Derivation of the density matrix of the harmonic oscillator through analytical matrix-squaring (section 3.2.2 of Werner's book).

For the classic derivations of the harmonic oscillator, see:

- R. P. Feynman "Statistical Mechanics: A set of lectures"
- L.L Landau, E.M Lifshitz "Quantum Mechanics" (Theoretical Physics, part 3)
- (and many articles on the web)

Matrix squaring was first applied by Storer (1968) to the convolution of density matrices. It 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 eqn (3.31) (see Alg. 3.3 (`matrix-square`)). We need not solve for eigenfunctions and eigenvalues of the Schrödinger equation. To test the program, we may iterate Alg. 3.3 (`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. 3.3.

procedure `matrix-square`
input $\{x_0, \ldots, x_K\}, \{\rho(x_k, x_l, \beta)\}$ (grid with step size Δ_x)
for $x = x_0, \ldots, x_K$ **do**
$\left\{ \begin{array}{l} \textbf{for } x' = x_0, \ldots, x_K \textbf{ do} \\ \quad \left\{ \rho(x, x', 2\beta) \leftarrow \sum_k \Delta_x \rho(x, x_k, \beta)\, \rho(x_k, x', \beta) \right. \end{array} \right.$
output $\{\rho(x_k, x_l, 2\beta)\}$
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Algorithm 3.3 `matrix-square`. Density matrix at temperature $1/(2\beta)$ obtained from that at $1/\beta$ by discretizing the integral in eqn (3.32).

3.2.2 Harmonic oscillator (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 (see Subsection 3.2.1). 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 in later sections and chapters.

The density matrix at high temperature,

$$\rho^{\text{h.o.}}(x, x', \beta) \xrightarrow[\beta\to 0]{\substack{\text{from} \\ \text{eqn (3.30)}}} \sqrt{\frac{1}{2\pi\beta}} \exp\left[-\frac{\beta}{4}x^2 - \frac{(x-x')^2}{2\beta} - \frac{\beta}{4}x'^2\right],$$

can be written as

$$\rho^{\text{h.o.}}(x, x', \beta) = c(\beta) \exp\left[-g(\beta)\frac{(x-x')^2}{2} - f(\beta)\frac{(x+x')^2}{2}\right], \quad (3.33)$$

where

$$f(\beta) \xrightarrow[\beta\to 0]{} \frac{\beta}{4},$$
$$g(\beta) \xrightarrow[\beta\to 0]{} \frac{1}{\beta} + \frac{\beta}{4}, \qquad (3.34)$$
$$c(\beta) \xrightarrow[\beta\to 0]{} \sqrt{\frac{1}{2\pi\beta}}.$$

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

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

must also have the functional form of eqn (3.33). We recast the exponential in the above integrand,

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

and obtain, using eqn (3.12),

$$\rho^{\text{h.o.}}(x, x'', 2\beta)$$
$$= c(2\beta)\exp\left[-\frac{f+g}{2}\left(x^2 + x''^2\right) + \frac{1}{2}\frac{(f-g)^2}{f+g}\frac{(x+x'')^2}{2}\right]. \qquad (3.35)$$

The argument of the exponential function in eqn (3.35) 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

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

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 eqn (3.34), and therefore

$$g(2\beta) = \frac{g(\beta) + (1/4)g^{-1}(\beta)}{2}. \tag{3.36}$$

We can easily check that the only function satisfying eqn (3.36) with the limit in eqn (3.34) 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

$$\begin{aligned} &\rho^{\text{h.o.}}(x, x', \beta) \\ &= \sqrt{\frac{1}{2\pi\sinh\beta}}\exp\left[-\frac{(x+x')^2}{4}\tanh\frac{\beta}{2} - \frac{(x-x')^2}{4}\coth\frac{\beta}{2}\right], \end{aligned} \tag{3.37}$$

and the diagonal density matrix is

$$\rho^{\text{h.o.}}(x, x, \beta) = \sqrt{\frac{1}{2\pi\sinh\beta}}\exp\left(-x^2\tanh\frac{\beta}{2}\right). \tag{3.38}$$

To introduce physical units into these two equations, we must replace

$$\begin{aligned} x &\to \sqrt{\frac{m\omega}{\hbar}}x, \\ \beta &\to \hbar\omega\beta = \frac{\hbar\omega}{k_{\mathrm{B}}T}, \end{aligned}$$

and also multiply the density matrix by a factor $\sqrt{m\omega/\hbar}$.

We used Alg. 3.2 (`harmonic-density`) earlier to compute the diagonal density matrix $\rho^{\text{h.o.}}(x, x, \beta)$ from the wave functions and energy eigenvalues. We now see that the resulting plots, shown in Fig. 3.3, are simply Gaussians of variance

$$\sigma^2 = \frac{1}{2\tanh(\beta/2)}. \tag{3.39}$$

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 eqn (3.39) for $\beta \to 0$). Integrating the diagonal density matrix over space gives the partition function of the harmonic oscillator:

$$Z^{\text{h.o.}}(\beta) = \int \mathrm{d}x\; \rho^{\text{h.o.}}(x, x, \beta) = \frac{1}{2\sinh(\beta/2)}, \tag{3.40}$$

where we have used the fact that

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