European Master on Nuclear Fusion Science and Engineering Physics.
Introductory Atomic and Molecular Physics. Problems (1).

1. A particle of mas m moving in one dimension is described by the wave packet:

$$\Psi(x,t) = \int_{-\infty}^{+\infty} A(k) \exp\left[\mathrm{i}(kx - \omega t)\right] \mathrm{d}k$$

with

$$A(k) = C \exp\left[-a^2(k-k_0)^2\right]$$

   (a) Taking $L = k - k_0$, show that $\Psi(x,t)$ is of the form:

$$C \int_{-\infty}^{+\infty} \mathrm{d}L \exp\left[-\alpha L^2 - 2\beta L - \gamma\right]$$

   (b) Using

$$\int_{-\infty}^{+\infty} \mathrm{d}u \exp(-cu^2) = \sqrt{(\pi/c)},$$

   express $\Psi(x,t)$ as a function of α, β and γ.

   (c) Find the values of Δx and Δk that fulfill $|\Psi(\Delta x, 0)|^2 = (1/\mathrm{e})|\Psi(0,0)|^2$ and $A(\Delta k) = (1/\mathrm{e})A(k_0)$.

2. The wavefunction $\Psi(x,t)$ must be a solution of the time-dependent Schrödinger equation. For a stationary state $|\Psi(x,t)|^2$ is constant in time. $\Psi(x,t)$ is expanded in terms of a set $\{u_n\}$ of eigefunctions of the time independent Hamiltonian :

$$\Psi(x,t) = \sum_n c_n \phi_n(t) u_n(x)$$

   (a) Obtain the form of $\phi_n(t)$ by substituting the expansion in the time-dependent Schrödinger equation.

   (b) Find the conditions that must verify the coefficients c_n so that $\Psi(x,t)$ is a stationary state.

3. Let E_n the energy eigenvalues of a one-dimensional system and $\psi_n(x)$ the corresponding energy eigenfunctions. Suppose that the normalized wave function of the system at $t = 0$ is given by:

$$\Psi(x, t=0) = \frac{1}{\sqrt{2}} \exp(\mathrm{i}\alpha_1)\psi_1(x) + \frac{1}{\sqrt{3}} \exp(\mathrm{i}\alpha_2)\psi_2(x) + \frac{1}{\sqrt{6}} \exp(\mathrm{i}\alpha_3)\psi_3(x)$$

   (a) Write down the wave function $\Psi(x,t)$ at time t.

(b) Find the probability that at time t a measurement of the energy of the system gives the value E_2.

(c) Does $< x >$ vary with time? Does $< p_x >$ vary with time? Does $< E >=< H >$ vary with time?

4. Which are the changes in the time-independent Schrödinger equation when a constant potential V_0 is added to the Hamiltonian?

5. Consider a free particle in one dimension.

   (a) Write down the time-dependent Schrödinger equation. Find the general solution and show that it can be interpreted as a sum of plane waves moving in directions $+x$ and $-x$.

   (b) Show that the initial conditions can be chosen to obtain a time-independent probability distribution.

   (c) The probability current density is defined as:

$$\boldsymbol{j}(\boldsymbol{r}, t) = \frac{\mathrm{i}\hbar}{2m}(\psi \nabla \psi^* - \psi^* \nabla \psi)$$

   Determine this vector for each plane wave of (a) and for the general solution.

6. Let Ψ a normalized solution of the time-dependent Schrödinger equation.

   (a) Show that the energy can be expressed as:

$$E = \int \mathrm{d}^3x \left[\frac{\hbar^2}{2m} \nabla \Psi^* \nabla \Psi + \Psi^* V(\boldsymbol{r}) \right]$$

   (Hint: Use the Green's theorem: $\int_V \nabla \cdot \boldsymbol{j} = \int_A j_n \mathrm{d}A$).

   (b) Show that the conservation of the energy can be written in the form:

$$\frac{\partial W}{\partial t} + \nabla \cdot \boldsymbol{S} = 0$$

   where W is the energy density.