# Algorithms and computations in physics (Oxford Lectures 2025)

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Third lecture: 4 February 2025 (version: 3 Februrary 2025)

In this third lecture, we consider Markov-chain sampling in an abstract setting in one dimension. We discuss some theory, but also seven ten-line pseudo-code algorithms, none of them approximate, and all of them as intricate as they are short. At the end, we discuss the foundations of statistical mechanics, as seen in a one-dimensional example.

## Contents



# 2 Markov-chain sampling

## 2.3 Reversible Markov chains

The material in this section is taken from Ref. [2], which presents a dozen of distinct Markov-chain Monte Carlo algorithms to sample the Boltzmann distribution of the anharmonic oscillator. We present two reversible Markov chains (plus a patch) before continuing with two non-reversible algorithms, in Sec. 2.4. In what follows, we consider the probability distribution

$$\pi_{24}(x) = \exp\left(-x^2/2 - x^4/4\right), \tag{2.11}$$

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This distribution (that we already encountered in Lecture 1) has—in principle—a normalization factor, but we will not worry about it. The harmonic part of this distribution is referred to as $\pi_2$ and the quartic term as $\pi_4$.

$$\pi_2(x) = \exp\left(-x^2/2\right), \quad \pi_4(x) = \exp\left(-x^4/4\right). \tag{2.12}$$

### 2.3.1 Metropolis algorithm

Algorithm 2.2 (`metropolis`) implements the symmetric *a priori* probability as a uniform displacement $\Delta = x' - x$ which is as likely as $-\Delta$. The Metropolis filter is implemented with a uniform random number $\Upsilon$ between 0 and 1, which we refer to as a "pebble." For large times $t$, when the initial configuration is forgotten, the algorithm samples $\pi_{24}$. In all the following Markov-chain algorithms, this large $t$ condition is understood.

**procedure** `metropolis`
**input** $x$ (sample at time $t$)
$\Delta \leftarrow \texttt{ran}(-\delta, \delta)$
$x' \leftarrow x + \Delta$
$\Upsilon \leftarrow \texttt{ran}(0, 1)$
**if** $\Upsilon < \min\left[1, \dfrac{\pi_{24}(x')}{\pi_{24}(x)}\right]$**:** $x \leftarrow x'$
**output** $x$ (sample at time $t+1$)
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**Algorithm 2.2:** `metropolis`. Sampling $\pi_{24}$ with the Metropolis algorithm.

### 2.3.2 Factorized Metropolis algorithm

The Metropolis algorithm is really famous, but it is not the end of history. A modern variant is the factorized Metropolis algorithm that we do not discuss here in detail, but only apply to the anharmonic oscillator, where it is written as:

$$\mathcal{P}_{24}^{\text{fact}}(x, x') = \min\left[1, \frac{\pi_2(x')}{\pi_2(x)}\right] \min\left[1, \frac{\pi_4(x')}{\pi_4(x)}\right]. \tag{2.13}$$

The factorized Metropolis algorithm satisfies detailed balance:

$$\begin{aligned} &\pi_{24}(x) P_{24}^{\text{fact}}(x, x') \\ &\propto \underbrace{\pi_2(x) \min\left[1, \frac{\pi_2(x')}{\pi_2(x)}\right]}_{\min[\pi_2(x), \pi_2(x')]:\ x \Leftrightarrow x'} \underbrace{\pi_4(x) \min\left[1, \frac{\pi_4(x')}{\pi_4(x)}\right]}_{\min[\pi_4(x), \pi_4(x')]:\ x \Leftrightarrow x'} \\ &\propto \pi_{24}(x') P_{24}^{\text{fact}}(x', x), \end{aligned} \tag{2.14}$$

where we have dropped the symmetric *a priori* probability $\mathcal{A}$. Algorithm 2.3 (`factor-metropolis`) implements the factorized Metropolis filter: Algorithm 2.3 (`factor-metropolis`) (which is naive) can be patched by replacing its random number $\Upsilon$ by two independent random numbers $\Upsilon_2$ and $\Upsilon_4$, as shown in Alg. 2.4 (`factor-metropolis(patch)`). There, a proposed move is accepted by *consensus* if all the factors accept it. In Alg. 2.4 (`factor-metropolis(patch)`), two independent decisions are taken,[1] one for the harmonic and one for the quartic factor, and the

[1] one can view this as the sampling of two independent Boolean random variables, (see Ref. [6]), of which the final decision is the *conjunction*.

**procedure** `factor-metropolis`
**input** $x$
$\Delta \leftarrow \texttt{ran}(-\delta, \delta)$
$x' \leftarrow x + \Delta$
$\Upsilon \leftarrow \texttt{ran}(0, 1)$
**if** $\Upsilon < \min\left[1, \dfrac{\pi_2(x')}{\pi_2(x)}\right] \min\left[1, \dfrac{\pi_4(x')}{\pi_4(x)}\right]$**:**
  $\{\ x \leftarrow x'$
**output** $x$
——

**Algorithm 2.3:** `factor-metropolis`. Sampling $\pi_{24}$ naively with the factorized Metropolis filter (see Ref. [2]).

proposed move is finally accepted only if it is accepted by both factors. The output is identical to that of Alg. 2.3 (`factor-metropolis`).

**procedure** `factor-metropolis(patch)`
**input** $x$
$\Delta \leftarrow \texttt{ran}(-\delta, \delta)$
$x' \leftarrow x + \Delta$
$\Upsilon_2 \leftarrow \texttt{ran}(0, 1)\,;\ \Upsilon_4 \leftarrow \texttt{ran}(0, 1)$
**if** $\Upsilon_2 < \min\left[1, \dfrac{\pi_2(x')}{\pi_2(x)}\right]$ **and** $\Upsilon_4 < \min\left[1, \dfrac{\pi_4(x')}{\pi_4(x)}\right]$**:**
  $\{\ x \leftarrow x'$   (move accepted by consensus)
**output** $x$
——

**Algorithm 2.4:** `factor-metropolis(patch)`. Patch of Alg. 2.3, implementing the consensus principle (see Ref. [2]).

### 2.3.3 More reversible Markov-chain algorithms . . .

A number of other reversible Markov chains for sampling $\pi_{24}$ are discussed in Ref. [2].

## 2.4 Non-reversible Markov chains

In a tradition that started with the Metropolis algorithm many decades ago, Markov chains are normally designed with the restrictive detailed-balance condition, although they are only required to satisfy global balance. In this section, we illustrate more recent attempts to overcome the detailed-balance condition in a systematic way, within the framework of "lifted" Markov chains. Background and references can be found in [2].

### 2.4.1 Lifting and the zig-zag algorithm

The Metropolis algorithm proposes positive and negative displacements $\Delta$ for the anharmonic oscillator with symmetric *a priori* probabilities (see Alg. 2.2 (`metropolis`)). The filter then imposes that the net flow vanishes, so there will be as many particles going from $x$ to $x + \Delta$ as in the reverse direction, even if, say, $\pi(x) \ll \pi(x + \Delta)$. To break detailed balance and only satisfy global balance, (while keeping $\pi_{24}$ as a stationary distribution), we first suppose that the positions $x$ lie on the grid $\{\dots, -2\Delta, -\Delta, 0, \Delta, 2\Delta, \dots\}$, with moves allowed only between nearest neighbors. Each configuration $x$ is duplicated into a forward-moving one $\{x, +1\}$, and a

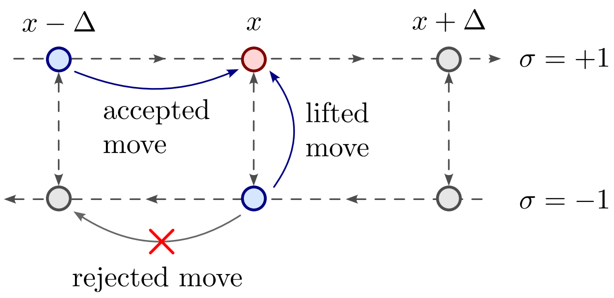


**Figure 2.1:** Discretized lifted Metropolis algorithm for the anharmonic oscillator. The flow into the lifted configuration $\{x,+1\}$ is indicated [see Eq. (2.18)].

backward-moving one $\{x,-1\}$. From a lifted configuration $\{x,\sigma\}$, the lifted Metropolis algorithm proposes only a forward move if $\sigma=1$, and only a backward move if $\sigma=-1$. In summary,

$$P^{\text{lift}}(\{x,\sigma\},\{x+\sigma\Delta,\sigma\}) = \min\left[1, \frac{\pi_{24}(x+\sigma\Delta)}{\pi_{24}(x)}\right], \tag{2.15}$$

where $\sigma=\pm1$. When this move is rejected by the Metropolis filter, the algorithm flips the direction and instead moves from $\{x,\sigma\}$ to $\{x,-\sigma\}$:

$$P^{\text{lift}}(\{x,\sigma\},\{x,-\sigma\}) = 1-\min\left[1, \frac{\pi_{24}(x+\sigma\Delta)}{\pi_{24}(x)}\right]. \tag{2.16}$$

This algorithm clearly violates detailed balance as there is thus no backward flow for $\sigma=+1$ and no forward flow for $\sigma=-1$. On the other hand, the lifted Metropolis algorithm satisfies the global-balance condition with the ansatz

$$\pi_{24}^{\text{lift}}(\{x,\sigma\}) = \frac{1}{2}\pi_{24}(x) \quad \text{for } \sigma=\pm1. \tag{2.17}$$

For example, the flow into the lifted configuration $\{x,+1\}$ satisfies

$$\begin{aligned}&\pi_{24}(\{x,+1\})\\ &= \pi_{24}(\{x-\Delta,+1\})P^{\text{lift}}(\{x-\Delta,+1\},\{x,+1\})\\ &+ \pi_{24}(\{x,-1\})P^{\text{lift}}(\{x,-1\},\{x,+1\}).\end{aligned} \tag{2.18}$$

The two contributions on the right-hand side of Eq. (2.18) correspond on the one hand to the accepted moves from $\{x-\Delta,+1\}$, and on the other hand to the lifted moves from $\{x,-1\}$, when the move from $\{x,-1\}$ toward $\{x-\Delta,-1\}$ is rejected (see Fig. 2.1). Equation (2.18) can be transformed into

$$\begin{aligned}\pi_{24}(x) &= \pi_{24}(x-\Delta)\min\left[1, \frac{\pi_{24}(x)}{\pi_{24}(x-\Delta)}\right]\\ &+ \pi_{24}(x)\left\{1-\min\left[1, \frac{\pi_{24}(x-\Delta\sigma)}{\pi_{24}(x)}\right]\right\},\end{aligned} \tag{2.19}$$

which is identically satisfied. We have shown that the lifted Metropolis algorithm satisfies the global-balance condition for the ansatz of Eq. (2.17), which splits $\pi_{24}(x)$ equally between $\{x,+1\}$ and $\{x,-1\}$. The sequence $\pi^{\{t\}}$ will actually converge to this stationary distribution.

In the lifted Metropolis algorithm, the particle, starting from $x_0=0$, climbs uphill in direction $\sigma$ until a move is rejected by the filter, when it remains at its current position but reverses its velocity to $-\sigma$. The following downhill moves, again without rejections, are followed by another uphill climb, and so on, criss-crossing between the two wings of the potential $U_{24}$. It outputs configurations $\{x, \sigma\}$ such that, remarkably, the $x$-component samples $\pi_{24}$. This curious algorithm is implemented in Alg. 2.5 (`lifted-metropolis`), where we (almost) silently replaced the fixed grid of positions by a sampling of $\Delta$.

**procedure** `lifted-metropolis`
**input** $\{x, \sigma\}$ (lifted sample at time $t$)
$\Delta \leftarrow \texttt{ran}(0, \delta)$ $(\delta > 0)$
$x' \leftarrow x + \sigma\Delta$ ($x'$ in direction $\sigma$ from $x$)
$\Upsilon \leftarrow \texttt{ran}(0, 1)$
**if** $\Upsilon < \min\left[1, \dfrac{\pi_{24}(x')}{\pi_{24}(x)}\right]$**:** $x \leftarrow x'$
**else:** $\sigma \leftarrow -\sigma$
**output** $\{x, \sigma\}$ (lifted sample at time $t+1$)
——

**Algorithm 2.5:** `lifted-metropolis`. Non-reversible lifted version of Alg. 2.2 (`metropolis`). The $x$-positions that are output by this program sample $\pi_{24}$ (see Ref. [2]).

### 2.4.2 Event-driven Markov processes

Markov chains in continuous time are called *Markov processes*. To approach these, we consider Algorithm 2.5 (`lifted-metropolis`) with a grid of positions $\{\dots, -2\Delta, -\Delta, 0, \Delta, 2\Delta, \dots\}$ and nearest-neighbor moves. In Alg. 2.5 (`lifted-metropolis`), we thus input a fixed $\Delta$ and scrap the line $\Delta \leftarrow \texttt{ran}(0, \delta)$, then study it in the limit of small $\Delta$. We rescale time such that a displacement $\pm\Delta$ is itself undertaken in a time interval $\Delta$. The particle in the anharmonic oscillator thus moves with unit absolute velocity, whose sense is reversed when there is a rejection. The downhill moves are all accepted, and even uphill moves are accepted with a probability close to one. We may simulate each of these steps, but it's preferable to *sample* the position of the next rejection. As an example, let us consider a sequence of uphill moves in positive direction from $x = 0$. The probability for accepting an entire sequence of $n$ subsequent uphill moves, at positions $0, \Delta, \dots, (n-1)\Delta$, and then rejecting the move $n + 1$, is

$$\mathbb{P}(0 \to x_{\text{ev}}) = \underbrace{\mathrm{e}^{-\beta\Delta U_{24}(0) \cdots \Delta U_{24}[(n-1)\Delta]}}_{n \text{ accept}} \underbrace{\left[1 - \mathrm{e}^{-\beta\Delta U_{24}(n\Delta)}\right]}_{\text{reject, expand to 1st order}} \to \beta \mathrm{e}^{-\beta U_{24}} \mathrm{d}U_{24}. \tag{2.20}$$

In the small-$\Delta$ limit, the rejection is here expanded to first order, and $\Delta U$ is replaced by $\mathrm{d}U$. In our example of the anharmonic oscillator starting at $x = 0$, all the increments of $\Delta U_{24}$ up to position $x$ add up to the potential $U_{24}(x)$. Equation (2.20) indicates that the value of $U_{24}$ at which the velocity is reversed follows an exponential distribution in $U_{24}$. Remembering from Lecture 1 how to sample an exponential random variable, we obtain

$$U_{24}(x_{\text{ev}}) = -\beta^{-1} \log \texttt{ran}(0, 1), \tag{2.21}$$

which can be inverted as $U_{24}(x_{\text{ev}}) = x_{\text{ev}}^2/2 + x_{\text{ev}}^4/4$, with

$$x_{\text{ev}} = \sigma\sqrt{-1 + \sqrt{1 - 4\beta^{-1} \log \texttt{ran}(0, 1)}}. \tag{2.22}$$

Algorithm 2.6 (`zig-zag`) implements this event-driven, continuous-time, Markov process and manages to move forward and backward. The equal-time samples again sample the Boltzmann distribution $\pi_{24}$ (see Fig. 2.2).

**procedure** `zig-zag`
**input** $\{x, \sigma\}, t$ (lifted sample with $\sigma x \leq 0$ )
$x_{\text{ev}} \leftarrow \sigma\sqrt{-1 + \sqrt{1 - 4\beta^{-1} \log \texttt{ran}(0,1)}}$ (see Eq. (2.22))
$t_{\text{ev}} \leftarrow t + |x_{\text{ev}} - x|$
**for** $t^* = \text{int}(t) + 1, \ldots, \text{int}(t_{\text{ev}})$**:**
$\quad\{$ **print** $x + \sigma(t^* - t)$ (equal-time samples)
$x \leftarrow x_{\text{ev}};\ \sigma \leftarrow -\sigma;\ t \leftarrow t_{\text{ev}}$ ("zig-zag")
**output** $\{x, \sigma\}, t$
——

**Algorithm 2.6:** `zig-zag`. Continuous-time, event-driven version of Alg. 2.5 (`lifted-metropolis`).' The $x$-positions output by the `print` statement sample $\pi_{24}$ (see Ref. [2]).

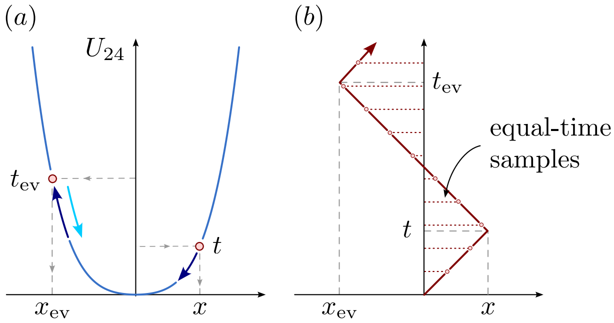


**Figure 2.2:** Zig-zag algorithm (continuous-time event-driven lifted Metropolis chain). (a): The particle swings about the origin, turning around at positions $x_{\text{ev}}$ [sampled by Eq. (2.22)]. (b): Piecewise deterministic constant-velocity trajectory. Particle positions are sampled at equal time steps (see Ref. [2]).

### 2.4.3 More non-reversible Markov-chain algorithms...

There are many more ideas in Markov-chain Monte Carlo (for a starter, try Ref. [2]), even if we restrict ourselves, as we did here, to true samplers of $\pi$, without any correction, in the limit of large times. From our modest beginnings, we already see a world of infinite possibilities.

# 3 Maxwell distribution, thermostats, Boltzmann distribution

In Lecture 2, and in the present Lecture 3, we were concerned with more and more adhoc Markov chains which sample a given distribution $\pi_{24}$ or a distribution $\pi_2$. These distributions were connected to potentials, for example $\pi_{24}$ was connected to the potential $U_{24}$. Here, we address the question of how the Boltzmann distribution $\pi_{24}$ actually arises from the potential $U_{24}$. This leads us to molecular dynamics with a heat bath. In molecular dynamics (as applied to our simple one-dimensional model), there is a position and a velocity whereas in Monte Carlo, we only saw the position $x$. We will deepen our understanding in a special case, in Lecture 4, so what we discuss here is only a preview.

### 3.0.1 Thermostats and the Boltzmann distribution

We consider the anharmonic oscillator as an isolated system that conserves the total energy. In between the turning points $-x_{\max}$ and $x_{\max}$ the kinetic energy (with the mass equal to unity)

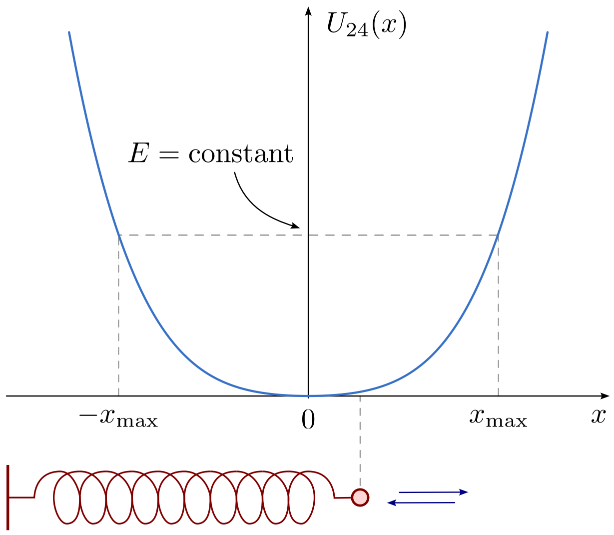


**Figure 3.1:** Isolated anharmonic oscillator

is $\frac{1}{2}(\mathrm{d}x/\mathrm{d}t)^2$, and conservation of energy can be written as

$$E = \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + U_{24}(x) \Leftrightarrow \frac{\mathrm{d}x}{\mathrm{d}t} = \pm\sqrt{2\left[E - U_{24}(x)\right]}, \tag{3.1}$$

which gives

$$\mathrm{d}t = \pm\sqrt{\frac{1}{2\left[E - U_{24}(x)\right]}}\mathrm{d}x. \tag{3.2}$$

To simulate the isolated anharmonic oscillator, we could numerically integrate the first-order ordinary differential equation on the right of Eq. (3.1) over a quarter period and then piece together the entire trajectory of Fig. 3.2a. However, this method is specific to one-dimensional dynamical systems. To reflect the general case, we numerically integrate Newton's law for the force $F$:

$$F = m\frac{\mathrm{d}^2 x(t)}{\mathrm{d}t^2}, \quad \text{with } F = -\frac{\mathrm{d}U_{24}}{\mathrm{d}x} = -x - x^3. \tag{3.3}$$

By substituting the time differential $\mathrm{d}t$ by a very small finite interval $\Delta t$, appropriate for stepping from $t$ to $t + \Delta t$, and to $t + 2\Delta t$, and so on, we obtain

$$x(t + \Delta t) = x(t) + v(t)\Delta t, \tag{3.4}$$
$$v(t + \Delta t) = v(t) - (x + x^3)\Delta t. \tag{3.5}$$

**procedure** `isolated-dynamics`
**input** $x, v, t$
$t \leftarrow t + \Delta t$
$x' \leftarrow x + v\Delta t$
$v \leftarrow v - \left(x + x^3\right)\Delta t$
$x \leftarrow x'$
**output** $x, v, t$
——

**Algorithm 3.1:** `isolated-dynamics`. Naive integration of Newton's equations for the isolated anharmonic oscillator (see Fig. 3.2).

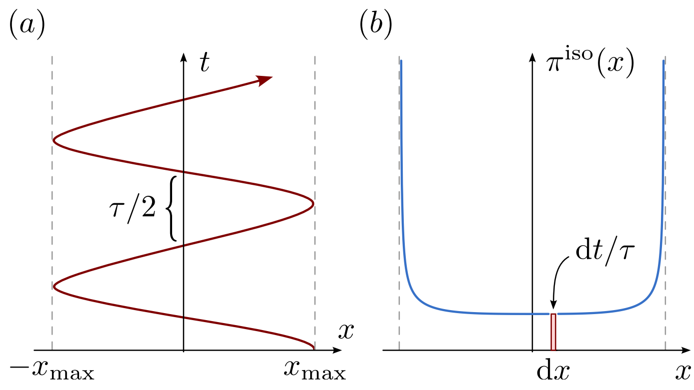


**Figure 3.2:** Trajectory of the isolated anharmonic oscillator

The outcome of this simulation corresponds not at all to the Boltzmann distribution.

### 3.0.2 Molecular dynamics with a thermostat

We return to the Newtonian dynamics of the anharmonic oscillator [2], but we take it out of isolation and have it interact with an infinite *bath* of hard spheres *via* thermostat (see Fig. 3.3.)

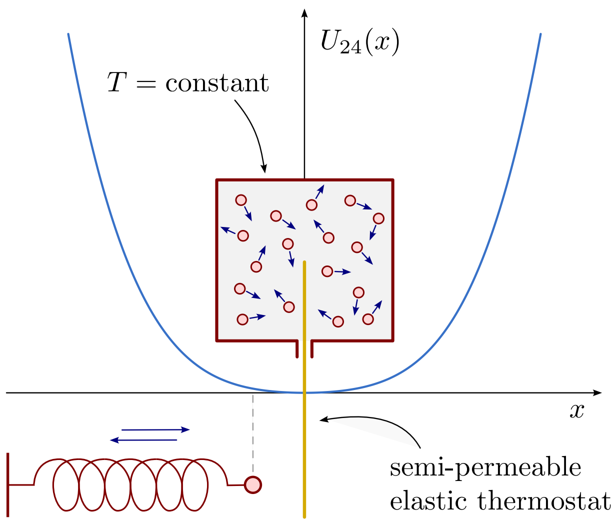


**Figure 3.3:** Anharmonic oscillator coupled to a heat bath

Statistical mechanics teaches us that the particles in the heat bath are Maxwell-distributed (we will discuss this point more in detail in Lecture 4).

$$\pi(v)\mathrm{d}v \propto \mathrm{e}^{-\beta v^2/2}\mathrm{d}v, \tag{3.6}$$

This is exactly the same problem as the sampling of positions on the surface of a hypersphere.

Particles that hit the thermostat behave differently. In particular, because the thermostat lies at a fixed position (up to an infinitesimal interval), its velocity follows the distribution

$$\pi^*(v)\mathrm{d}v = \beta|v|\mathrm{e}^{-\beta v^2/2}\mathrm{d}v, \tag{3.7}$$

often called the Maxwell boundary condition. It differs by the prefactor $\beta|v|$ from the Maxwell distribution of one velocity component. The velocity distribution of the thermostat in Eq. (3.7) can be sampled as

$$v = \pm\sqrt{\frac{-2\log \mathtt{ran}(0,1)}{\beta}}, \tag{3.8}$$

(it is an exponential distribution of the random variable $v^2$).

**procedure** `thermostat-dynamics`
**input** $x, v, t$
$x' \leftarrow x + v\Delta t$
$t \leftarrow t + \Delta t$
$\Upsilon \leftarrow \mathtt{ran}(0,1)$
**if** $x \cdot x' < 0$ **and** $\Upsilon < 1/2$**:**
$\{\ v \leftarrow -\mathtt{sign}(v)\sqrt{-2\beta^{-1}\log \mathtt{ran}(0,1)}$ (see Eq. (3.8))
**else:**
$\left\{\begin{array}{l} v \leftarrow v - (x + x^3)\Delta t \\ x \leftarrow x' \end{array}\right.$
**output** $x, v, t$
——

**Algorithm 3.2:** `thermostat-dynamics`. Naive solution of Newton's equations for the anharmonic oscillator with the semi-permeable thermostat at $x = 0$ (see Fig. 3.4).

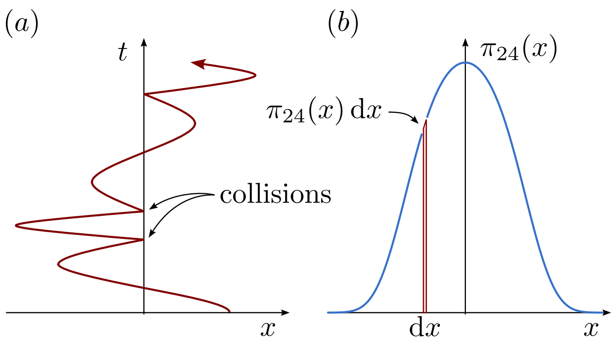


**Figure 3.4:** Trajectory of the anharmonic oscillator coupled to a heat bath.

Output of Alg. 3.2 (`thermostat-dynamics`) can be histogrammed to see that the distribution of positions is exactly (up to discretization errors in $\Delta t$) the Boltzmann distribution of the anharmonic oscillator, proving (experimentally but by our own means) that the Boltzmann distribution describes a subsystem interacting with a heat bath. But what about the distribution of velocities? As we only give our particle a kick at $x = 0$, we'd surely suppose that it runs out of steam as it climbs up the potential. But this is not the case, and Fig. 3.5 illustrates it by histogramming probability distributions of the velocities at different values up the hill. As statistical mechanics dictates, we have independence of distributions of positions and velocities.

# References

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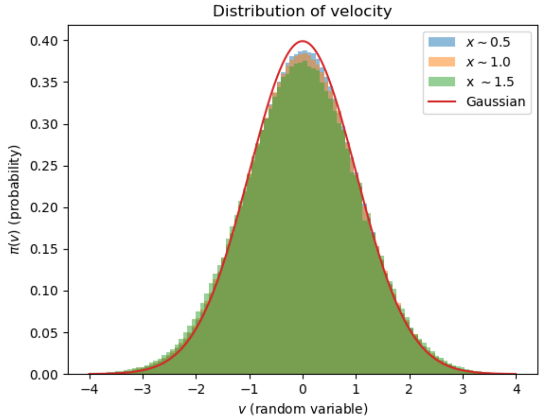


**Figure 3.5:** Velocity distributions of the anharmonic oscillator (Algorithm 3.2) at different approximate positions of $x$. Up to discretization effects, they all agree with the Maxwell distribution at inverse temperature $\beta = 1$.

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