1 ELEC1204 Lab P3 - Wavepackets

This lab is going to get you started with designing and constructing your own classes. By the end of the lab you will be able to numerically evaluate a wavepacket and verify that it is plausible.

![Electron wave packet evolution](image)
2 Preparation

2.1 Complex Number Class

Design a complex number class yourself (not copied from any other source).
Your class must include:
- complex conjugation
- modulus and argument functions.
- square root of a complex type.
- exponentiation of a complex type ($e^z$)
- appropriate Constructors

Outside of the class definition (by overloading + - * /) support
addition, subtraction, multiplication and division of complex types.
multiplication of a double by a complex type.
equality and inequality tests of complex types ==, !=.

2.2 Wave packets

$\psi(x,t)$ is a Gaussian wavefunction.

$$\psi(x,t) = \left(\frac{\alpha}{2\pi}\right)^{\frac{1}{4}} \exp\left(-\alpha \kappa_0^2\right) \frac{1}{\sqrt{(\alpha + j\beta t)}} \exp\left(\frac{(2\alpha \kappa_0 + jx)^2}{4(\alpha + j\beta t)}\right)$$ (1)

When $\beta \approx 0.5785 \text{cm}^2/\text{sec}$ it represents an electron with an energy determined by $\kappa_0$ which is set to 4 in the MATLAB code below. Its on the web site is you want to play but is not part of the required preparation.

```matlab
alpha = 0.5;
k0 = 4.0;
beta = 0.5785; %h/2m for electron cm^2/sec
x = linspace(-10,10,400);
t = linspace(0,3,400);
gamma = alpha + i*beta*t;
norm = exp(-k0*k0*alpha)*((2*alpha*k0)/pi)^0.25;
```
\[ X, T = \text{meshgrid}(x, t); \]
\[ \gamma = \alpha + i\beta T; \]
\[ \phi = \left( \frac{\text{norm}}{\sqrt{\gamma}} \right) \cdot \exp\left( \frac{(2\alpha k_0 + iX) 
\cdot (2\alpha k_0 + iX)}{4\gamma} \right); \]
\[ \text{figure(1)}; \]
\[ \text{mesh}(X, T, \text{real}(\phi \cdot \phi^*)); \]
\[ \text{title('amplitude of the real part of } \psi)'; \]
\[ \text{ylabel('time');} \]
\[ \text{zlabel('amplitude of the real part of } \psi'); \]
\[ \text{xlabel('x');} \]
\[ \text{figure(2)}; \]
\[ \text{hold off;} \]
\[ t_0 = 0.0; \]
\[ \phi_{0} = \text{PSI}(\alpha, \beta, k_0, x, t_0); \]
\[ \text{plot}(x, \text{real}(\phi_{0})); \]
\[ \text{pause;} \]
\[ \text{hold on;} \]
\[ t_1 = 0.5; \]
\[ \phi_{1} = \text{PSI}(\alpha, \beta, k_0, x, t_1); \]
\[ \text{plot}(x, \text{real}(\phi_{1}), 'r-'); \]
\[ \text{pause;} \]
\[ t_2 = 1.0; \]
\[ \phi_{2} = \text{PSI}(\alpha, \beta, k_0, x, t_2); \]
\[ \text{plot}(x, \text{real}(\phi_{2}), 'g-'); \]
\[ \text{ylabel('amplitude of the real part of } \psi); \]
\[ \text{xlabel('t=0 (blue), t=1/2s (red), t=1s (green)');} \]
\[ \text{title('electron wave packet evolution');} \]

and you will need

function psi = PSI(a, b, k0, x, t)
\[ \gamma = a + i b t; \]
\[ \text{norm} = \exp(-k_0 k_0 a) \cdot ((2a)/\pi)^{0.25}; \]
\[ L = 2a k_0 + i x; \]
\[ \psi = \frac{\text{norm}}{\sqrt{\gamma}} \cdot \exp(\frac{(L \cdot L)}{4\gamma}); \]

3 Lab work

3.1 Write and test your complex numbers

Implement and test your complex number class.
3.2 Evaulate a wavepacket

Use your complex number class to evaluate an electron wavepacket at $t = 0$, $t = 0.5$ and $t = 1$. These are the values used for the front cover picture.

3.3 Test that it is normalised

Do this at $t = 0$ seconds only, so the only variable is $x$. When we discretise the x-axis in $\delta x$ size intervals and write $\psi(x,0) = \psi(j\delta x,0) = \psi_j(t)$ where $-N \leq j \leq N$ Verify that the Gaussian wavepacket, equation (2) of the notes is normalised at $t = 0$ secs

I used $N = 4096$, $L = 25$ (length of positive x axis), $\beta = 0.5785$ (an electron), $\alpha = 0.5$, $\kappa_0 = 1$, $x_0 = -L$, $x_N = L$, $\delta x = \frac{2L}{N}$

You need to show that:

$$\int_{-L}^{L} \overline{\psi}(x)\psi(x)dx = 1$$

Use the extended Trapezoidal rule

$$\int_{x_0}^{x_m} f(x)dx = \delta x [\frac{f_0}{2} + f_1 + f_2 + \ldots f_{m-1} + \frac{f_m}{2}]$$

with $f = \psi^*\psi$

4 Extra work

Output the real part of your wavepacket in a form suitable for display in matlab. Display it in MATLAB for the 3 time values that you have.

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