NB: The graded, first version of the report must be returned if you hand in a second time!

H3b: Time dependent quantum mechanics

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Task №	Points	Avail. points
Σ		

Introduction

Problem 1

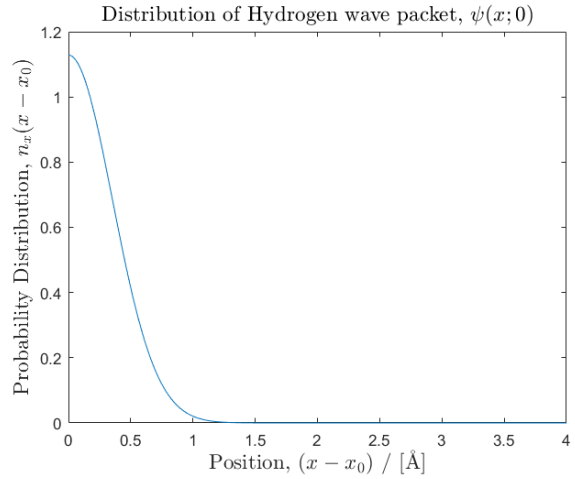
In this first problem we use FFT to transition between the space and momentum wave packet for a hydrogen atom. We also compare the wave packet obtained to the analytically derived packet, via Fourier transform.

It was suggested that Å, fs and eV should be the units used for length, time and energy respectively. Expressed in these units the mass of the atom has the approximate numerical value 103.7500 and the expected momentum p_0 has the numerical value 4.5552. The constant $\hbar$ gets the approximate numerical value 0.6579.

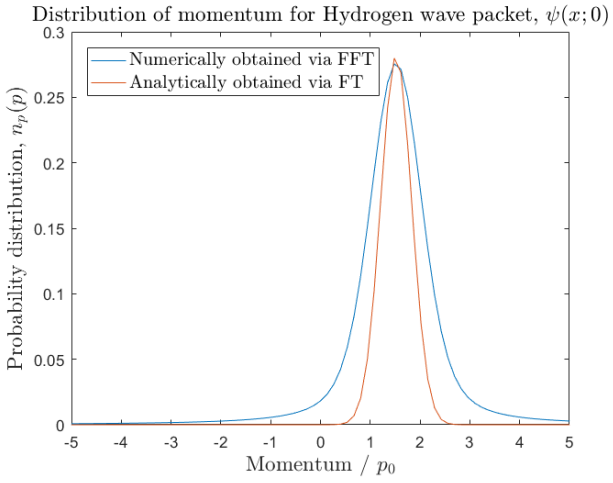
The initial distribution of the Gaussian wave packet is given by

$$\psi(x;0) = \frac{1}{(\pi d^2)^{1/4}} \exp(-\frac{(x-x_0)^2}{2d^2}) \exp(ip_0(x-x_0)/\hbar), \tag{1}$$

where d is the witdth of the packet, x_0 and p_0 are the corresponding initial position and momenta.



(a)



(b)

Figure 1: *(a):* The positive half of the wave packet in space. Given that it is a Gaussian distribution with zero mean, it is symmetrical around the y-axis. *(b):* The wave packet in momentum space. The blue graph is the result obtained from numerically doing FFT on the initial wave packet. The red dashed graph is the analytical solution.

The analytical derivation of the Fourier transform is given below.

$$
\begin{aligned}
\mathcal{F}\left[\psi(x;0)\right](p) &= \int_{-inf}^{inf} e^{-ipx}\psi(x;0)dx \\
&= \frac{1}{(\pi d^2)^{1/4}} \int_{-inf}^{inf} e^{-ipx} e^{-\frac{(x-x_0)^2}{2d^2}} e^{ip_0(x-x_0)/\hbar} dx \\
\left\{a = \frac{e^{-ipx_0}}{(\pi d^2)^{1/4}}\right\} &= a \int_{-inf}^{inf} e^{-ip(x-x_0)} e^{-\frac{(x-x_0)^2}{2d^2}} e^{ip_0(x-x_0)/\hbar} dx \\
\left\{\begin{array}{lll} x' & = x - x_0 \\ dx' & = dx \\ x' & \to x \end{array}\right\} &= a \int_{-inf}^{inf} e^{-i(p-p_0/\hbar)x} e^{-\frac{x^2}{2d^2}} dx \\
\left\{\begin{array}{lll} p' & = p - p_0/\hbar \\ b & = \frac{1}{2d^2} \\ x' & = x - \frac{ip}{2b} \\ dx' & = dx \\ x' & \to x \end{array}\right\} &= a \int_{-inf}^{inf} e^{-bx^2} e^{-p'^2/4b} dx \\
&= a e^{-p'^2/4b} \int_{-inf}^{inf} e^{-bx^2} dx \\
\left\{\int_{-int}^{int} e^{-bx^2} dx = \sqrt{\frac{\pi}{2b}}\right\} &= a e^{-p'^2/4b} \sqrt{\frac{\pi}{2b}} \\
&= (\pi d^2)^{1/4} e^{-ipx_0 - (p\hbar - p_0)^2 d^2/2\hbar^2}
\end{aligned}
\tag{2}
$$

A Source code

A.1 `main1.m`

```
% ===================================
% HOMEWORK 3B IN COMP.PHYS. - TASK 1
% ===================================
% By Victor Nilsson, Simon Nilsson
% 2016
%
% Length scale: 1
% Time scale:   1 fs = 1e-15 s
% Energy scale: 1 eV

clear all, clc, close all

% ------ SIMULATION PARAMETERS ---------
hbar        = 1.054/1.602; % JS -> f eV s
d           = 0.5;
m           = 1.66/1.6*1e2;
p_0         = sqrt(0.1*2*m);
x_0         = 0;
dx          = 0.01;
n_points    = 1024;
dp          = 2*pi/(n_points*dx);


% ----------- VARIABLES ------------
% space samples
x = x_0 + dx*(0:n_points-1);
% and the corresponding samples in momentum space
p = dp*((0:n_points-1)-n_points/2);
% ---- Functions handles ----
Gaussian_Wave_Packet = @(x)1/(pi*d^2)^(1/4)*exp(-(x-x_0).^2/(2*d^2)).*exp(1i*p_0*(x-x_0)/hbar);
% Fourier transform obtained via Mathematica as the 'Inverse Fourier
% Transform', due to differences in FT defintion
Gaussian_Packet_Fourier = @(p)exp(-1i*p*x_0 - (d^2*(p*hbar - p_0).^2)./(2*hbar^2))*(pi*d^2)^(1/4);
% ---------------------------------

% Sample-discretize the wave packet function
wave_packet = Gaussian_Wave_Packet(x)*dx;
theoretic_prob = abs(Gaussian_Packet_Fourier(p)).^2;

prob = abs(wave_packet/dx).^2;
fft_prob_momentum = abs(fftshift(fft(wave_packet))).^2*dp;

% Plot prob.distr. in momentum space
```

```
figure(1); clf;
plot(p/p_0, fft_prob_momentum)
hold on
plot(p/p_0, theoretic_prob)
hold off
xlim([-5 5])
xlabel('Momentum / $p_0$', 'interpreter', 'latex', 'fontsize', 14)
ylabel('Probability distribution, $n_p(p)$','interpreter','latex', 'fontsize', 14)
title('Distribution of momentum for Hydrogen wave packet, $\psi(x;0)$','interpreter','latex','fontsize',14)
L = legend({'Numerically obtained via FFT', 'Analytically obtained via FT'},'interpreter','latex','fontsize',12);
set(L, 'location', 'northwest')

% Plot prob.distr. in normal space
figure(2); clf;
plot(x, prob)
xlim([0 4])
ylabel('Probability Distribution, $n_x(x-x_0)$','interpreter','latex', 'fontsize', 14)
xlabel('Position, $(x-x_0)$ / [\AA]', 'interpreter', 'latex', 'fontsize', 14)
title('Distribution of Hydrogen wave packet, $\psi(x;0)$','interpreter','latex','fontsize',14)
```

A.2 main2.m

```
% ==================================
% HOMEWORK 3B IN COMP.PHYS. - TASK 2
% ==================================
% By Victor Nilsson, Simon Nilsson
% 2015
%
% Length scale: 1
% Time scale:   1 fs = 1e-15 s
% Energy scale: 1 eV

clear all, clc, close all

% ------ SIMULATION PARAMETERS ---------
hbar        = 1.054/1.602; % JS -> f eV s
d           = 0.5;
m           = 1.66/1.6*1e2;
p_0         = sqrt(0.1*2*m);
x_0         = 0;
dx          = 0.1;
n_points    = 2^10;
dp          = 2*pi/(n_points*dx);
dt          = 1;


% ------------ VARIABLES ------------
% space samples
x = x_0+dx*(0:n_points-1);
% and the corresponding samples in momentum space
p = ((0:n_points-1)-n_points/2)*dp;
% Functions handles
Gaussian_Wave_Packet = @(x)1/(pi*d^2)^(1/4)*exp(-(x-x_0).^2/(2*d^2)).*exp(1i*p_0*(x-x_0)/hbar);
Potential_Function = @(x) 0;
% ----
step_three=Gaussian_Wave_Packet(x);

potential = Potential_Function(x);
exp_potential = exp(-1i/hbar.*potential*dt);
inv_pot = exp(-1i/hbar*(hbar^2*p.^2./(2*m))*dt);


% Plot initial prob.distr.
figure(1); clf;
plot(x(1:n_points/2), abs(step_three(1:n_points/2).^2))
xlim([0 2])
xlabel('Position / [\AA]', 'interpreter', 'latex', 'fontsize', 14)
ylabel('Probability distribution', 'fontsize', 14)
title('$\left| \psi (0) \right|^2$', 'interpreter', 'latex', 'fontsize', 18)

% Plot the rest in a separate figure
figure(2); clf;
step_one = step_three;
step_two = fftshift(fft(step_one.*exp_potential));
step_three = ifft(ifftshift(inv_pot.*step_two));

plotHandle = plot(x(1:n_points/2), abs(step_three(1:n_points/2).^2));
xlabel('Position / [\AA]', 'interpreter', 'latex', 'fontsize', 14)
ylabel('Probability distribution', 'fontsize', 14)
```

```
title('$\left| \psi (t = 256 \mathrm{fs}) \right|^2$', 'interpreter', 'latex', 'fontsize', 18)

for j=1:n_points/4-1
    step_one = step_three;

    step_two = fftshift(fft(step_one.*exp_potential));
    step_three = ifft(ifftshift(inv_pot.*step_two));
    set(plotHandle, 'YData', abs(step_three(1:n_points/2).^2))
    pause(0.01)
end
```

A.3 main3.m

```
% ===================================
% HOMEWORK 3B IN COMP.PHYS. - TASK 2
% ===================================
% By Victor Nilsson, Simon Nilsson
% 2015
%
% Length scale: 1
% Time scale:   1 fs = 1e-15 s
% Energy scale: 1 eV

clear all, clc, close all

% ------ SIMULATION PARAMETERS ---------
hbar         = 1.054/1.602; % JS -> f eV s
d            = 0.5;
m            = 1.66/1.6*1e2;
p_0          = sqrt(0.12*2*m);
x_0          = 0;
dx           = 0.1;
n_points     = 2^10;
dp           = 2*pi/(n_points*dx);
dt           = 1;
v_0=0.1;
alpha=2.0;


% ------------ VARIABLES ------------
% space samples
x = x_0+dx*(0:n_points-1);
% and the corresponding samples in momentum space
p = ((0:n_points-1)-n_points/2)*dp;
% Functions handles
Gaussian_Wave_Packet = @(x)1/(pi*d^2)^(1/4)*exp(-(x-x_0).^2/(2*d^2)).*exp(1i*p_0*(x-x_0)/hbar);
Potential_Function = @(x) v_0*cosh(x/alpha).^(-2);
% ----
step_three=Gaussian_Wave_Packet(x);

potential = Potential_Function(x);
exp_potential = exp(-1i/hbar.*potential*dt);
inv_pot = exp(-1i/hbar*(hbar^2*p.^2./(2*m))*dt);

for j=1:n_points/4
    step_one = step_three;

    step_two = fftshift(fft(step_one.*exp_potential));
    step_three = ifft(ifftshift(inv_pot.*step_two));

    plot(x-max(x)/2,abs(ifftshift(step_three)).^2)
    pause(0.01)
end
```

A.4 main4.m

```
% ===================================
% HOMEWORK 3B IN COMP.PHYS. - TASK 2
% ===================================
% By Victor Nilsson, Simon Nilsson
% 2015
%
% Length scale: 1
% Time scale:   1 fs = 1e-15 s
% Energy scale: 1 eV

clear all, clc, close all

% ------ SIMULATION PARAMETERS ---------
```

```
hbar         = 1.054/1.602; % JS -> f eV s
d            = 0.5;
m            = 1.66/1.6*1e2;
p_0          = sqrt(0.12*2*m);
x_0          = 0;
dx           = 0.1;
n_points     = 2^10;
dp           = 2*pi/(n_points*dx);
dt           = 1;
a            = 0.3;
b            = 0.4;
d            = 0.7;
c            = 0.05; % 0.1;

tmp = V_d(0,a,b,c,d);
[R,v]=eig(tmp);
```