a Monte Carlo algorithm

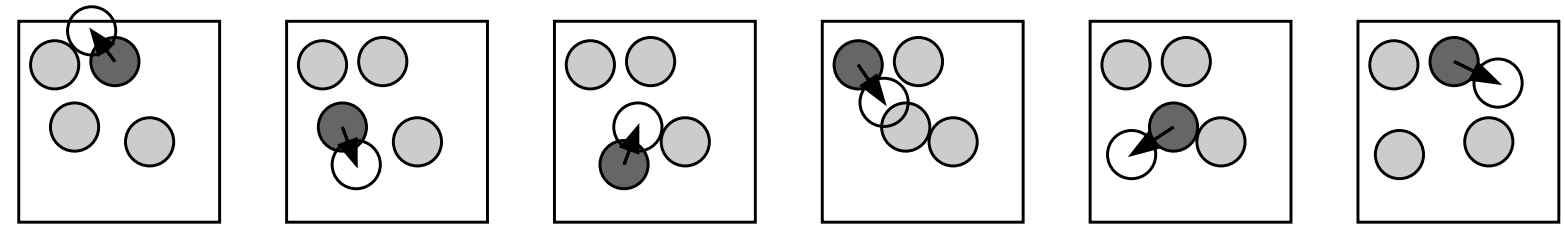
- MC algorithms approach thermal equilibrium (the stationary probability distribution) as $\exp\left[-t/\tau\right]$.
- No need to go to $t \to \infty$ to get one good sample. The condition $t \gg \tau$ (for example, $10 \times \tau$) is enough.
- τ can only be estimated from simulations that run for much longer than τ
- #1 problem.
- Do not confuse with the 'ergodicity problem'.

Monte Carlo $\neq$ Molecular dynamics

- Exponential convergence is a property of statistical physics (Monte Carlo algorithms).
- In hydrodynamics (molecular dynamics), convergence is proven (Simanyi ’03, ’04), but it is power-law rather than exponential.
- This is the fascinating subject of long-time tails (other talk).

The role of rejections

- The local moves in the following example . . .



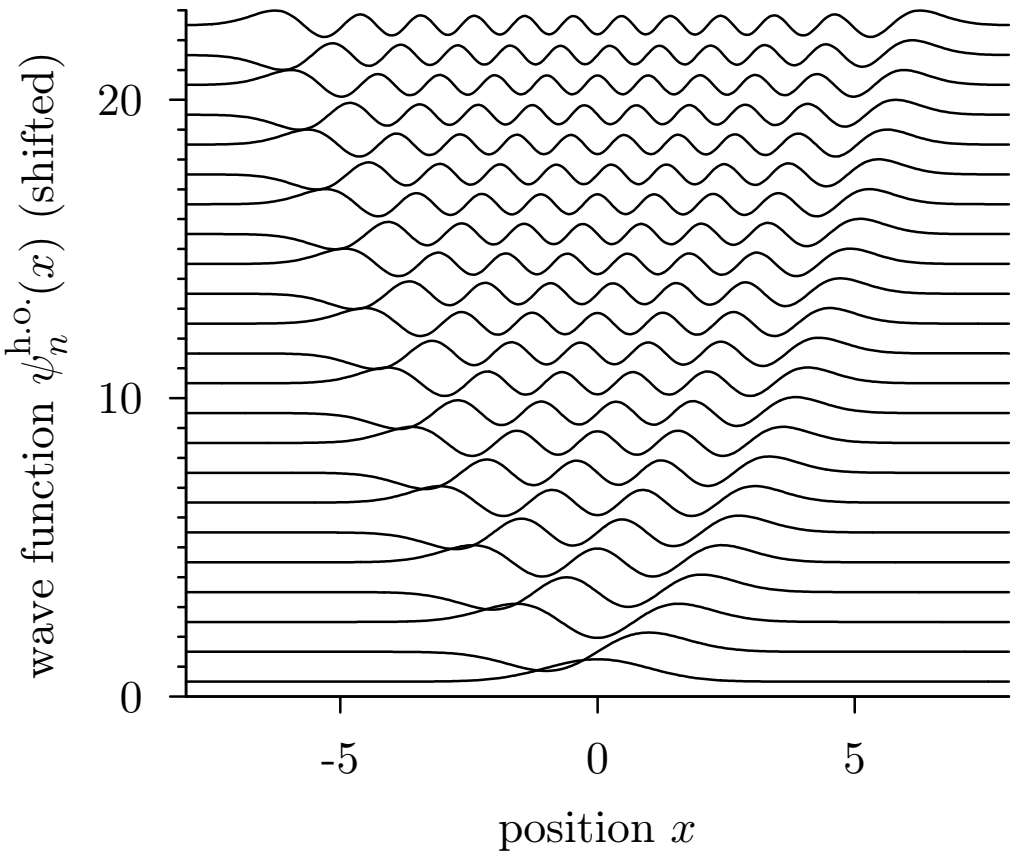
- . . . work best at zero density η . . .
- . . . $[\eta = 0] \Rightarrow [\eta =$ finite] through *rejections* . . .
- . . . this can only work in small boxes, or for small correlation lengths.
- one-half rule determines optimal step size.

Exercises II

The following exercises probe the convergence of direct-sampling methods. This is often difficult enough.

- Sampling difficult integrals (Alg. `direct-gamma`)
- Importance sampling (Alg. `direct-gamma-zeta`)
- Checking for finite *m*th moment of a distribution (Alg. `markov-zeta`)

Quantum system: harmonic oscillator



- $V(x) = \frac{1}{2}x^2$ (harmonic potential).
- Wave functions ψ_n, with energies E_n.
- NB: $\pi(x) \not\propto \exp[-\beta V(x)]$.

Density matrix in Quantum statistical physics

- A quantum system can be in different 'energy levels' ψ_n, with energies E_n.
- The weight of a configuration is given by the density matrix, not the Boltzmann weight:

$$\pi(\mathbf{x}) \propto \underbrace{\rho(\mathbf{x},\mathbf{x},\beta)}_{\text{density matrix}} = \sum_n \underbrace{\exp\left[-\beta E_n\right]}_{\text{stat mech}} \underbrace{\psi_n(\mathbf{x})\psi_n^*(\mathbf{x})}_{\text{quant mech}}.$$

- We can evaluate $\pi(\mathbf{x})$ with path integrals, but also sometimes with other methods.

Convolution of the density matrix

- The density matrix satisfies an exact convolution condition:

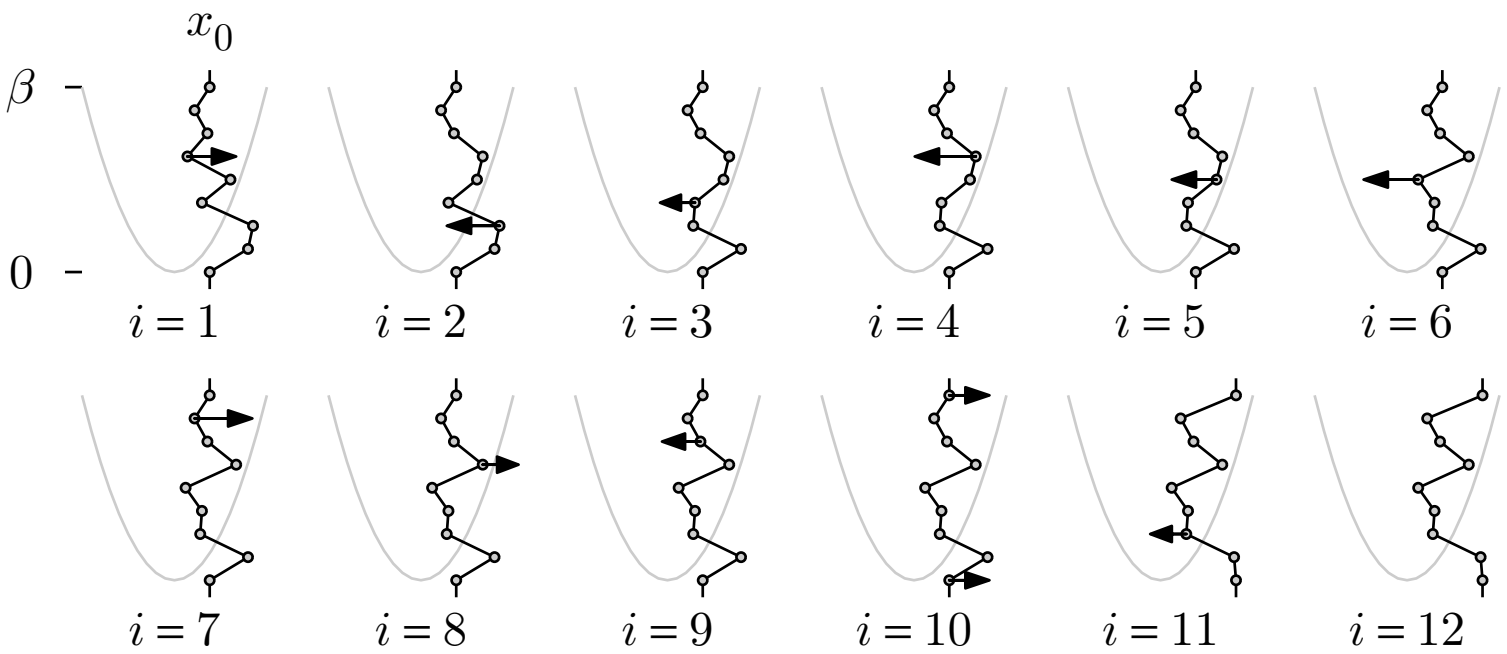
$$\rho(x, x', \beta) = \int \dots \int \mathrm{d}x_1 \ \dots \mathrm{d}x_{N-1} \times \rho(x_0, x_1, \tfrac{\beta}{N}) \dots \rho(x_{N-1}, x_N, \tfrac{\beta}{N}).$$

- $\frac{\beta}{N}$ is small $\Rightarrow$ high temperature ....
- At high temperature, the density matrix is essentially Gaussian.

$$\rho(x, x', \tau = \tfrac{\beta}{N}) \sim e^{-\frac{\tau}{2}V(x)} e^{-\frac{(x-x')^2}{2\tau}} e^{-\frac{\tau}{2}V(x')}$$

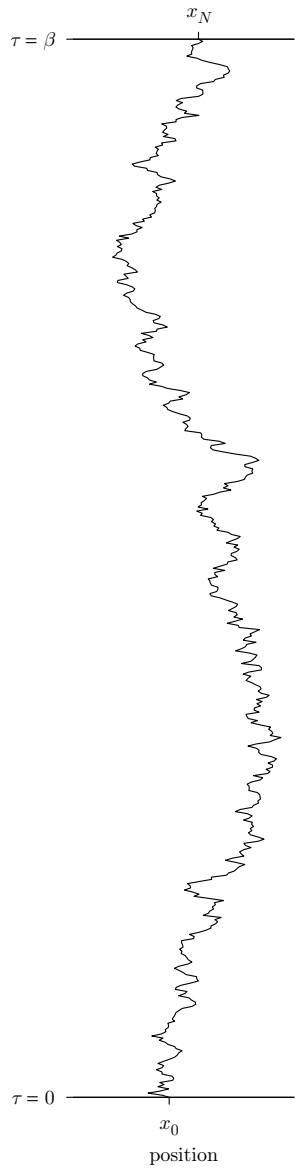
Naive path sampling (schematic)

- Naively sample $\pi(x_0) = \rho(x_0, x_0, \beta)$ through local algorithm:



- Rejections even for free particle.
- correlation time τ is enormous.

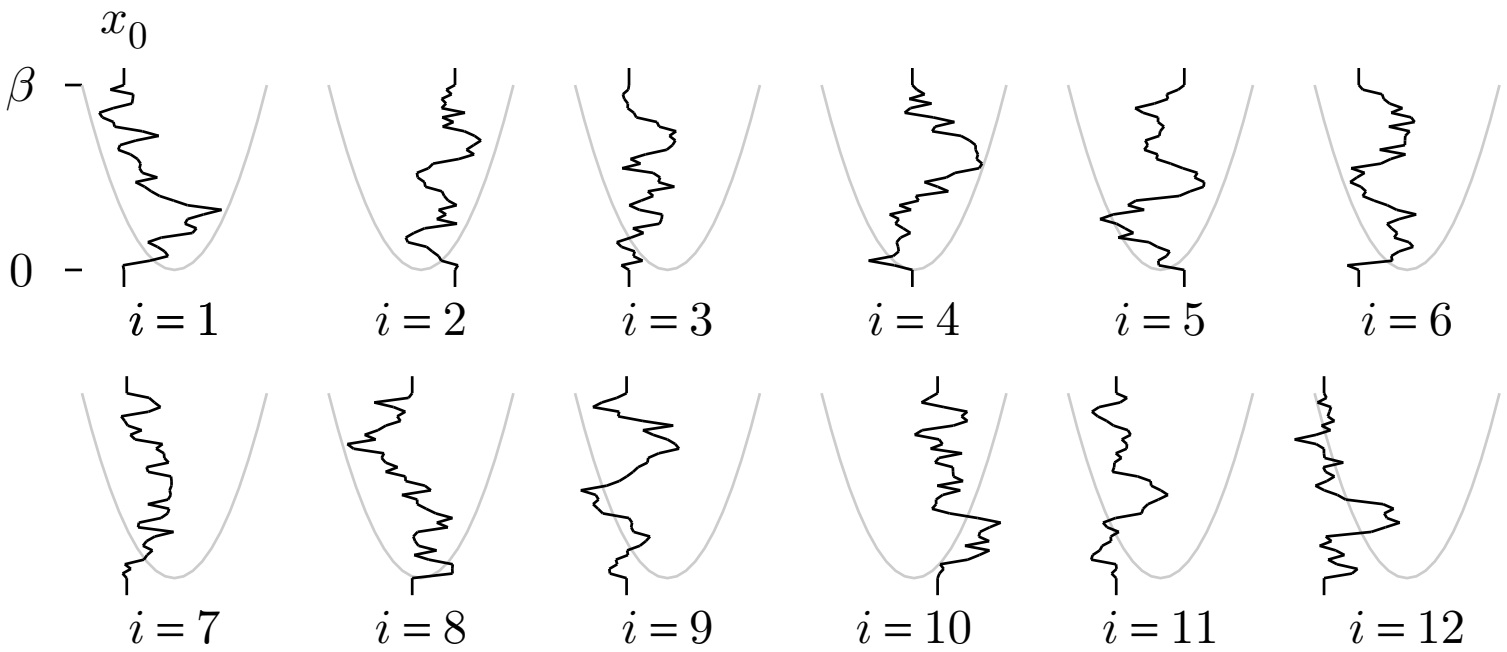
Lévy construction for free quantum particle



- Free path can be sampled without rejections.
- This is the Lévy construction (1940) . . .
- . . . aka Gaussian bridge . . .
- . . . aka stochastic interpolation . . .
- . . . aka free path integral.
- Works also in harmonic external potential.

Lévy construction and interacting quantum systems

- The Lévy construction allows to solve exactly the many-body quantum problem without interactions.
- The corresponding MC algorithm has $\tau = 0$.
- $\tau = 0$ also for free bosons.



- Incorporate interactions through Metropolis algorithm.

Exercises III

- Harmonic density matrix (from Alg. `harmonic-wavefunctions` and Alg. `harmonic-density`)
- Harmonic density matrix (from Alg. `matrix-square`)
- Harmonic density matrix (from Alg. `naive-harmonic-path`)
- Harmonic density matrix (from Alg. `levy-free-path`)
- ...

Conclusion

We discussed Monte Carlo methods in statistical mechanics:

- Equiprobability—Boltzmann distribution.
- Direct sampling – Markov-chain sampling.
- Exponential convergence.
- . . .
- Quantum Monte Carlo.
- Density matrix, matrix squaring
- Path integral
- Lévy construction
- ...

References

- W. Krauth "Statistical Mechanics: Algorithms and Computations" (Oxford University Press, 2006). Wikimedia site **http://www.smac.lps.ens.fr**