

atoms in the other rings through an interparticle potential. If the quantum system is a fluid where indistinguishability is important, then we must consider the effect of exchange by treating the quantum system as a classical polymer system where the “atoms” represent the monomers of a polymer, and where polymers can split up and reform. Chandler and Wolynes discuss how the quantum mechanical effects due to exchanging identical particles can be associated with the chemical equilibrium of the polymers. They also discuss Bose condensation using path integral techniques.

**Problem 16.31.** Path integral calculation

- Write a program to implement the path integral algorithm for the one-dimensional harmonic oscillator potential with  $V(x) = x^2/2$ . Use the structure of your Monte Carlo Lennard-Jones program from Chapter 15 as a guide.
- Let  $N\Delta\tau = 15$  and consider  $N = 10, 20, 40,$  and  $80$ . Equilibrate for at least 2000 Monte Carlo steps per atom and average over at least 5000 mcs. Compare your results with the exact result for the ground state energy given by  $E_0 = 0.5$ . Estimate the equilibration time for your calculation. What is a good initial configuration? Improve your results by using larger values of  $N\Delta\tau$ .
- Find the mean energy,  $\langle E \rangle$ , of the harmonic oscillator at the temperature  $T$  determined by  $\beta = N\Delta\tau$ . Find  $\langle E \rangle$  for  $\beta = 1, 2,$  and  $3$ , and compare it with the exact result  $\langle E \rangle = \frac{1}{2} \coth(\beta/2)$ .
- Repeat the above calculations for the Morse potential  $V(x) = 2(1 - e^{-x})^2$ .

## 16.11 Projects

Many of the techniques described in this chapter can be extended to two-dimensional quantum systems. The `Complex2DFrame` tool in the frames package is designed to show two-dimensional complex scalar fields such as quantum wave functions. Listing 16.13 in Appendix A shows how this class is used to show a two-dimensional Gaussian wave packet with a momentum boost.

**Project 16.32.** Separable systems in two dimensions

The shooting method is inappropriate for the calculation of eigenstates and eigenvalues in two or more dimensions with arbitrary potential energy functions,  $V(\mathbf{r})$ . However, the special case of separable potentials can be reduced to several one-dimensional problems that can be solved using the numerical methods described in this chapter. Many molecular modeling programs use the Hartree-Fock self-consistent field approximation to model non-separable systems as a set of one-dimensional problems. Recently, there has been significant progress motivated by a molecular dynamics algorithm developed by Car and Parrinello.

Write a two-dimensional eigenstate class, `Eigenstate2d`, that calculates eigenstates and eigenvalues for a separable potential of the form:

$$V(x, y) = V_1(x) + V_2(y). \quad (16.106)$$