Quantum Molecular Dynamics Homework 3 Spring, 2000

1. Consider a particle in a harmonic well, starting at $t = 0$ with $q = -q_0$ and $p = 0$. Sketch the location of the particle in phase space at $t = 0$, $1/4\tau$, $1/2\tau$, $3/4\tau$, andτ, where τ is a period of motion. Connect the points and show that the orbit is an ellipse. Which way does the phase space orbit circulate, clockwise or counterclockwise?

2. Consider a pendulum, starting at $t = 0$ with $q = 0$ and $p = p_0$. Sketch the location of the particle in phase space at $t = 0$, $1/4\tau$, $1/2\tau$, $3/4\tau$, andτ, where τ is a period of motion. You should get discover three different regions, two corresponding to rotation and one to libration, depending on the value of p_0. Show that the direction of the rotational orbits in phase space correlate smoothly with those of the libration at separatrix.

3. To understand why the Fourier transform variable p in the definition of the Wigner function has the physical meaning of a momentum, examine the structure of the quantity $<x'|\Psi><\Psi|x>$ for the case where $\Psi(x) = Ne^{-\alpha(x-x_0)^2+ip_0(x-x_0)}$. This product is a function of the variables x and x' and is complex. Plot the real part of this product and discuss the wavelength of oscillations along the $s = x - x'$ coordinate. If the object is Fourier transformed along the $s = x - x'$ coordinate, where will its peak be in the Fourier variable, p?

4. The Wigner distribution has several important properties which suggest its interpretation as a probability distribution:

$$\int_{-\infty}^{\infty} f_W(p,q)\,dp = <q|\Psi><\Psi|q> = |\Psi(q)|^2 \tag{4.1}$$

$$\int_{-\infty}^{\infty} f_W(p,q)\,dq = <p|\Psi><\Psi|p> = |\tilde{\Psi}(p)|^2 \tag{4.2}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_W(p,q)\,dpdq = 1 \tag{4.3}$$

where $\tilde{\Psi}(p)$ is the momentum representation of the wavefunction $|\Psi>$. Derive these relations.

5. Consider the normalized wavepacket

$$\Psi(q,t) = (\frac{2Re\alpha_t}{\pi})^{1/4} e^{-\alpha_t(q-q_t)^2+\frac{i}{\hbar}p_t(q-q_t)+\frac{i}{\hbar}\gamma_t}, \tag{5.1}$$

and assume that γ_t is real.

a. Taking $\alpha_t = \frac{m\omega}{2\hbar}$, show that

$$f_W(q,p) = \frac{1}{\pi\hbar} e^{-\frac{m\omega}{\hbar}(q-q_t)^2} e^{-\frac{1}{m\omega\hbar}(p-p_t)^2}. \tag{5.2}$$

b. Show that in the more general case, where

$$\alpha_t = a(\frac{\alpha_0 \cos\omega t + ia\sin\omega t}{i\alpha_0 \sin\omega t + a\cos\omega t}) \tag{5.3}$$

($a = \frac{m\omega}{2\hbar}$), the Wigner distribution takes the form:

$$f_W(q,p) = \frac{1}{\pi\hbar} e^{-\frac{2|\alpha_t|^2}{\mathrm{Re}\,\alpha_t}(q-q_t)^2} e^{-\frac{1}{2\hbar^2 \mathrm{Re}\,\alpha_t}(p-p_t)^2} e^{-\frac{2\mathrm{Im}\,\alpha_t}{\hbar \mathrm{Re}\,\alpha_t}(q-q_t)(p-p_t)}. \tag{5.4}$$

6. Calculate $\mathrm{Tr}(\rho)$ and $\mathrm{Tr}(\rho^2)$ for the generic 2x2 density matrix:

$$\rho_{mn} = \begin{pmatrix} |a|^2 & a^*b \\ ab^* & |b|^2 \end{pmatrix} \tag{6.1}$$

Then repeat, this time with the off-diagonal elements set equal to 0. Show that in the first case $Tr(\rho^2) = 1$ (pure state) and in the second case $Tr(\rho^2) \leq 1$ (mixed state).

7. Verify that

$$Tr(\rho^2) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq \rho_W^2(p,q)$$

for the harmonic oscillator potential. First calculate the LHS using both the energy representation for ρ:

$$< \psi_n|\rho|\psi_m >= e^{-\beta E_n}/Q\delta_{nm} \qquad Q = \sum_n e^{-\beta E_n}. \tag{7.1}$$

Then repeat the calculation using the x representation for ρ:

$$\frac{< x'|e^{-\beta H}|x >}{Q} = (\frac{m\omega}{\pi\hbar}\tanh(f/2))^{1/2} exp\{\frac{-m\omega}{2\hbar\sinh(f)}[(x^2 + x'^2)\cosh(f) - 2xx']\} \tag{7.2}$$

where $f = \hbar\omega/kT$ and $Q = \int_{-\infty}^{\infty} < x|e^{-\beta H}|x > dx$. Note that the higher the temperature, the farther ρ gets from a pure state, i.e. $Tr(\rho^2)$ decreases with temperature. Plot $Tr(\rho^2)$ as a function of T.