Solution Exercise 1

Problem 1: Classical and Quantum statistics

a) See `solution01.py`. The normal distribution with mean μ and standard deviation σ,

$$\frac{1}{\sqrt{2\pi\sigma^2}}\mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{1.1}$$

can be sampled using the command `numpy.random.normal`(μ, σ, N), which returns a one-dimensional array of N samples. Comparing Eq. (1.1) with the distribution in the exercise, we have $\mu_x = \mu_p = 0,\ \sigma_x = \sqrt{1/\beta m\omega^2},\ \sigma_p = \sqrt{m/\beta}$.

b) See `solution01.py`. The only difference to the classical case are the standard deviations, which for the Wigner distribution are $\sigma_x = \sqrt{\hbar/2m\omega\alpha}$ and $\sigma_p = \sqrt{m\hbar\omega/2\alpha}$, where $\alpha = \tanh(\beta\hbar\omega/2)$.

Side note: While in the present case the Wigner distributions is positive definite, in general it is not guaranteed to be so. It is therefore more properly called a quasiprobability distribution. For example, the Wigner distribution of an excited state of the harmonic oscillator can take on negative values. In such cases numerical evaluation of integrals by sampling becomes considerably more challenging due to slow convergence.

c) See Figure 1-1.

d) See Figure 1-1.

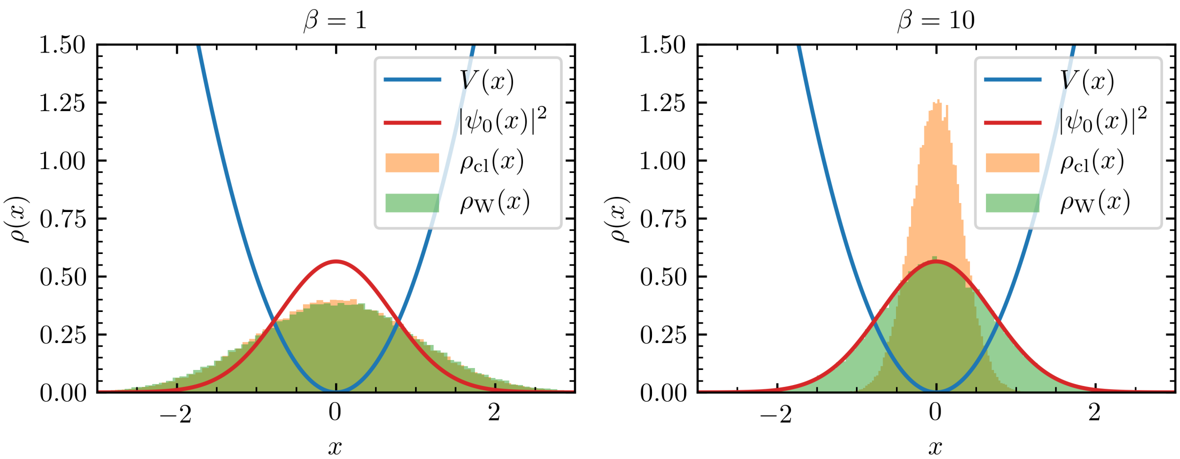

Figure 1-1: Classical and Wigner densities for $\beta = 1$ and 10, calculated using 10^5 samples. The two distributions are similar for $\beta\hbar\omega \leq 1$, because then $\tanh(\beta\hbar\omega/2) \approx \beta\hbar\omega/2$. For $\beta\hbar\omega \gg 1$, the Wigner distribution is wider since it takes quantum effects into account. In the limit as $\beta \to \infty$, $\tanh(\beta\hbar\omega/2) \to 1$, so that the Wigner distribution approaches the correct ground-state probability density $|\psi_0(x)|^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \mathrm{e}^{-m\omega x^2/\hbar}$.

e) Typical stretch modes have frequencies in the range of 1000–3000 cm^{-1}, while at room temperature $k_\mathrm{B}T$ corresponds to ≈ 200 cm^{-1}. This means that $\beta\hbar\omega \gg 1$ [like in 1d)], so that the mode is overwhelmingly likely to be found in its vibrational ground state. As seen in Figure 1-1, the classical distribution would then be too narrow (because it neglects quantum effects), while the Wigner distribution approaches the correct ground-state probability density.

f) Odd functions like $x\,\mathrm{e}^{-ax^2}$ integrate to zero, so $\langle x\rangle = \langle xp\rangle = 0$. Your numerical results will not be exactly zero, but should tend to zero as you increase the number of samples. The remaining observable of interest is

$$\langle x^2\rangle = \frac{\iint_{\mathbb{R}^2} x^2 \rho(x,p)\,\mathrm{d}x\,\mathrm{d}p}{\iint_{\mathbb{R}^2} \rho(x,p)\,\mathrm{d}x\,\mathrm{d}p}. \tag{1.2}$$

For both the classical and the Wigner densities, $\rho(x,p)$ is a product of two Gaussians. The momentum integral is the same in the numerator and the denominator, and therefore cancels. The position integrals can be evaluated using the hint in 1f) or by noting that for a normal distribution [Eq. (1.1)], $\langle x^2\rangle = \sigma^2$. The final results are given in Table 1.1. For $\beta = 1$, $\langle x^2\rangle$ is close to 1 for both distributions, whereas for $\beta = 10$, you should get 0.1 in the classical case and approximately 0.5 in the quantum (Wigner) case.

Table 1.1: Analytical expressions for the expectation values.

	$\langle x\rangle$	$\langle x^2\rangle$	$\langle xp\rangle$
Classical	0	$\frac{1}{m\beta\omega^2}$	0
Wigner	0	$\frac{\hbar}{2m\omega}\coth\left(\frac{\beta\hbar\omega}{2}\right)$	0

g) See Figure 1-2 overleaf.

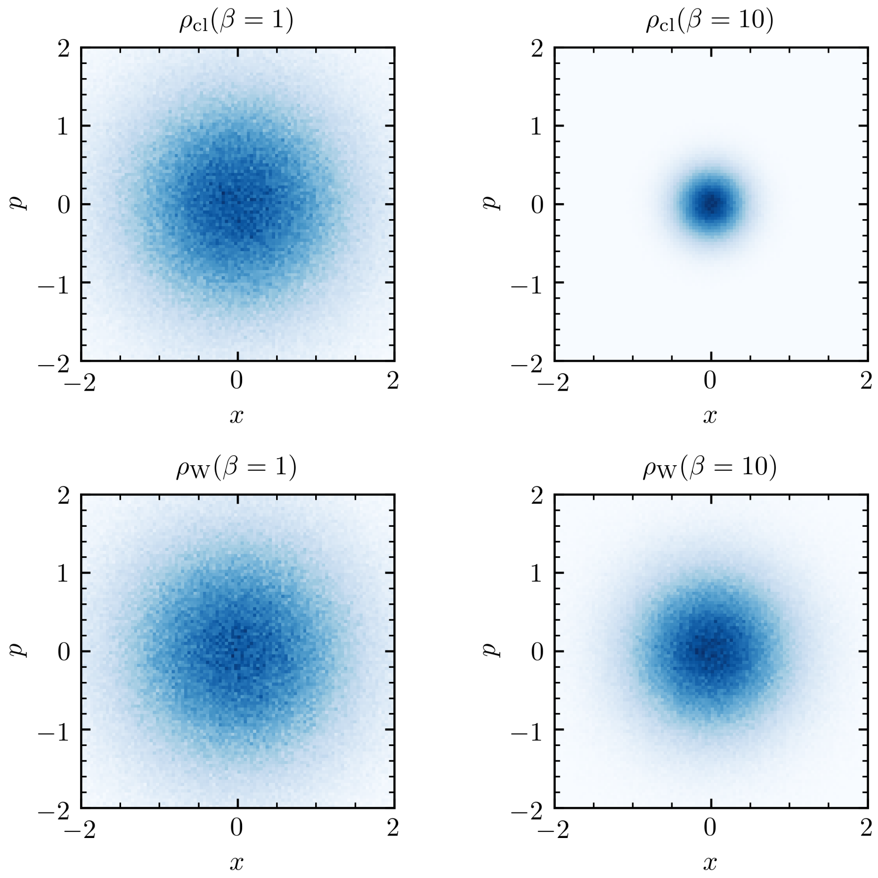

Figure 1-2: Like in Figure 1-1, the classical and Wigner densities are similar at $\beta = 1$ (high temperature), whereas at $\beta = 10$ (low temperature), the classical density is considerably narrower than the Wigner distribution.