Quantum Molecular Dynamics **Autumn 2001-2002**

Home Work 2

1. (Ch. 3, EOC ex. 3) Let $\psi(x,0) = e^{-\alpha x^2}$. Find an expression for the free particle evolution $\psi(x,t)$ by using the Fourier integral theorem. Show that $\psi(x,t)$ can be written in the form $\psi(x,t) = e^{-\alpha_t x^2 + \gamma_t}$.

2. (Ch. 3, EOC ex. 4) An alternative approach to the previous problem is: guess that $\psi(x,t) = e^{-\alpha_t x^2 + \gamma_t}$. Substitute this form into the time dependent Schrodinger equation and, by matching equations in powers of x find expressions for α_t and γ_t. Show that these expressions are equal to those derived in the previous problem.

3. (Ch. 3, EOC ex. 5) Take the more general trial form $\psi(x,t) = e^{-\alpha_t(x-x_t)^2 + \frac{i}{\hbar}p_t(x-x_t) + \frac{i}{\hbar}\gamma_t}$, where x_t and p_t are real. Substitute this form into the TDSE and obtain expressions for α_t, x_t, p_t, and γ_t.

4. (Ch. 3 EOC ex. 6) Find $\overline{x}(t)$ and $\overline{\Delta x^2}(t)$, $\overline{p}(t)$ and $\overline{\Delta p^2}(t)$ for exercise 2 above. Show that the uncertainty principle is satisfied:
$$\Delta x(t)\Delta p(t) \geq \frac{\hbar}{2}. \tag{4.1}$$

5. (Ch. 3, EOC ex. 8) Take the form for the gaussian wavepacket, $\psi(x,t) = \exp(-\alpha_t(x-x_t)^2 + \frac{i}{\hbar}p_t(x-x_t) + \frac{i}{\hbar}\gamma_t)$, and substitute it into the Time Dependent Schrödinger Equation for the harmonic oscillator potential, $V(x) = \frac{1}{2}m\omega^2x^2$. Obtain expressions for the parameters α_t, x_t, p_t, and γ_t. [Hint: to simplify the algebra, write $\frac{1}{2}m\omega^2x^2 = \frac{1}{2}m\omega^2[(x-x_t)+x_t]^2$. To solve the differential equation for α_t and γ_t it is convenient to introduce the substitution $\alpha_t = \frac{a\dot{z}}{z}$, where a is a constant which gives the harmonic equation $\ddot{z} = -\omega z$.] What happens when $\alpha_0 = \frac{m\omega}{2\hbar}$? In this case the wavepacket is sometimes called a 'coherent state', a confusing but widely used label.

6. (Ch. 3, EOC ex. 1) Optional: Show that the product of two gaussians is a third gaussian centered between the first two.

7. (Ch. 3, EOC ex. 2) Optional: Find an expression for the overlap integral of two complex gaussians of the form $\psi(x,t) = e^{-\alpha_t(x-x_t)^2 + \frac{i}{\hbar}p_t(x-x_t) + \frac{i}{\hbar}\gamma_t}$, the first with center at x',p', and the second with center at x'',p''. Note that this expression depends only on the differences $|p'-p''|$ and $|x'-x''|$. Interpret the exponent in terms of the phase space distance between the centers of the two gaussians by finding a quantitative relationship between the two.

8. (Ch. 3, EOC ex. 7) Optional: Take the form for the gaussian wavepacket, $\psi(x,t) = \exp(-\alpha_t(x-x_t)^2 + \frac{i}{\hbar}p_t(x-x_t) + \frac{i}{\hbar}\gamma_t)$, and substitute it into the Time Dependent Schrödinger Equation for the linear potential, $V(x) = -kx$. Obtain expressions for the parameters α_t, x_t, p_t, and γ_t.

9. (Ch. 3, EOC ex. 9) Optional: Consider the forced harmonic oscillator, *i.e.*, $V(x) = 1/2m\omega^2x^2 - F(t)x$.

   a. Show that the wavepacket given by $\psi(x,t) = \exp(-\alpha_t(x-x_t)^2 + \frac{i}{\hbar}p_t(x-x_t) + \frac{i}{\hbar}\gamma_t)$ is a solution to this problem. Substitute this form into the Time Dependent Schrödinger Equation and obtain expressions for x_t, p_t, α_t, and γ_t.

   b. A convenient way of solving the differential equations for x_t and p_t is to define a complex quantity $z(t) = p_t + im\omega x_t$. Then $z(t) = e^{i\omega t}\int_0^t F(t')e^{-i\omega t'}\,dt' + e^{i\omega t}z(0)$. Differentiate $z(t)$ with respect to time and show that the resulting equation for $\dot{z}(t)$ is consistent with Hamilton's equations of motion for x_t and p_t.

   c. Solve for $z(t)$ for

i. $F(t) = \sin(\omega t)$

ii. $F(t) = A$

iii. $F(t) = At$.

Draw pictures in the complex plane of $z(t)$ for all these cases.

d. Show that in general, if $t(dF/dt) \ll F$, then $z(t) = iF(t)/\omega$ (taking $x_0 = p_0 = 0$). *Hint: Integrate by parts.* This is the limit of adiabatic forcing, i.e. if the change in the Hamiltonian is slow enough an initial eigenstate will stay an eigenstate for all time.