

**Problem 1.** Consider the Hamiltonian for a particle in a harmonic potential in one dimension.

$$\mathcal{H}(r, p) = K(p) + U(x) = \frac{p^2}{2m} + \frac{1}{2}kx^2 \quad (1)$$

Use Hamilton's equations to find the time derivatives of the position and momentum of the particle. For initial conditions  $x(0) = 1$  and  $p(0) = 0$ , determine  $x(t)$  and  $p(t)$ . Use these solutions to plot the trajectory of the particle in phase space (let the  $y$  axis be momentum and the  $x$  axis be position) and label the initial position of the particle. In a separate plot, draw  $x(t)$  as a function of  $t$ .

**Problem 2.** Gibbs's paradox. Using the canonical partition function for an ideal gas derived in class, calculate the dimensionless entropy using

$$\frac{S}{k} = \beta \langle E \rangle - \beta A = -\beta \frac{\partial \ln Q}{\partial \beta} + \ln Q \quad (2)$$

and argue that this quantity is extensive. Now, pretend that you're Gibbs back in the nineteenth century before the formulation of quantum mechanics and you've derived the partition function

$$Q_G(\beta, N, V) = \frac{1}{g^{3N}} \int dr^N dp^N e^{-\beta \mathcal{H}(r^N, p^N)} \quad (3)$$

where  $g$  has units of momentum times length and makes  $Q$  dimensionless. Note the absence of the  $(N!)^{-1}$  factor. For an ideal gas, calculate the partition function and the entropy  $S_G/k$ . Is the entropy extensive?

Now consider the mixing of two gases. To begin, the gas is separated by a partition into two regions with equal density:  $\rho = N_1/V_1 = N_2/V_2$ . Then we remove the partition and allow the particles to mix. Calculate the entropy of mixing

$$\frac{\Delta S_m}{k} = \frac{S_f}{k} - \frac{S_i}{k} \quad (4)$$

using both  $Q$  given in class and  $Q_G$  assuming that the initial entropy  $S_i$  is the sum of the entropies of the two regions. Explain the differences in the two answers.

**Problem 3.** Consider the integral

$$J = \int_{-\infty}^{\infty} e^{-ax^2+bx} dx \quad (5)$$

and evaluate the answer. (Hint: manipulate the argument of the exponent until it looks like the Gaussian integral discussed in class.) This integral is the basis for particle to field transformations used to understand polymer physics. Use the result in this quantum mechanics problem. Let

$$\psi(x) = \frac{1}{(\Delta^2 \pi)^{1/4}} e^{-x^2/(2\Delta^2)} \quad (6)$$

be a Gaussian wave function normalized such that  $\int |\psi(x)|^2 dx = 1$  and where  $\Delta$  is the uncertainty in position. Quantum mechanics stipulates that the wave function in the momentum basis is

$$\psi(p) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{h}} e^{ip(2\pi/h)x} \psi(x) dx \quad (7)$$

Calculate this wave function and determine the product of the uncertainty in position and the uncertainty in momentum. Look familiar? Calculating the wave function in the momentum basis amounts to taking a Fourier transform with  $k = 2\pi p/h$ , and the Fourier transform of a Gaussian is a Gaussian.