PHY3011 Quantum Mechanics—Assignment 1

Please do this assignment and hand in the answers to the Departmental Office by 4pm Monday 16th November.

WAVEPACKETS

Free electrons, *ie,* those moving in a constant potential, are infinitely extended so it's hard to treat them as particles. We could second-quantise them, but a cheap and cheerful scheme is to make them into **wavepackets**. That's what this problem is about. You will need a computer graph plotting program, and the help of a textbook (it's all in *Cassells*). Please don't use the internet; I don't want any downloaded grafix.

In this problem just consider a free electron plane wave, moving in one dimension, in the x-direction,

$$\psi_k = \mathrm{e}^{\mathrm{i}(kx-\omega t)}. \tag{1}$$

This wave has wavelength $2\pi/k$, energy

$$\varepsilon = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m}$$

and angular frequency ω. It is a solution of the time dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \mathrm{i}\hbar\frac{\partial\psi}{\partial t} \tag{2}$$

where t is time. Actually equation (1) is just one particular solution of the wave equation (2), in fact any wavevector is allowed for a free electron so a more general solution is a linear combination of waves of different k:

$$\psi = \sum_k C(k)\,\mathrm{e}^{\mathrm{i}(kx-\omega t)}$$

where $C(k)$ are any coefficients. It's handy to write this instead as an integral,

$$\psi = \int_{-\infty}^{\infty} A(k)\,\mathrm{e}^{\mathrm{i}(kx-\omega t)}\,\mathrm{d}k \tag{3}$$

where A can be any function within reason. But if we want to *localise* the plane waves to make the electron particle-like we want to choose a function that is large only in the neighbourhood of some chosen wavevector k_0. A good choice is a Gaussian,

$$A(k) = c\,\mathrm{e}^{-a^2(k-k_0)^2}, \qquad c = \frac{a}{\sqrt{\pi}} \tag{4}$$

where a and c are constants, a determines the *width* of the Gaussian and c is a normalising constant; of course really there's only one constant because they are related by the factor $\sqrt{\pi}$. You may want to check at this point that you remember what a Gaussian looks like—it's a "bell curve."

From now on, work in *Rydberg atomic units* in which $\hbar = 1$, $2m = 1$ and the energy is in Rydbergs (1 Ry = 13.6 eV). Then we have

$$\varepsilon = \omega = k^2.$$

If we put (4) into (3) we get our wavepacket

$$\psi = \frac{a}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-a^2(k-k_0)^2 + \mathrm{i}(kx - k^2 t)} \, \mathrm{d}k \tag{5a}$$

$$= \frac{a}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha\xi^2 - 2\beta\xi - \gamma} \, \mathrm{d}\xi \tag{5b}$$

where

$$\xi = k - k_0$$

and

$$\alpha = a^2 + \mathrm{i}t \qquad \beta = \frac{1}{2}\mathrm{i}\,(-x + 2k_0 t) \qquad \gamma = \mathrm{i}k_0\,(-x + k_0 t)\,. \tag{5c}$$

The integral (5b) can be done like this.

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha\xi^2 - 2\beta\xi - \gamma} \, \mathrm{d}\xi &= \mathrm{e}^{(\beta^2/\alpha) - \gamma} \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha(\xi + \beta/\alpha)^2} \, \mathrm{d}\xi \\ &= \mathrm{e}^{(\beta^2/\alpha) - \gamma} \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha u^2} \, \mathrm{d}u \\ &= \sqrt{\frac{\pi}{\alpha}}\, \mathrm{e}^{(\beta^2/\alpha) - \gamma}. \end{aligned}$$

So substituting back for α, β and γ from (5c) we get

$$\psi(x,t) = \frac{a}{\sqrt{a^2 + \mathrm{i}t}} \exp\left(-\frac{(x - 2k_0 t)^2}{4(a^2 + \mathrm{i}t)} + \mathrm{i}k_0(x - k_0 t)\right). \tag{6}$$

This is the wavefunction for your wavepacket centred at wavevector k_0 as a function of position x and time t. The probability density is

$$|\psi(x,t)|^2 = \frac{a^2}{\sqrt{a^4 + t^2}} \exp\left(-\frac{a^2(x - 2k_0 t)^2}{2(a^4 + t^2)}\right). \tag{7}$$

The argument to the exponential is clearly negative, so the maximum value of the probability at any time t is when the argument is largest (*ie*, zero) which is when

$$x = 2k_0 t$$

so the velocity of the wavepacket must be $2k_0$ in Rydberg units, or in any units

$$v_g = \frac{\hbar k_0}{m}. \tag{8}$$

This is the *group velocity*.

Here are now your problems.

1. Consider the single plane wave (1). Explain why it cannot be normalised. What is the *phase velocity* of this wave? Compare this with the *group velocity* (8) of the wavepacket centred on the same wavevector. You may like to make a comment on this.
2. Using equation (6) find $\psi(x, 0)$ and $|\psi(x, 0)|^2$. Normalise these. Plot these functions and comment on exactly what they are. For complex functions, plot the real and imaginary parts separately.
3. Is $\psi(x, 0)$ a stationary state? That is, is it a solution of the time independent Schrödinger equation?
4. What can you say about the momentum of the particle you have created? What are the uncertainties in the momentum and position and do they agree with the uncertainty principle? Do all this at $t = 0$. What is the role of the constant a in all of this?
5. Make some plots of equations (6) and (7) at a few times, for example $t = 0$, $t = t_0$, $t = 2t_0$, $t = 4t_0$ to find out how the shape and position of the wavepacket evolves over time. Don't bother about the complex amplitude, just plot the exponential parts of the function.
6. Using some sensible values of the parameters, find out roughly how long the wavepacket survives as a localised object. How far does it travel in that time?