Chapter 3 Problems

1. For a Hamiltonian of the form $\hat{H}^2 = \hat{p}^2/2\mathrm{m} + V(x)$ calculate the quantities

$$\frac{\partial}{\partial t}\langle x^2 \rangle \text{ and } \frac{\partial}{\partial t}\langle \hat{p}^2 \rangle.$$

   Note that the commutator $[\hat{A}, \hat{B}^2]$ can be written as $[\hat{A}, \hat{B}]\hat{B} + \hat{B}[\hat{A}, \hat{B}]$.

2. An H_2 or a D_2 molecule can be idealized as a harmonic oscillator with force constant $k = 575\ \mathrm{Nm}^{-1}$. In this idealization the ground state wavefunctions for H_2 and D_2 are Gaussians.

$$\Phi_0(x) = N_0 e^{-\alpha x^2/2}$$

   where $\alpha = 2\pi\mu\upsilon/\hbar$ and $\upsilon = \frac{1}{2\pi}\sqrt{k/\mu}$, which μ the reduced mass of either H_2 or D_2.

   (a) Express the FWHM in terms of μ and k.

   (b) What is the FWHM for H_2 and D_2 in m?

   Suppose that the potential holding the atoms together is suddenly "removed" and the molecule travels through a potential-free region.

   (c) Give an expression for the time-dependence of the FWHM.

   (d) Calculate the FWHM for both molecules after one vibrational period $T = 1/\upsilon$.

   (e) Calculate the FWHM for both molecules after $t = 1$ second.

3. (a) Show that

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-x^2/4\beta^2} e^{-ikx} \mathrm{d}x = e^{-\beta^2 k^2}\sqrt{2\beta^2}$$

   using the standard integral

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\alpha x^2} \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}$$

   (b) Use the result from (a) to prove Eq. (3.37) from Eq. (3.36).

4. Using Eqs. (B3.5.1)–(B3.5.5) of Study Box 3.5, explicitly derive the elements of the local R-matrix of Eq. (3.62).
5. Eq. (3.88) gives the relation between gives the relation between $\psi(\boldsymbol{q}, t)$ and $\psi(\boldsymbol{q}, t + \Delta t)$ *via* the time evolution propagator.
   (a) Give an expression for the relation between $\psi(t)$ and $\psi(\boldsymbol{q}, t - \Delta t)$.
   (b) Use this relation and Eq. (7.18) to derive an expression for the propagation of $\psi(t - \Delta t)$ to $\psi(t + \Delta t)$.
   (c) If you use the above result to propagate a wavefunction, do the real part and the imaginary part of the wavefunction have to be propagated simultaneously or can they be propagated separately? Why?
6. Explicitly derive Eqs. (3.97) (a) and (b).