Exercise: Evaluate the Feynman path integral for the free particle by means of discretization. Why is the result independent of the number N of discretization steps?

Solution:

The discretized version of the propagator of a free particle is given by

$$K(q_\mathrm{f}, q_\mathrm{i}, t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}} \int_{-\infty}^{+\infty} \prod_{n=1}^{N-1} \left(\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}} \mathrm{d}q_n\right) \exp\left(\frac{\mathrm{i}}{\hbar} \sum_{n=1}^{N} \frac{m}{2} \frac{(q_n - q_{n-1})^2}{\Delta t}\right) . \tag{1}$$

Here, $q_N = q_\mathrm{f}$ and $q_0 = q_\mathrm{i}$.

For a multidimensional Gaussian integral, we have

$$\int_{-\infty}^{+\infty} \mathrm{d}x^N \mathrm{e}^{-\mathbf{x}^\mathrm{T}\mathbf{A}\mathbf{x}} = \sqrt{\frac{\pi^N}{\det(\mathbf{A})}} . \tag{2}$$

Without loss of generality, the matrix $\mathbf{A}$ can be assumed to be symmetric, because an antisymmetric matrix will not contribute to the bilinear form. The relation (2) can then be proven by transforming into the eigenbasis of $\mathbf{A}$ and carrying out the individual integrals. The right-hand side is then obtained by realizing that the product of eigenvalues equals the determinant of the corresponding matrix.

The same line of reasoning can be applied to a Fresnel integral and we find

$$\int_{-\infty}^{+\infty} \mathrm{d}x^N \mathrm{e}^{\mathrm{i}\mathbf{x}^\mathrm{T}\mathbf{A}\mathbf{x}} = \sqrt{\frac{(\mathrm{i}\pi)^N}{\det(\mathbf{A})}} . \tag{3}$$

We thus aim at bringing (1) into such a form.

In a first step, we consider the sum in the exponent.

$$\sum_{n=1}^{N} (q_n - q_{n-1})^2 = q_{N-1}^2 + q_1^2 + \sum_{n=2}^{N-1} (q_n - q_{n-1})^2 - 2q_\mathrm{f}q_{N-1} - 2q_\mathrm{i}q_1 + q_\mathrm{f}^2 + q_\mathrm{i}^2 . \tag{4}$$

Realizing that all squares of $q_i, i = 1, \ldots, N-1$ appear twice and that the mixed terms arising from the squares in the sum have to be splitted into two contributions in a bilinear form, we obtain

$$\sum_{n=1}^{N} (q_n - q_{n-1})^2 = \mathbf{x}^T\mathbf{A}\mathbf{x} - 2\mathbf{b}^T\mathbf{x} + q_\mathrm{f}^2 + q_\mathrm{i}^2 . \tag{5}$$

Here, we have introduced the tridiagonal $(N-1) \times (N-1)$ matrix

$$\mathbf{A} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix} \tag{6}$$

and the vectors

$$\mathbf{x} = \begin{pmatrix} q_{N-1} \\ q_{N-2} \\ \vdots \\ q_2 \\ q_1 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} q_{\mathrm{f}} \\ 0 \\ \vdots \\ 0 \\ q_{\mathrm{i}} \end{pmatrix} \tag{7}$$

In (5) we can now complete the square to obtain

$$\sum_{n=1}^{N}(q_n - q_{n-1})^2 = (\mathbf{x}^T - \mathbf{b}^T\mathbf{A}^{-1})\mathbf{A}(\mathbf{x} - \mathbf{A}^{-1}\mathbf{b}) - \mathbf{b}^T\mathbf{A}^{-1}\mathbf{b} + q_{\mathrm{f}}^2 + q_{\mathrm{i}}^2\,. \tag{8}$$

Carrying out the Fresnel integrals with the help of (3) we find as a first result

$$K(q_{\mathrm{f}}, q_{\mathrm{i}}, t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t\det(\mathbf{A})}}\exp\left(\frac{\mathrm{i}m}{2\hbar\Delta t}(q_{\mathrm{f}}^2 + q_{\mathrm{i}}^2 - \mathbf{b}^T\mathbf{A}^{-1}\mathbf{b})\right)\,. \tag{9}$$

In order to proceed further, we need to evaluate the determinant of the matrix $\mathbf{A}$ defined in (6). One possibility is to realize that $\mathbf{A}$ is a tridiagonal Toeplitz matrix for which the eigenvalues are known analytically. For our special case, the eigenvalues read

$$\lambda_k = 2\left(1 + \cos\left(\frac{\pi k}{N}\right)\right) \qquad k = 1, \dots, N-1 \tag{10}$$

The determinant D_{N-1} of the $(N-1)\times(n-1)$ matrix $\mathbf{A}$ then becomes

$$\begin{aligned} D_{N-1} = \det(\mathbf{A}) &= \prod_{k=1}^{N-1} 2\left(1 + \cos\left(\frac{\pi k}{N}\right)\right) \\ &= \lim_{x\to -1}\prod_{k=1}^{N-1}\left(x^2 - 2x\cos\left(\frac{\pi k}{N}\right) + 1\right) \\ &= \lim_{x\to -1}\frac{x^{2N}-1}{x^2-1} \\ &= N\,. \end{aligned} \tag{11}$$

This result can also be obtained by induction. The determinant of $\mathbf{A}$ satisfies the recursion relation

$$D_n = 2D_{n-1} - D_{n-2} \tag{12}$$

with the initial conditions

$$D_1 = 2, D_2 = 3\,. \tag{13}$$

It can easily be checked that this recursion problem is indeed solved by $D_{N-1} = N$.

In view of the exponent of (9), we need the entries in the corners of the matrix $\mathbf{A}^{-1}$ which can easily be obtained by directly determining the corresponding elements of the adjugate matrix. On the diagonal, we find

$$(\mathbf{A}^{-1})_{11} = (\mathbf{A}^{-1})_{N-1,N-1} = \frac{D_{N-2}}{D_{N-1}} = 1 - \frac{1}{N}\,. \tag{14}$$

In the off-diagonal corners, the adjugate matrix takes the value 1 and we obtain

$$(\mathbf{A}^{-1})_{N-1,1} = (\mathbf{A}^{-1})_{1,N-1} = \frac{1}{D_{N-1}} = \frac{1}{N}\,. \tag{15}$$

In the exponent of (9), we thus have

$$\mathbf{b}^T\mathbf{A}^{-1}\mathbf{b} = \left(1 - \frac{1}{N}\right)(q_{\mathrm{f}}^2 + q_{\mathrm{i}}^2) + \frac{2}{N}q_{\mathrm{f}}q_{\mathrm{i}} = q_{\mathrm{f}}^2 + q_{\mathrm{i}}^2 - \frac{(q_{\mathrm{f}} - q_{\mathrm{i}})^2}{N} \tag{16}$$

Inserting this result together with (11) into (9), we arrive at

$$K(q_{\mathrm{f}}, q_{\mathrm{i}}, t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar N\Delta t}} \exp\left(\frac{\mathrm{i}m}{2\hbar}\frac{(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{N\Delta t}\right) . \tag{17}$$

Since we had divided the original time interval of length t into N equidistant pieces, we have $\Delta t = t/N$ and thus find the exact propagator of the free particle

$$K(q_{\mathrm{f}}, q_{\mathrm{i}}, t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}} \exp\left(\frac{\mathrm{i}m}{2\hbar}\frac{(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{t}\right) . \tag{18}$$

The fact that we obtain the correct result for any value of N and do not need to take the limit $N \to \infty$ is exceptional. The reason is that for vanishing potential energy $V = 0$, the Lie-Trotter formula is exact not only in the limit $N \to \infty$ but also for any finite N. Another way of viewing it is that the decomposition in the initial expression (1) is nothing else than a multiple application of the semigroup property which we had proven in another exercise.