Algorithms and computations in physics (Oxford Lectures 2024)

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This is the first of two lectures on computational quantum statistical mechanics. Starting from the quantum harmonic oscillator, we introduce to density matrices and the Feynman path integral (sixth lecture), before arriving at a *bona fide* quantum Monte Carlo algorithm for bosons, that will illustrate the phenomenon of Bose–Einstein condensation (seventh lecture). The computational techniques that we concentrate on during these two weeks have widespread use in statistics and physics, and the fundamental matrix-squaring property of density matrices corresponds to the convolution of probability densities. The Lévy algorithm for the sampling of path integrals, on the other hand, is mathematically equivalent to what is known in electrical engineering and other fields as the "Gaussian bridge".

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6 Quantum statistical mechanics: Density matrix, path integral

6.1 The density matrix

In this section, we discuss the density matrix, the fundamental object in quantum statistical mechanics.

6.1.1 The quantum harmonic oscillator

The one-dimensional quantum mechanical harmonic oscillator, which consists of a particle of mass m in a potential

$$V(x) = \frac{1}{2} m\omega^2 x^2,$$

is governed by the Schrödinger equation:

$$H\psi_n^{\text{h.o.}} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \right) \psi_n^{\text{h.o.}} = E_n \psi_n^{\text{h.o.}}. \tag{6.1}$$

The eigenfunctions of the harmonic oscillator are analyzed in detail in elementary quantum-mechanics lectures, and their content is encapsulated in Alg. 6.1 (`harmonic-wavefunction`).

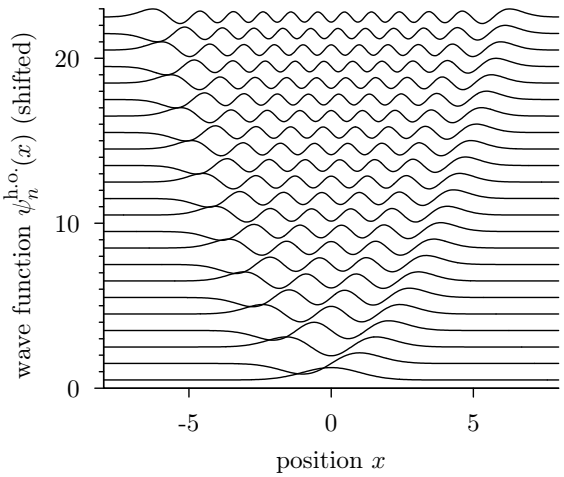

Figure 6.1: Harmonic-oscillator wave functions $\psi_n^{\text{h.o.}}(x)$ shifted by E_n (from Alg. 6.1 (`harmonic-wavefunction`)).

procedure `harmonic-wavefunction`
input x
$\psi_{-1}^{\text{h.o.}}(x) \leftarrow 0$ (unphysical, starts recursion)
$\psi_0^{\text{h.o.}}(x) \leftarrow \pi^{-1/4} \exp\left(-x^2/2\right)$ (ground state)
for $n = 1, 2, \ldots$ **:**
$\left\{ \psi_n^{\text{h.o.}}(x) \leftarrow \sqrt{\frac{2}{n}} x \psi_{n-1}^{\text{h.o.}}(x) - \sqrt{\frac{n-1}{n}} \psi_{n-2}^{\text{h.o.}}(x) \right.$
output $\{\psi_0^{\text{h.o.}}(x), \psi_1^{\text{h.o.}}(x), \ldots\}$

Algorithm 6.1: `harmonic-wavefunction`. Eigenfunctions of the one-dimensional harmonic oscillator (with $\hbar = m = \omega = 1$).

In general, the wave functions $\{\psi_0, \psi_1, \dots\}$ satisfy a completeness condition

$$\sum_{n=0}^{\infty} \psi_n^*(x)\psi_n(y) = \delta(x-y),$$

where $\delta(x-y)$ is the Dirac δ-function, and form an orthonormal set:

$$\int_{-\infty}^{\infty} \mathrm{d}x\ \psi_n^*(x)\psi_m(x) = \delta_{nm} = \begin{cases} 1 & \text{if } n=m \\ 0 & \text{otherwise} \end{cases}, \tag{6.2}$$

where δ_{nm} is the discrete Kronecker δ-function. The wave functions of the harmonic oscillator can be computed recursively[1] (see Alg. 6.1 (`harmonic-wavefunction`)). We can easily write down the first few of them, and verify that they are indeed normalized and mutually orthogonal, and that $\psi_n^{\text{h.o.}}$ satisfies the above Schrödinger equation (for $m=\hbar=\omega=1$) with $E_n = n + \frac{1}{2}$.

In thermal equilibrium, a quantum particle occupies an energy state n with a Boltzmann probability proportional to $\mathrm{e}^{-\beta E_n}$, and the partition function is therefore

$$\begin{aligned} Z^{\text{h.o.}}(\beta) = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta E_n} &= \mathrm{e}^{-\beta/2} + \mathrm{e}^{-3\beta/2} + \mathrm{e}^{-5\beta/2} + \cdots \\ &= \mathrm{e}^{-\beta/2}\left(\frac{1}{1-\mathrm{e}^{-\beta}}\right) = \frac{1}{\mathrm{e}^{\beta/2}-\mathrm{e}^{-\beta/2}} = \frac{1}{2\sinh(\beta/2)}. \end{aligned} \tag{6.3}$$

The complete thermodynamics of the harmonic oscillator follows from eq. (6.3). The normalized probability of being in energy level n is

$$\left\{\begin{matrix}\text{probability of being} \\ \text{in energy level } n\end{matrix}\right\} = \frac{1}{Z}\ \mathrm{e}^{-\beta E_n}.$$

When it is in energy level n (see Fig. 6.1), a quantum system is at a position x with probability $\psi_n^*(x)\psi_n(x)$. (The asterisk stands for the complex conjugate; for the real-valued wave functions used in most of these lecture notes, $\psi^* = \psi$.) The probability of being in level n at position x is

$$\left\{\begin{matrix}\text{probability of being} \\ \text{in energy level } n \\ \text{at position } x\end{matrix}\right\} = \frac{1}{Z}\ \mathrm{e}^{-\beta E_n}\psi_n(x)\psi_n^*(x). \tag{6.4}$$

This expression generalizes the Boltzmann distribution to quantum physics. However, the energy levels and wave functions are generally unknown for complicated quantum systems, and eq. (6.4) is not useful for practical computations. To make progress, we discard the information about the energy levels and consider the (diagonal) density matrix

$$\pi(x) = \left\{\begin{matrix}\text{probability of being} \\ \text{at position } x\end{matrix}\right\} \propto \rho(x,x,\beta) = \sum_n \mathrm{e}^{-\beta E_n}\psi_n(x)\psi_n^*(x),$$

as well as a more general object, the nondiagonal density matrix (in the position representation)

$$\left\{\begin{matrix}\text{density} \\ \text{matrix}\end{matrix}\right\} : \rho\big(x,x',\beta\big) = \sum_n \psi_n(x)\mathrm{e}^{-\beta E_n}\psi_n^*(x'), \tag{6.5}$$

which is the central object of quantum statistics. For example, the partition function $Z(\beta)$, that we already computed in eq. (6.3), is the trace of the density matrix, i.e. the sum or the integral

[1] In most formulas in these lecture notes, we use units such that $\hbar = m = \omega = 1$.

of its diagonal terms:

$$Z(\beta) = \mathrm{Tr}\ \rho = \int \mathrm{d}x\ \rho(x, x, \beta)\,. \tag{6.6}$$

We shall compute the density matrix in different settings, and often without knowing the eigenfunctions and eigenvalues. For the case of the harmonic oscillator, however, we have all that it takes to compute the density matrix from our solution of the Schrödinger equation (see Alg. 6.2 (`harmonic-density`) and Fig. 6.2). The output of this program will allow us to check less basic approaches.

procedure `harmonic-density`
input $\{\psi_0^{\text{h.o.}}(x), \dots, \psi_N^{\text{h.o.}}(x)\}$ (from Alg. 6.1 (`harmonic-wavefunction`))
input $\{\psi_0^{\text{h.o.}}(x'), \dots, \psi_N^{\text{h.o.}}(x')\}$
input $\{E_n = n + \frac{1}{2}\}$
$\rho^{\text{h.o.}}(x, x', \beta) \leftarrow 0$
for $n = 0, \dots, N$**:**
  $\{\ \rho^{\text{h.o.}}(x, x', \beta) \leftarrow \rho^{\text{h.o.}}(x, x', \beta) + \psi_n^{\text{h.o.}}(x)\psi_n^{\text{h.o.}}(x')\mathrm{e}^{-\beta E_n}$
output $\{\rho^{\text{h.o.}}(x, x', \beta)\}$

Algorithm 6.2: `harmonic-density`. Density matrix for the harmonic oscillator obtained from the lowest-energy wave functions (see eq. (6.5)).

For the perturbation theory of Sec. 6.2.1, we need the fact that the density matrix is generally given by the operator

$$\rho = \mathrm{e}^{-\beta H} = 1 - \beta H + \frac{1}{2}\beta^2 H^2 - \cdots\,. \tag{6.7}$$

The matrix elements of H in an arbitrary basis are $H_{kl} = \langle k|H|l\rangle$, and the matrix elements of ρ are

$$\langle k|\rho|l\rangle = \langle k|\mathrm{e}^{-\beta H}|l\rangle = \delta_{kl} - \beta H_{kl} + \frac{1}{2}\beta^2 \sum_n H_{kn}H_{nl} - \cdots\,.$$

In the energy basis, ρ is diagonal, and we recover

$$\rho\big(x, x', \beta\big) = \sum_{kl} \underbrace{\langle x|k\rangle}_{\psi_k(x)} \langle k|\rho|l\rangle \underbrace{\langle l|x'\rangle}_{\psi_l^*(x')}$$

because $\langle k|\rho|l\rangle = \delta_{kl} \exp\left(-\beta E_k\right)$.

6.1.2 Free density matrix

We move on to our first analytic calculation, a prerequisite for further developments: the density matrix of a free particle, with the Hamiltonian

$$H^{\text{free}}\psi = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi = E\psi.$$

We put the particle in a box of length L with periodic boundary conditions, that is, a torus. The solutions of the Schrödinger equation in a periodic box are plane waves that are periodic in

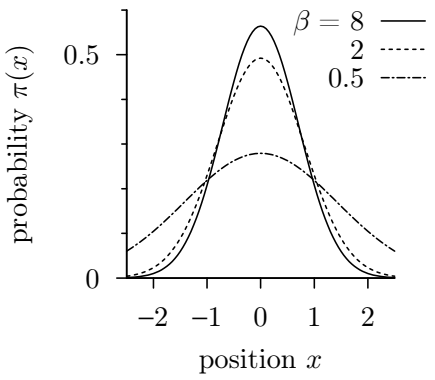

Figure 6.2: Probability to be at position x, $\pi(x) = \rho^{\text{h.o.}}(x, x, \beta)\,/Z$ (from Alg. 6.2 (`harmonic-density`). We will later compute this function exactly, and also obtain it from path-integral Monte Carlo.

L:

$$\psi_n^{\text{a}}(x) = \sqrt{\frac{2}{L}} \sin\left(2n\pi\frac{x}{L}\right) \;\; (n = 1, 2, \dots), \tag{6.8}$$

$$\psi_n^{\text{s}}(x) = \sqrt{\frac{2}{L}} \cos\left(2n\pi\frac{x}{L}\right) (n = 0, 1, \dots) \tag{6.9}$$

(see Fig. 6.3), where the superscripts denote wave functions that are antisymmetric and symmetric with respect to the center of the interval $[0, L]$. Equivalently, we can use complex wave functions

$$\psi_n^{\text{per},L}(x) = \sqrt{\frac{1}{L}} \exp\left(\text{i}2n\pi\frac{x}{L}\right) \quad (n = -\infty, \dots, \infty), \tag{6.10}$$

$$E_n = \frac{2n^2\pi^2}{L^2}, \tag{6.11}$$

which give

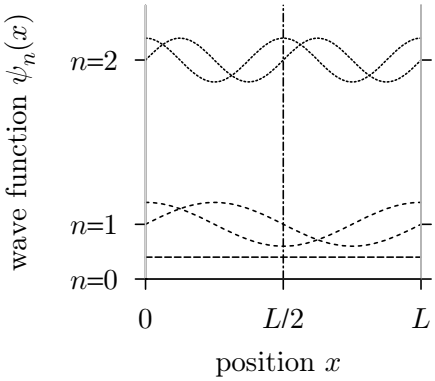

Figure 6.3: Wave functions of a one-dimensional free particle in a torus of length L (shifted; see eq. (6.9)).

$$\rho^{\text{per},L}\left(x,x',\beta\right) = \sum_n \psi_n^{\text{per},L}(x)\mathrm{e}^{-\beta E_n}\left[\psi_n^{\text{per},L}(x')\right]^* = \frac{1}{L}\sum_{n=-\infty}^{\infty} \exp\left[\mathrm{i}2\pi n\frac{x-x'}{L}\right]\exp\left(-\frac{\beta 2n^2\pi^2}{L^2}\right). \quad (6.12)$$

We now let L tend to infinity (the exact expression for finite L is discussed in Ref. [1]) In this limit, we can transform the sum in eq. (6.12) into an integral. It is best to introduce a dummy parameter $\Delta_n = 1$, the difference between two successive n-values:

$$\rho^{\text{per},L}\left(x,x',\beta\right) = \frac{1}{L}\sum_{n=-\infty}^{\infty} \overbrace{\Delta_n}^{=1} \exp\left[\mathrm{i}2n\pi\frac{x-x'}{L}\right]\exp\left(-\frac{\beta 2n^2\pi^2}{L^2}\right).$$

Changing variables from n to λ, where $\lambda = 2n\pi/L$, and thus $\Delta_\lambda = 2\pi\Delta_n/L$, gives the term-by-term equivalent sum

$$\rho^{\text{per},L}\left(x,x',\beta\right) = \frac{1}{2\pi}\sum_{\lambda=\ldots,-\frac{2\pi}{L},0,\frac{2\pi}{L},\ldots} \Delta_\lambda \exp\left[\mathrm{i}\lambda(x-x')\right]\exp\left(-\frac{\beta}{2}\lambda^2\right) \xrightarrow[L\to\infty]{} \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\lambda\ \exp\left[\mathrm{i}\lambda(x-x')\right]\exp\left(-\frac{\beta}{2}\lambda^2\right).$$

[2] This Gaussian integral can be evaluated (see eq. (6.13)). We arrive at the free density matrix, the periodic density matrix in the limit of an infinite torus:

$$\rho^{\text{free}}\left(x,x',\beta\right) = \sqrt{\frac{m}{2\pi\hbar^2\beta}}\exp\left[-\frac{m(x-x')^2}{2\hbar^2\beta}\right], \quad (6.14)$$

where we have reinserted the Planck constant and the particle mass. In the limit of high temperature, $\rho^{\text{free}}(x,x',\beta)$ is infinitely peaked at $x = x'$, and it continues to satisfy $\int_{-\infty}^{\infty}\mathrm{d}x\ \rho^{\text{free}}(x,x',\beta) = 1$. This means that it realizes the Dirac δ-function:

$$\lim_{\beta\to 0}\rho^{\text{free}}\left(x,x',\beta\right) \to \delta(x-x'). \quad (6.15)$$

6.1.3 Density matrix in a box

As we just saw, the density matrix can be computed for the free particle. It can also be computed for the particle in a harmonic potential (see Sec. 6.2.3), and the particle in a fixed, a periodic, and even a rotating box (see Ref. [1]). These subjects would all be treated if we had a little more time...

6.2 Matrix squaring

A classical equilibrium system is at coordinates $\mathbf{x}$ with a probability $\pi(\mathbf{x})$ given by the Boltzmann distribution. In contrast, a quantum statistical system is governed by the diagonal density matrix, defined through wave functions and energy eigenvalues. The problem is that we usually do not know the solutions of the Schrödinger equation, so that we need other methods to compute the density matrix. In this section, we discuss matrix squaring, a practical approach to computing the density matrix at any temperature from a high-temperature limit with the help

[2] We use

$$\int_{-\infty}^{\infty}\mathrm{d}\lambda\ \exp\left(-\frac{1}{2}\frac{\lambda^2}{\sigma^2}\pm\lambda\tilde{c}\right) = \sqrt{2\pi}\sigma\exp\left(\frac{1}{2}\tilde{c}^2\sigma^2\right), \quad (6.13)$$

of a convolution principle, which yields the density matrix at low temperature once we know it at high temperature.

6.2.1 High-temperature limit (Trotter formula)

In the limit of high temperature, the density matrix of a quantum system described by a Hamiltonian $H = H^{\text{free}} + V$ is given by a general expression known as the Trotter formula:

$$\rho\left(x, x', \beta\right) \xrightarrow[\beta\to 0]{} \mathrm{e}^{-\frac{1}{2}\beta V(x)} \rho^{\text{free}}\left(x, x', \beta\right) \; \mathrm{e}^{-\frac{1}{2}\beta V(x')}. \tag{6.16}$$

To verify eq. (6.16), we expand the exponentials of operators, but observe that terms may not commute, that is, $H_{\text{free}} V \neq V H_{\text{free}}$. We then compare the result with the expansion in eq. (**??**) of the density matrix $\rho = \mathrm{e}^{-\beta H}$. The above Trotter formula gives

$$\left(1 - \underbrace{\frac{\beta}{2} V}_{a} + \underbrace{\frac{\beta^2}{8} V^2}_{b} \ldots\right) \left[1 - \underbrace{\beta H^{\text{free}}}_{c} + \underbrace{\frac{\beta^2}{2} (H^{\text{free}})^2}_{d} \ldots\right] \left(1 - \underbrace{\frac{\beta}{2} V}_{e} + \underbrace{\frac{\beta^2}{8} V^2}_{f} \ldots\right),$$

which yields

$$1 - \underbrace{\beta(V + H^{\text{free}})}_{a+e+c} + \frac{\beta^2}{2} \Big[\underbrace{V^2}_{ae+b+f} + \underbrace{V H^{\text{free}}}_{ac} + \underbrace{H^{\text{free}} V}_{ce} + \underbrace{(H^{\text{free}})^2}_{d} \Big] - \cdots .$$

This agrees up to order β^2 with the expansion of

$$\mathrm{e}^{-\beta(V + H^{\text{free}})} = 1 - \beta(V + H^{\text{free}}) + \frac{\beta^2}{2} \underbrace{(V + H^{\text{free}})(V + H^{\text{free}})}_{V^2 + V H^{\text{free}} + H^{\text{free}} V + (H^{\text{free}})^2} + \cdots .$$

The above manipulations are generally well defined for operators and wave functions in a finite box.

6.2.2 Convolution

In addition to the high-temperature limit, any density matrix $\rho(x, x', \beta)$ possesses a fundamental convolution property:

$$\begin{aligned} &\underline{\int \mathrm{d}x' \; \rho\left(x, x', \beta_1\right) \rho\left(x', x'', \beta_2\right)} \qquad\qquad (6.17) \\ &= \int \mathrm{d}x' \sum_{n,m} \psi_n(x) \mathrm{e}^{-\beta_1 E_n} \psi_n^*(x') \psi_m(x') \mathrm{e}^{-\beta_2 E_m} \psi_m^*(x'') \\ &= \sum_{n,m} \psi_n(x) \mathrm{e}^{-\beta_1 E_n} \underbrace{\int \mathrm{d}x' \; \psi_n^*(x') \psi_m(x')}_{\delta_{nm},\ \text{see eq. (6.2)}} \mathrm{e}^{-\beta_2 E_m} \psi_m^*(x'') \\ &= \sum_n \psi_n(x) \mathrm{e}^{-(\beta_1+\beta_2) E_n} \psi_n^*(x'') = \underline{\rho\left(x, x'', \beta_1 + \beta_2\right)}. \qquad\qquad (6.18) \end{aligned}$$

We can thus express the density matrix in eq. (6.18) at the inverse temperature $\beta_1 + \beta_2$ (low temperature) as an integral (eq. (6.17)) over density matrices at higher temperatures corresponding to β_1 and β_2. Let us suppose that the two temperatures are the same ($\beta_1 = \beta_2 = \beta$) and that the positions x are discretized. The integral in eq. (6.17) then turns into a sum $\sum_l$, and $\rho(x, x', \beta)$ becomes a discrete matrix ρ_{kl}. The convolution turns into a product of a matrix

with itself, a matrix squared:

$$\begin{array}{ccccc} \int \mathrm{d}x' \, \rho(x, x', \beta) \, \rho(x', x'', \beta) & = & \rho(x, x'', 2\beta) \, . \\ \Updownarrow & \Updownarrow & \Updownarrow & & \Updownarrow \\ \sum_l & \rho_{kl} & \rho_{lm} & = & \left(\rho^2\right)_{km} \end{array}$$

Matrix squaring can be iterated: after computing the density matrix at 2β, we go to 4β, then to 8β, etc., that is, to lower and lower temperatures. Together with the Trotter formula, which gives a high-temperature approximation, we thus have a systematic procedure for computing the low-temperature density matrix. The procedure works for any Hamiltonian provided we can evaluate the integral in eq. (6.17) (see Alg. 6.3 (`matrix-square`)). We need not solve for eigenfunctions and eigenvalues of the Schrödinger equation. To test the program, we may iterate Alg. 6.3 (`matrix-square`) several times for the harmonic oscillator, starting from the Trotter formula at high temperature. With some trial and error to determine a good discretization of x-values and a suitable initial temperature, we can easily recover the plots of Fig. 6.2.

procedure `matrix-square`
input $\{x_0, \ldots, x_K\}, \{\rho(x_k, x_l, \beta)\}$ (grid with step size Δ_x)
for $x = x_0, \ldots, x_K$**:**
  for $x' = x_0, \ldots, x_K$**:**
    $\rho(x, x', 2\beta) \leftarrow \sum_k \Delta_x \rho(x, x_k, \beta) \, \rho(x_k, x', \beta)$
output $\{\rho(x_k, x_l, 2\beta)\}$

Algorithm 6.3: `matrix-square`. Density matrix at temperature $1/(2\beta)$ obtained from that at $1/\beta$ by discretizing the integral in eq. (6.18).

6.2.3 Density matrix in a harmonic potential (exact solution)

Quantum-statistics problems can be solved by plugging the high-temperature approximation for the density matrix into a matrix-squaring routine and iterating down to low temperature. This strategy works for anything from the simplest test cases to complicated quantum systems in high spatial dimensions, interacting particles, bosons, fermions, etc. How we actually do the integration inside the matrix-squaring routine depends on the specific problem, and can involve saddle point integration or other approximations, Riemann sums, Monte Carlo sampling, etc. For the harmonic oscillator, all the integrations can be done analytically. This yields an explicit formula for the density matrix for a harmonic oscillator at arbitrary temperature, which we shall use later in this and the following lecture.

The density matrix at high temperature,

$$\rho^{\text{h.o.}}\left(x, x', \beta\right) \xrightarrow[\beta \to 0]{\text{from eq. (6.16)}} \sqrt{\frac{1}{2\pi\beta}} \exp\left[-\frac{\beta}{4}x^2 - \frac{(x-x')^2}{2\beta} - \frac{\beta}{4}x'^2\right],$$

can be written as

$$\rho^{\text{h.o.}}\left(x, x', \beta\right) = c(\beta) \exp\left[-g(\beta)\frac{(x-x')^2}{2} - f(\beta)\frac{(x+x')^2}{2}\right], \tag{6.19}$$

where

$$\begin{aligned} f(\beta) &\xrightarrow[\beta\to 0]{} \frac{\beta}{4}, \\ g(\beta) &\xrightarrow[\beta\to 0]{} \frac{1}{\beta}+\frac{\beta}{4}, \\ c(\beta) &\xrightarrow[\beta\to 0]{} \sqrt{\frac{1}{2\pi\beta}}. \end{aligned} \tag{6.20}$$

The convolution of two Gaussians is again a Gaussian, so that the harmonic-oscillator density matrix at inverse temperature 2β,

$$\rho^{\text{h.o.}}\big(x,x'',2\beta\big)=\int_{-\infty}^{\infty}\mathrm{d}x'\;\rho^{\text{h.o.}}\big(x,x',\beta\big)\,\rho^{\text{h.o.}}\big(x',x'',\beta\big)\,,$$

must also have the functional form of eq. (6.19). We recast the exponential in the above integrand,

$$\begin{aligned} -\frac{f}{2}\left[(x+x')^2+(x'+x'')^2\right]-\frac{g}{2}\left[(x-x')^2+(x'-x'')^2\right] \\ =\underbrace{-\frac{f+g}{2}\left(x^2+x''^2\right)}_{\text{independent of } x'}\underbrace{-2(f+g)\frac{x'^2}{2}-(f-g)(x+x'')x'}_{\text{Gaussian in } x',\ \text{variance } \sigma^2=(2f+2g)^{-1}}, \end{aligned}$$

and obtain, using eq. (6.13),

$$\rho^{\text{h.o.}}\big(x,x'',2\beta\big)=c(2\beta)\exp\left[-\frac{f+g}{2}\left(x^2+x''^2\right)+\frac{1}{2}\frac{(f-g)^2}{f+g}\frac{(x+x'')^2}{2}\right]. \tag{6.21}$$

The argument of the exponential function in eq. (6.21) is

$$-\underbrace{\left[\frac{f+g}{2}-\frac{1}{2}\frac{(f-g)^2}{f+g}\right]}_{f(2\beta)}\frac{(x+x'')^2}{2}-\underbrace{\left(\frac{f+g}{2}\right)}_{g(2\beta)}\frac{(x-x'')^2}{2}.$$

We thus find

$$\begin{aligned} f(2\beta)&=\frac{f(\beta)+g(\beta)}{2}-\frac{1}{2}\frac{[f(\beta)-g(\beta)]^2}{f(\beta)+g(\beta)}=\frac{2f(\beta)g(\beta)}{f(\beta)+g(\beta)}, \\ g(2\beta)&=\frac{f(\beta)+g(\beta)}{2}, \\ c(2\beta)&=c^2(\beta)\sqrt{\frac{2\pi}{2[f(\beta)+g(\beta)]}}=c^2(\beta)\frac{\sqrt{2\pi}}{2\sqrt{g(2\beta)}}. \end{aligned}$$

The recursion relations for f and g imply

$$f(2\beta)g(2\beta)=f(\beta)g(\beta)=f(\beta/2)g(\beta/2)=\cdots=\frac{1}{4},$$

because of the high-temperature limit in eq. (6.20), and therefore

$$g(2\beta)=\frac{g(\beta)+(1/4)g^{-1}(\beta)}{2}. \tag{6.22}$$

We can easily check that the only function satisfying eq. (6.22) with the limit in eq. (6.20) is

$$g(\beta) = \frac{1}{2}\coth\frac{\beta}{2} \implies f(\beta) = \frac{1}{2}\tanh\frac{\beta}{2}.$$

Knowing $g(\beta)$ and thus $g(2\beta)$, we can solve for $c(\beta)$ and arrive at

$$\rho^{\text{h.o.}}(x, x', \beta) = \sqrt{\frac{1}{2\pi\sinh\beta}}\exp\left[-\frac{(x+x')^2}{4}\tanh\frac{\beta}{2} - \frac{(x-x')^2}{4}\coth\frac{\beta}{2}\right], \tag{6.23}$$

and the diagonal density matrix is

$$\rho^{\text{h.o.}}(x, x, \beta) = \sqrt{\frac{1}{2\pi\sinh\beta}}\exp\left(-x^2\tanh\frac{\beta}{2}\right) \tag{6.24}$$

(see Ref. [1] for formulas with physical units).

We earlier used Alg. 6.2 (`harmonic-density`) to compute $\rho^{\text{h.o.}}(x, x, \beta)$ from the wave functions and energy eigenvalues. We now see that the resulting plots, shown in Fig. 6.2, are simply Gaussians of variance

$$\sigma^2 = \frac{1}{2\tanh(\beta/2)}. \tag{6.25}$$

For a classical harmonic oscillator, the analogous probabilities are obtained from the Boltzmann distribution

$$\pi^{\text{class.}}(x) \propto \mathrm{e}^{-\beta E(x)} = \exp\left(-\beta x^2/2\right).$$

This is also a Gaussian, but its variance ($\sigma^2 = 1/\beta$) agrees with that in the quantum problem only in the high-temperature limit (see eq. (6.25) for $\beta \to 0$). Integrating the diagonal density matrix over space gives the partition function of the harmonic oscillator:

$$Z^{\text{h.o.}}(\beta) = \int \mathrm{d}x\ \rho^{\text{h.o.}}(x, x, \beta) = \frac{1}{2\sinh(\beta/2)}, \tag{6.26}$$

where we have used the fact that

$$\tanh\frac{\beta}{2}\sinh\beta = 2\left(\sinh\frac{\beta}{2}\right)^2.$$

This way of computing the partition function agrees with what we obtained from the sum of energies in eq. (6.3). Matrix squaring also allows us to compute the ground-state wave function without solving the Schrödinger equation because, in the limit of zero temperature, eq. (6.24) becomes $\rho^{\text{h.o.}}(x, x, \beta) \propto \exp\left(-x^2\right) \propto \psi_0^{\text{h.o.}}(x)^2$ (see Alg. 6.1 (`harmonic-wavefunction`)).

In conclusion, we have obtained in this subsection an analytic expression for the density matrix of a harmonic oscillator, not from the energy eigenvalues and eigenfunctions, but using matrix squaring down from high temperature. We shall need this expression several times in this lecture and the next one.

6.3 The Feynman path integral

In matrix squaring, we convolute two density matrices at temperature T to produce the density matrix at temperature $T/2$. By iterating this process, we can obtain the density matrix at any temperature from the quasi-classical high-temperature limit. Most often, however, it is impossible to convolute two density matrices analytically. With increasing numbers of particles and in high dimensionality, the available computer memory soon becomes insufficient even to store a reasonably discretized matrix $\rho(\mathbf{x}, \mathbf{x}', \beta)$, so that one cannot run Alg. 6.3 (`matrix-square`) on a discretized approximation of the density matrix. Monte Carlo methods are able to resolve

this problem. They naturally lead to the Feynman path integral for quantum systems and to the idea of path sampling, as we shall see in the present section.

Instead of evaluating the convolution integrals one after the other, as is done in matrix squaring, we can write them out all together:

$$\rho(x,x',\beta) = \int \mathrm{d}x''\ \rho(x,x'',\beta/2)\,\rho(x'',x',\beta/2)$$
$$= \iiint \mathrm{d}x''\mathrm{d}x'''\mathrm{d}x''''\rho\left(x,x''',\frac{\beta}{4}\right)\rho\left(x''',x'',\frac{\beta}{4}\right)\rho\left(x'',x'''',\frac{\beta}{4}\right)\rho\left(x'''',x',\frac{\beta}{4}\right)$$
$$= \dots.$$

This equation continues to increasingly deeper levels, with the kth applications of the matrix-squaring algorithm corresponding to $\simeq 2^k$ integrations. Writing $\{x_0, x_1, \dots\}$ instead of the cumbersome $\{x, x', x'', \dots\}$, this gives

$$\rho(x_0, x_N, \beta) = \int \cdots \int \mathrm{d}x_1 \dots \mathrm{d}x_{N-1}\ \rho\left(x_0, x_1, \frac{\beta}{N}\right) \dots \rho\left(x_{N-1}, x_N, \frac{\beta}{N}\right), \tag{6.27}$$

where we note that, for the density matrix $\rho(x_0, x_N, \beta)$, the variables x_0 and x_N are fixed on both sides of eq. (6.27). For the partition function, there is one more integration, over the variable x_0, which is identified with x_N:

$$Z = \int \mathrm{d}x_0\ \rho(x_0, x_0, \beta) = \int \cdots \int \mathrm{d}x_0 \dots \mathrm{d}x_{N-1}$$
$$\times\, \rho\left(x_0, x_1, \frac{\beta}{N}\right) \dots \rho\left(x_{N-1}, x_0, \frac{\beta}{N}\right). \tag{6.28}$$

The sequence $\{x_0, \dots, x_N\}$ in eqs. (6.27) and (6.28) is called a path, and we can imagine the variable x_k at the value $k\beta/N$ of the imaginary-time variable τ, which goes from 0 to β in steps of $\Delta_\tau = \beta/N$ (see Feynman (1972)). Density matrices and partition functions are thus represented as multiple integrals over paths, called path integrals, both at finite N and in the limit $N \to \infty$. The motivation for this representation is again that for large N, the density matrices under the multiple integral signs are at small $\Delta_\tau = \beta/N$ (high temperature) and can thus be replaced by their quasi-classical high-temperature approximations. To distinguish between the density matrix with fixed positions x_0 and x_N and the partition function, where one integrates over $x_0 = x_N$, we shall refer to the paths in eq. (6.27) as contributing to the density matrix $\rho(x_0, x_N, \beta)$, and to the paths in eq. (6.28) as contributing to the partition function.

After presenting a naive sampling approach in Sec. 6.3.1, we discuss direct path sampling using the Lévy construction in free space, in Sec. 6.3.2 and in a harmonic potential, in Sec. 6.3.3.

6.3.1 Naive path sampling

The Feynman path integral describes a single quantum particle in terms of paths $\{x_0, \dots, x_N\}$ (often referred to as world lines), with weights given by the high-temperature density matrix or another suitable approximation:

$$Z = \underbrace{\int \int \mathrm{d}x_0, \dots, \mathrm{d}x_{N-1}}_{\text{sum of paths}} \underbrace{\rho(x_0, x_1, \Delta_\tau) \cdot \dots \cdot \rho(x_{N-1}, x_0, \Delta_\tau)}_{\text{weight } \pi \text{ of path}}.$$

More generally, any variable x_k can represent a d-dimensional quantum system. The full path then lies in $d+1$ dimensions.

Let us first sample the paths contributing to the partition function of a harmonic oscillator using a local Markov-chain algorithm (see Fig. 6.4). We implement the Trotter formula, as

procedure `naive-harmonic-path`
input $\{x_0, \ldots, x_{N-1}\}$
$\Delta_\tau \leftarrow \beta/N$
$k \leftarrow \texttt{nran}\,(0, N-1)$
$k_\pm \leftarrow k \pm 1$
if $k_- = -1$**:** $k_- \leftarrow N$
$x'_k \leftarrow x_k + \texttt{ran}(-\delta, \delta)$
$\pi_a \leftarrow \rho^{\text{free}}\big(x_{k_-}, x_k, \Delta_\tau\big)\, \rho^{\text{free}}\big(x_k, x_{k_+}, \Delta_\tau\big) \exp\left(-\frac{1}{2}\Delta_\tau x_k^2\right)$
$\pi_b \leftarrow \rho^{\text{free}}\big(x_{k_-}, x'_k, \Delta_\tau\big)\, \rho^{\text{free}}\big(x'_k, x_{k_+}, \Delta_\tau\big) \exp\left(-\frac{1}{2}\Delta_\tau x_k'^2\right)$
$\Upsilon \leftarrow \pi_b/\pi_a$
if $\texttt{ran}(0,1) < \Upsilon$**:** $x_k \leftarrow x'_k$
output $\{x_0, \ldots, x_{N-1}\}$

Algorithm 6.4: `naive-harmonic-path`. Markov-chain sampling of paths contributing to $Z^{\text{h.o.}} = \int \mathrm{d}x_0\ \rho^{\text{h.o.}}(x_0, x_0, \beta)$.

we would for an arbitrary potential. Each path comes with a weight containing terms as the following:

$$\underbrace{\ldots \rho^{\text{free}}(x_{k-1}, x_k, \Delta_\tau)\, \mathrm{e}^{-\frac{1}{2}\Delta_\tau V(x_k)}}_{\rho(x_{k-1}, x_k, \Delta_\tau) \text{ in Trotter formula}} \underbrace{\mathrm{e}^{-\frac{1}{2}\Delta_\tau V(x_k)} \rho^{\text{free}}(x_k, x_{k+1}, \Delta_\tau) \ldots}_{\rho(x_k, x_{k+1}, \Delta_\tau) \text{ in Trotter formula}}.$$

As shown, each argument x_k appears twice, and any two contributions $\exp\left[-\frac{1}{2}\Delta_\tau V(x_k)\right]$, where $V(x) = \frac{1}{2}x^2$, can be combined into a single term $\exp\left[-\Delta_\tau V(x_k)\right]$. To move from one position of the path to the next, we choose a random element k and accept the move $x_k \to x_k + \delta_x$ using the Metropolis algorithm. The ratio of the weights of the new and the old path involves only two segments of the path and one interaction potential (see Alg. 6.4 (`naive-harmonic-path`)). A move of x_k, for $k \neq 0$, involves segments $\{x_{k-1}, x_k\}$ and $\{x_k, x_{k+1}\}$. Periodic boundary conditions in the τ-domain have been worked in: for $k = 0$, we consider the density matrices between $\{x_{N-1}, x_0\}$ and $\{x_0, x_1\}$. Such a move across the horizon $k = 0$ changes x_0 and x_N, but they are the same (see the iteration $i = 10$ in Fig. 6.4).

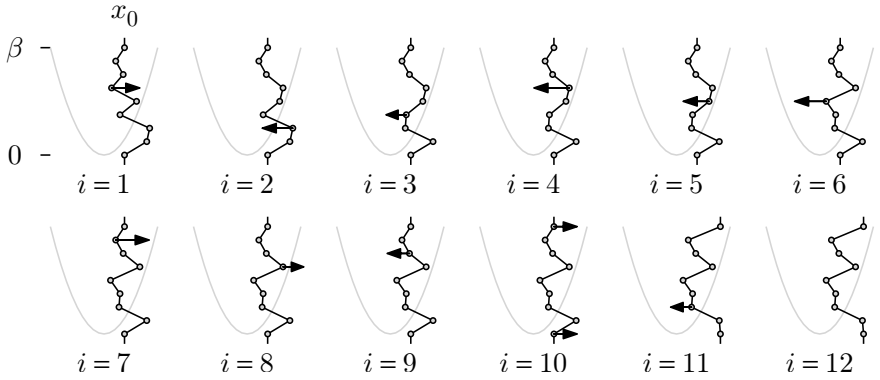

Figure 6.4: Markov-chain path sampling for a harmonic potential (from Alg. 6.4 (`naive-harmonic-path`)).

Algorithm 6.4 (`naive-harmonic-path`) is an elementary path-integral Monte Carlo program. To test it, we can generate a histogram of positions for any of the x_k. For large N, the error in the Trotter formula is negligible. The histogram must then agree with the analytical result for the probability $\pi(x) = \rho^{\text{h.o.}}(x, x, \beta)\,/Z$, which we can also calculate from eqs. (6.24) and (6.26). This simple path-integral Monte Carlo program can in principle, but rarely in practice, solve

problems in equilibrium quantum statistical physics.

6.3.2 Direct path sampling, Lévy construction

procedure `levy-free-path`
input $\{x_0, x_N\}$
$\Delta_\tau \leftarrow \beta/N$
for $k = 1, \ldots, N-1$**:**
$\quad \Delta'_\tau \leftarrow (N-k)\Delta_\tau$
$\quad \langle x_k \rangle \leftarrow (\Delta'_\tau x_{k-1} + \Delta_\tau x_N)/(\Delta_\tau + \Delta'_\tau)$
$\quad \sigma^{-2} \leftarrow \Delta_\tau^{-1} + \Delta_\tau'^{-1}$
$\quad x_k \leftarrow \langle x_k \rangle + \texttt{gauss}\,(\sigma)$
output $\{x_0, \ldots, x_N\}$

Algorithm 6.5: `levy-free-path`. Sampling a path contributing to $\rho^{\text{free}}(x_0, x_N, \beta)$, using the Lévy construction (see Fig. 6.6).

To overcome the limitations of local path sampling, we must analyze the origin of the high rejection rate. As discussed in several other places in this book, a high rejection rate signals an inefficient Monte Carlo algorithm, because it forces us to use small displacements δ. This is what happens in Alg. 6.4 (`naive-harmonic-path`). We cannot move x_k very far away from its neighbors, and are also prevented from moving larger parts of the path, consisting of positions $\{x_k, \ldots, x_{k+l}\}$. For concreteness, we first consider paths contributing to the density matrix of a free particle, and later on the paths for the harmonic oscillator. Let us sample the integral

$$\rho^{\text{free}}(x_0, x_N, \beta) = \int \cdots \int \mathrm{d}x_1 \ldots \mathrm{d}x_{N-1} \underbrace{\rho^{\text{free}}(x_0, x_1, \Delta_\tau)\, \rho^{\text{free}}(x_1, x_2, \Delta_\tau) \ldots \rho^{\text{free}}(x_{N-1}, x_N, \Delta_\tau)}_{\pi(x_1, \ldots, x_{N-1})}. \quad (6.29)$$

We focus for a moment on Monte Carlo moves where all positions except x_k are frozen, in particular x_{k-1} and x_{k+1}. Slightly generalizing the problem, we focus on a position x_k sandwiched in between fixed positions x' and x'', with two intervals in τ, Δ'_τ and Δ''_τ (see Fig. 6.5). In the

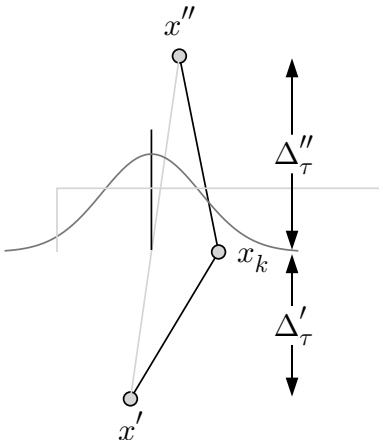

Figure 6.5: Proposed and accepted moves in Alg. 6.4 (`naive-harmonic-path`). The position x_k is restrained by x' and x''.

naive path-sampling algorithm, the move is drawn randomly between $-\delta$ and $+\delta$, around the current position x_k (see Fig. 6.5, again). The distribution of the accepted moves in Fig. 6.5 is given by

$$\pi^{\text{free}}(x_k|x',x'') \propto \rho^{\text{free}}\left(x',x_k,\Delta'_\tau\right)\rho^{\text{free}}\left(x_k,x'',\Delta''_\tau\right),$$

where

$$\rho^{\text{free}}\left(x',x_k,\Delta'_\tau\right) \propto \exp\left[-\frac{(x'-x_k)^2}{2\Delta'_\tau}\right],$$
$$\rho^{\text{free}}\left(x_k,x'',\Delta''_\tau\right) \propto \exp\left[-\frac{(x_k-x'')^2}{2\Delta''_\tau}\right].$$

Expanding the squares and dropping all multiplicative terms independent of x_k, we find the following for the probability of x_k:

$$\underline{\pi^{\text{free}}(x_k|x',x'')} \propto \exp\left(-\frac{\cancel{x'^2}-2x'x_k+x_k^2}{2\Delta'_\tau}-\frac{x_k^2-2x_kx''+\cancel{x''^2}}{2\Delta''_\tau}\right)$$
$$\propto \underline{\exp\left[-\frac{(x_k-\langle x_k\rangle)^2}{2\sigma^2}\right]}, \quad (6.30)$$

where

$$\langle x_k\rangle = \frac{\Delta''_\tau x' + \Delta'_\tau x''}{\Delta'_\tau+\Delta''_\tau}$$

and

$$\sigma^2 = (1/\Delta''_\tau + 1/\Delta'_\tau)^{-1}.$$

The mismatch between the proposed moves and the accepted moves generates the rejections in the Metropolis algorithm. We could modify the naive path-sampling algorithm by choosing x_k from a Gaussian distribution with the appropriate parameters (taking $x' \equiv x_{k-1}$ (unless $k=0$), $x'' \equiv x_{k+1}$, and $\Delta'_\tau = \Delta''_\tau = \beta/N$). In this way, no rejections would be generated.

The conditional probability in eq. (6.30) can be put to much better use than just to suppress a few rejected moves in a Markov-chain algorithm. In fact, $\pi^{\text{free}}(x_k|x',x'')$ gives the weight of all paths which, in Fig. 6.5, start at x', pass through x_k and end up at x''. We can sample this distribution to obtain x_1 (using $x'=x_0$ and $x''=x_N$). Between the freshly sampled x_1 and x_N, we may then pick x_2, and thereafter x_3 between x_2 and x_N and, eventually, the whole path $\{x_1,\ldots,x_N\}$ (see Fig. 6.7 and Alg. 6.5 (`levy-free-path`)). A directly sampled path with $N=50\,000$ is shown in Fig. 6.6; it can be generated in a split second, has no correlations with previous paths, and its construction has caused no rejections. In the limit $N\to\infty$, $x(\tau)$ is a differentiable continuous function of τ.

Direct path sampling—in other words, the Lévy construction—was introduced by Lévy (1940) as a stochastic interpolation between points x_0 and x_N. This generalizes interpolations using polynomials, trigonometric functions, splines, wavelets etc. The Lévy construction is local: the path $x(\tau)$, in any interval $[\tau_1,\tau_2]$, is the stochastic interpolation of its end points $x(\tau_1)$ and $x(\tau_2)$, but the behavior of the path outside the interval plays no role.

6.3.3 Lévy construction in a harmonic potential

We now consider the Lévy construction for a harmonic oscillator. The algorithm can be generalized to this case because the harmonic density matrix is a Gaussian (the exponential of a

Figure 6.6: A path contributing to $\rho^{\text{free}}(x_0, x_N, \beta)$ (from Alg. 6.5 (`levy-free-path`), with $N = 50\,000$).

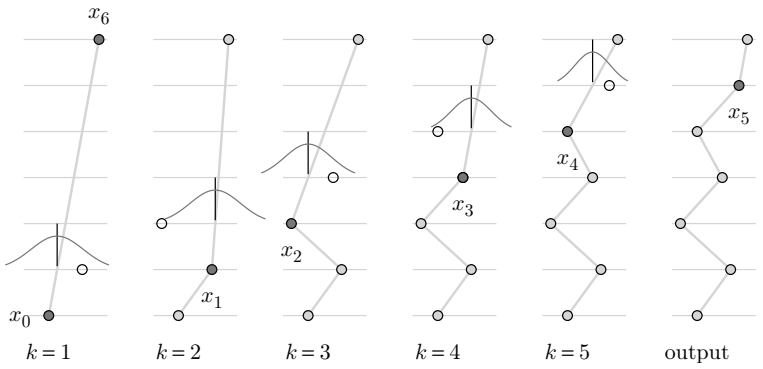

Figure 6.7: Lévy construction of a free-particle path from x_0 to x_6 (see Alg. 6.5 (`levy-free-path`)).

procedure `levy-harmonic-path`
input $\{x_0, x_N\}$
$\Delta_\tau \leftarrow \beta/N$
for $k = 1, \ldots, N-1$**:**

$$\left\{\begin{array}{l} \Upsilon_1 \leftarrow \coth \Delta_\tau + \coth\left[(N-k)\Delta_\tau\right] \\ \Upsilon_2 \leftarrow x_{k-1}/\sinh \Delta_\tau + x_N/\sinh\left[(N-k)\Delta_\tau\right] \\ \langle x_k\rangle \leftarrow \Upsilon_2/\Upsilon_1 \\ \sigma \leftarrow 1/\sqrt{\Upsilon_1} \\ x_k \leftarrow \langle x_k\rangle + \texttt{gauss}\,(\sigma) \end{array}\right.$$

output $\{x_0, \ldots, x_N\}$

Algorithm 6.6: `levy-harmonic-path`. Sampling a path contributing to $\rho^{\text{h.o.}}(x_0, x_N, \beta)$, using the Lévy construction (see Fig. 6.8).

quadratic polynomial), and the convolution of two Gaussians is again a Gaussian:

$$\rho^{\text{h.o.}}\left(x', x'', \Delta'_\tau + \Delta''_\tau\right) = \int \mathrm{d}x_k \underbrace{\rho^{\text{h.o.}}\left(x', x_k, \Delta'_\tau\right) \rho^{\text{h.o.}}\left(x_k, x'', \Delta''_\tau\right)}_{\pi^{\text{h.o.}}(x_k|x',x'')}.$$

Because of the external potential, the mean value $\langle x_k\rangle$ no longer lies on the straight line between x' and x''. From the nondiagonal harmonic density matrix in eq. (6.23), and proceeding as in eq. (6.30), we find the following:

$$\pi^{\text{h.o.}}(x_k|x', x'') \propto \exp\left[-\frac{1}{2\sigma^2}\left(x_k - \langle x_k\rangle\right)^2\right],$$

with parameters

$$\begin{aligned} \langle x_k\rangle &= \frac{\Upsilon_2}{\Upsilon_1}, \\ \sigma &= \Upsilon_1^{-1/2}, \\ \Upsilon_1 &= \coth\ \Delta'_\tau + \coth\ \Delta''_\tau, \\ \Upsilon_2 &= \frac{x'}{\sinh \Delta'_\tau} + \frac{x''}{\sinh \Delta''_\tau}, \end{aligned}$$

as already used in the analytic matrix squaring for the harmonic oscillator. We can thus directly sample paths contributing to the harmonic density matrix $\rho^{\text{h.o.}}(x_0, x_N, \beta)$ (see Alg. 6.6

(`levy-harmonic-path`)), and also paths contributing to $Z^{\text{h.o.}} = \int \mathrm{d}x_0 \; \rho^{\text{h.o.}}(x_0, x_0, \beta)$, if we first sample x_0 from the Gaussian diagonal density matrix in eq. (6.24).

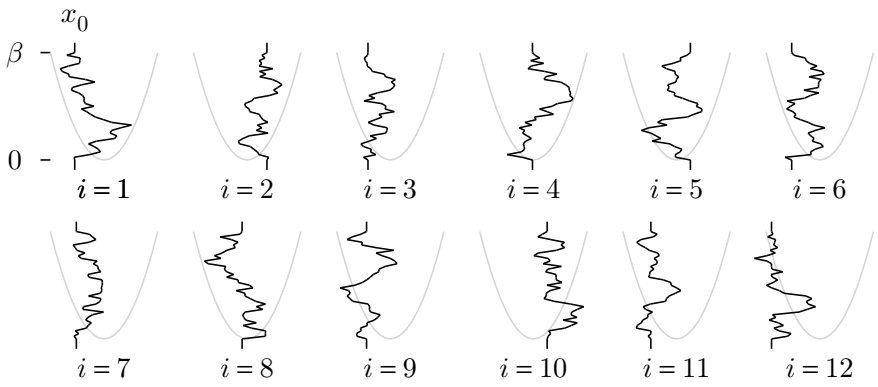

Figure 6.8: Paths contributing to $Z^{\text{h.o.}} = \int \mathrm{d}x_0 \; \rho^{\text{h.o.}}(x_0, x_0, \beta)$ (from Alg. 6.6 (`levy-harmonic-path`), with x_0 first sampled from eq. (6.24)).

In Alg. 6.5 (`levy-free-path`), we were not obliged to sample the path in chronological order (first x_0, then x_1, then x_2, etc.). After fixing x_0 and x_N, we could have chosen to sample the midpoint $x_{N/2}$, then the midpoint between x_0 and $x_{N/2}$ and between $x_{N/2}$ and x_N, etc..

References

[1] W. Krauth, *Statistical Mechanics: Algorithms and Computations*. Oxford University Press, 2006.