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Basic Physics Course with MATLAB's Symbolic Toolbox and Live Editor

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5.3 Gaussian wave packet as solution of the free Schrödinger equation (Computational example)

A Gaussian wave packet is formed by the superposition of plane waves g_p with a Gaussian momentum distribution $f(p)$ (see below).

Free Schrödinger equation (FSE): $-\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$

Wave function of the Gaussian wave packet: $\psi(x,t) = \int_{-\infty}^{\infty} f(p)g_p(x,t)dp$

```
clear all
syms hbar m b x x0 X p p0 t positive
Par=[m==1 hbar==1 b==1 x0==-5 p0==5/2]
```

Par =

$$\left(m = 1 \quad \text{hbar} = 1 \quad b = 1 \quad x_0 = -5 \quad p_0 = \frac{5}{2}\right)$$

1 Plane waves

Plane wave as a solution of the FSE: $g_p = \sqrt{\frac{1}{2\pi\hbar}}e^{iS/\hbar}$, where $S = p(x-x_0) - \frac{p^2}{2m}t$

```
syms g_p f S
g_p=sqrt(1/(2*pi*hbar))*exp(i*S/hbar)
```

g_p =

$$\frac{\sqrt{2}\ \mathrm{e}^{\frac{S\,\mathrm{i}}{\mathrm{hbar}}}}{2\ \sqrt{\mathrm{hbar}}\ \sqrt{\pi}}$$

```
S=p*(x-x0)-p^2*t/(2*m)
```

S =

$$p\ (x-x_0)-\frac{p^2\,t}{2\,m}$$

```
g_p=sube(g_p,'S'==S)
```

g_p =

$$\frac{\sqrt{2}\ \mathrm{e}^{\frac{\left(p\ (x-x_0)-\frac{p^2\,t}{2\,m}\right)\,\mathrm{i}}{\mathrm{hbar}}}}{2\ \sqrt{\mathrm{hbar}}\ \sqrt{\pi}}$$

2 Momentum distribution of the Gaussian wave packet

Gaussian momentum distribution: $f\ =\sqrt{\frac{b}{\hbar\sqrt{\pi}}}e^{-b^2\frac{(p-p_0)^2}{2\hbar^2}}$

```
f=sqrt(b)/sqrt(hbar*sqrt(sym(pi)))*exp(-b^2*(p-p0)^2/(2*hbar^2))
```

f =

$$\frac{\sqrt{b}\ \mathrm{e}^{-\frac{b^2\ (p-p_0)^2}{2\,\mathrm{hbar}^2}}}{\sqrt{\mathrm{hbar}}\ \pi^{1/4}}$$

3 Integration (Fourier transform)

$$\psi(x,t)=\int_{-\infty}^{\infty} f(p)g_p(x,t)dp=\int_{-\infty}^{\infty}\left(f(p)g_p(x,t)e^{-i\frac{(x-x_0)p}{\hbar}}\right)e^{iXp}dp,\quad \text{where } X=\frac{x-x_0}{\hbar}$$

Argument

```
f*g_p*exp(-i*p*(x-x0)/hbar)
```

ans =

$$\frac{\sqrt{2}\ \sqrt{b}\ \mathrm{e}^{-\frac{b^2\ (p-p_0)^2}{2\,\mathrm{hbar}^2}}\ \mathrm{e}^{-\frac{p\ (x-x_0)\ \mathrm{i}}{\mathrm{hbar}}}\ \mathrm{e}^{\frac{\left(p\ (x-x_0)-\frac{p^2\,t}{2\,m}\right)\,\mathrm{i}}{\mathrm{hbar}}}}{2\,\mathrm{hbar}\ \pi^{3/4}}$$

```
expand(ans)
```

```
ans =
```

$$\frac{\sqrt{2}\ \sqrt{b}\ \mathrm{e}^{\frac{b^2\,p\,p_0}{\mathrm{hbar}^2}}\ \mathrm{e}^{-\frac{p^2\,t\,\mathrm{i}}{2\,\mathrm{hbar}\,m}}}{2\,\mathrm{hbar}\,\pi^{3/4}\ \sqrt{\mathrm{e}^{\frac{b^2\,p^2}{\mathrm{hbar}^2}}}\ \sqrt{\mathrm{e}^{\frac{b^2\,{p_0}^2}{\mathrm{hbar}^2}}}}$$

```
sube(ans,[m==1]);
simplify(ans);
2*pi*ifourier(ans,p,X);
psi=sube(ans,X==(x-x0)/hbar)
```

```
psi =
```

$$\frac{\sqrt{2}\ \sqrt{b}\ \mathrm{e}^{-\frac{b^2\,{p_0}^2}{2\,\mathrm{hbar}^2}-\frac{\mathrm{hbar}^2\,\left(\frac{x-x_0}{\mathrm{hbar}}-\frac{b^2\,p_0\,\mathrm{i}}{\mathrm{hbar}^2}\right)^2}{2\,\left(b^2+\mathrm{hbar}\,t\,\mathrm{i}\right)}}}{2\,\pi^{1/4}\ \sqrt{\frac{b^2}{2}+\frac{\mathrm{hbar}\,t\,\mathrm{i}}{2}}}$$

```
psi=simplify(psi)
```

```
psi =
```

$$\frac{\sqrt{b}\ \mathrm{e}^{-\frac{\left(\mathrm{i}\,p_0\,b^2-\mathrm{hbar}\,x+\mathrm{hbar}\,x_0\right)^2}{2\,\mathrm{hbar}^2\,\left(b^2+\mathrm{hbar}\,t\,\mathrm{i}\right)}-\frac{b^2\,{p_0}^2}{2\,\mathrm{hbar}^2}}}{\pi^{1/4}\ \sqrt{b^2+\mathrm{hbar}\,t\,\mathrm{i}}}$$

4 Density

Density: $\rho = \psi^*\psi = |\psi|^2$

```
rho=abs(psi)^2;
rho=simplify(rho,'Steps',80)
```

```
rho =
```

$$\frac{b\,\mathrm{e}^{-\frac{b^2\,\left(x_0-x+p_0\,t\right)^2}{b^4+\mathrm{hbar}^2\,t^2}}}{\sqrt{\pi}\ \sqrt{b^4+\mathrm{hbar}^2\,t^2}}$$

5 Plots

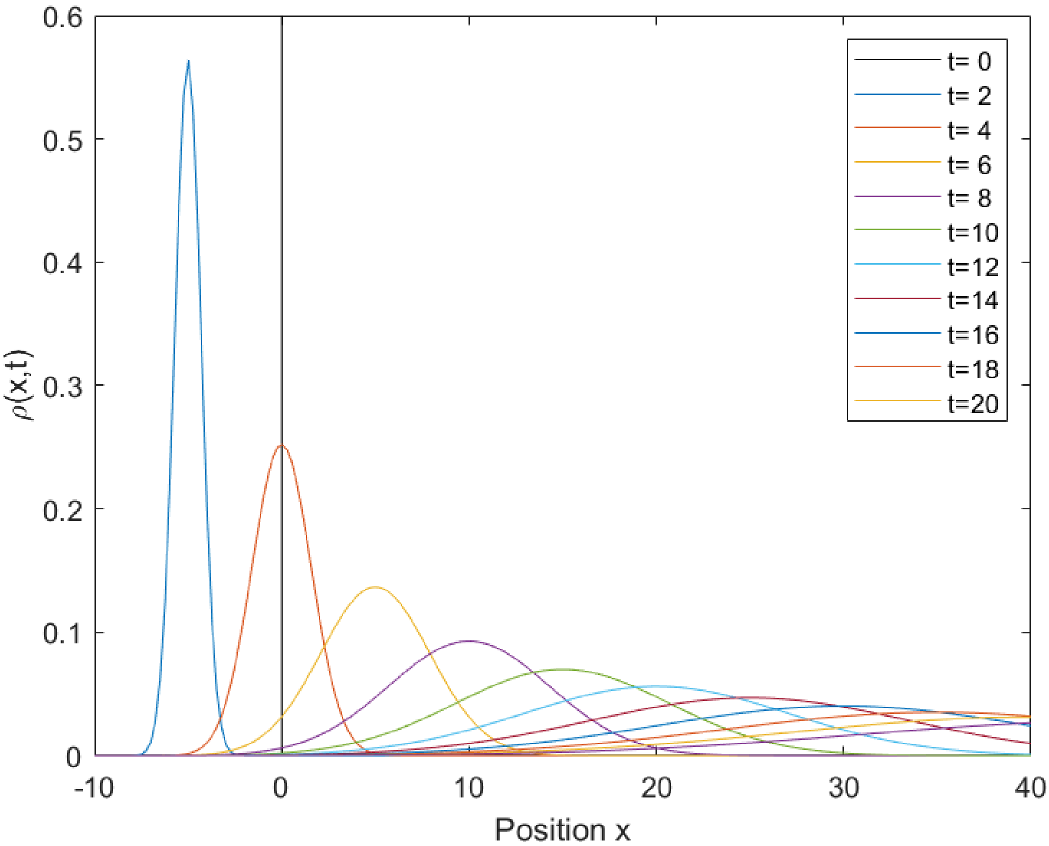
```
t=0:2:20;
```

```
x=linspace(-10,40,200);
sube(rho,Par)
```

ans =

$$\frac{e^{-\frac{\left(x-\frac{5\,t}{2}+5\right)^2}{t^2+1}}}{\sqrt{\pi}\,\sqrt{t^2+1}}$$

```
RHO=matlabFunction(ans);
plot([0 0],[0 0.6],'k')
hold on
for n=1:size(t,2)
    plot(x,RHO(t(n),x))
    txt{n}=sprintf('t=%2.f',t(n));
end
axis([-10 40 0 0.6])
xlabel('Position x')
ylabel('\rho(x,t)')
legend(txt)
```



6 Heisenberg's uncertainty relation $\Delta x \Delta p \geq \frac{\hbar}{2}$

It states that the position and momentum of an action quantum cannot be measured arbitrarily exactly. This is examined here for the Gaussian wave packet.

Mean value of position: $\langle x \rangle = \int_{-\infty}^{\infty} x\rho dx \equiv \overline{x}$

Variance of position: $(\Delta x)^2 = \langle (x-\overline{x})^2 \rangle = \langle x^2 \rangle - 2\overline{x}\langle x \rangle + \overline{x}^2 = \langle x^2 \rangle - \overline{x}^2$

Eigenvalue of the momentum: $p_{EW} = (\hat{p}\psi)\frac{1}{\psi} = \left(\frac{\hbar}{i}\frac{\partial\psi}{\partial x}\right)\frac{1}{\psi} = p_{c0} + p_{c1}x$

Mean value of the momentum: $\overline{p} = \langle \hat{p} \rangle = \int_{-\infty}^{\infty} p_{EW}\rho dx = p_{c0} + p_{c1}\overline{x}$

Variance of the momentum: $(\Delta p)^2 = \left\langle \hat{p}^2 \right\rangle - \overline{p}^2 = \left\langle |p_{c0} + p_{c1}x|^2 \right\rangle - |p_{c0} + p_{c1}\overline{x}|^2$

$$= \left(|p_{c0}|^2 + 2\mathrm{Re}(p_{c0}p_{c1})\overline{x} + |p_{c1}|^2\langle x^2 \rangle\right) - \left(|p_{c0}|^2 + 2\mathrm{Re}(p_{c0}p_{c1})\overline{x} + |p_{c1}|^2\overline{x}^2\right)$$

$$= |p_{c1}|^2(\Delta x)^2$$

```
syms x t positive
int(x*rho,x,-inf,inf);
x_m=simplify(ans)
```

x_m = $x_0 + p_0\, t$

```
int(x^2*rho,x,-inf,inf);
dx2=simplify(simplify(ans)-x_m^2)
```

dx2 =

$$\frac{b^4 + \mathrm{hbar}^2\, t^2}{2\, b^2}$$

```
p_EW=hbar/i*diff(psi,x)/psi;
p_EW=expand(simplify(p_EW))
```

p_EW =

$$\frac{b^2\, p_0}{b^2 + \mathrm{hbar}\, t\, \mathrm{i}} + \frac{\mathrm{hbar}\, x\, \mathrm{i}}{b^2 + \mathrm{hbar}\, t\, \mathrm{i}} - \frac{\mathrm{hbar}\, x_0\, \mathrm{i}}{b^2 + \mathrm{hbar}\, t\, \mathrm{i}}$$

```
[s,q]=coeffs(p_EW,x)
```

s =

$$\left(\frac{\mathrm{hbar}\,\mathrm{i}}{b^2+\mathrm{hbar}\,t\,\mathrm{i}} \quad \frac{b^2\,p_0}{b^2+\mathrm{hbar}\,t\,\mathrm{i}}-\frac{\mathrm{hbar}\,x_0\,\mathrm{i}}{b^2+\mathrm{hbar}\,t\,\mathrm{i}}\right)$$

q = $\left(x \quad 1\right)$

```
p_c0=s(2)
```

p_c0 =

$$\frac{b^2\,p_0}{b^2+\mathrm{hbar}\,t\,\mathrm{i}}-\frac{\mathrm{hbar}\,x_0\,\mathrm{i}}{b^2+\mathrm{hbar}\,t\,\mathrm{i}}$$

```
p_c1=s(1)
```

p_c1 =

$$\frac{\mathrm{hbar}\,\mathrm{i}}{b^2+\mathrm{hbar}\,t\,\mathrm{i}}$$

```
p_mean=simplify(p_c0+p_c1*x_m)
```

p_mean = p_0

```
dp2=simplify(abs(p_c1)^2,'Steps',20)*dx2
```

dp2 =

$$\frac{\mathrm{hbar}^2}{2\,b^2}$$

```
figure
dxdp=simplify(sqrt(dx2*dp2))
```

dxdp =

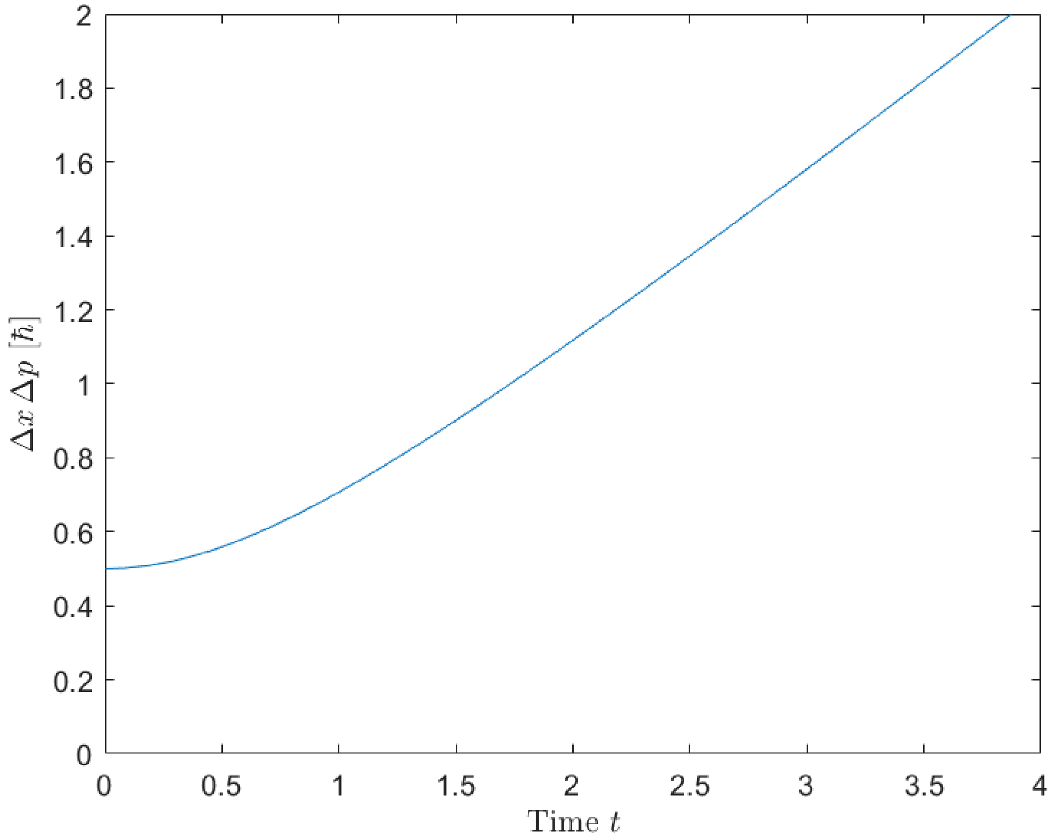
$$\frac{\mathrm{hbar}\,\sqrt{b^4+\mathrm{hbar}^2\,t^2}}{2\,b^2}$$

```
sube(dxdp,Par)
```

ans =

$$\frac{\sqrt{t^2+1}}{2}$$

```
fplot(ans,[0,4])
set(gcf,'DefaultTextInterpreter','Latex')
axis([0 4 0 2]);xlabel('${\rm Time}\ t$');ylabel('$\Delta x\, \Delta p\ [\hbar]$')
```



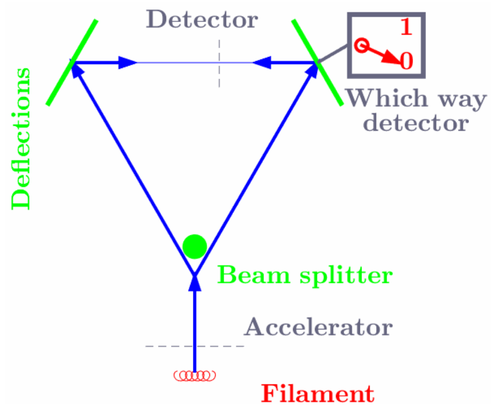
7 Animation of the interference $\rightarrow$ 'Gauss_Interference.gif'

A beam with action quanta is split and superimposed by deflections again.

For simplification, the measuring probability is calculated only after the deflections.

Three cases are distinguished in the wave function ψ_{ab} (see below):

- No which-way detector (WWD): $a = b = \sqrt{1/2}$
- WWD does not respond: $a = 1, \; b = 0$
- WWD responds: $a = 0, \; b = 1$



Wave function: $\psi_{ab}(x,t) = a \cdot \psi(x,t)\big|_{x_0=-5, p_0=\frac{5}{2}} + b \cdot \psi(x,t)\big|_{x_0=5, p_0=-\frac{5}{2}}$

and $(a,b) \in \left\{ \underbrace{(\sqrt{1/2}, \sqrt{1/2})}_{\text{no WWD}}, \underbrace{(1,0)}_{\text{does not respond}}, \underbrace{(0,1)}_{\text{responds}} \right\}$

```
psi7=sube(psi,[hbar==1,b==1])
```

psi7 =

$$\frac{e^{-\frac{p_0^2}{2}-\frac{(x_0-x+p_0\,\mathrm{i})^2}{2\,(1+t\,\mathrm{i})}}}{\pi^{1/4}\,\sqrt{1+t\,\mathrm{i}}}$$

```
psia=sube(psi7,[x0==-5 p0==5/2 ]);
psib=sube(psi7,[x0==5 p0==-5/2]);
rhoa=matlabFunction(abs(psia)^2);
rhob=matlabFunction(abs(psib)^2);
rhoab=matlabFunction(abs(psia+psib)^2/2);

XMa=20;
YMa=0.8;
x=linspace(-XMa,XMa,200);
t=linspace(0,10,50);
```

```
figure
subplot(3,1,1)
ha=plot(x(:),rhoa(t(1),x(:)));
axis([-XMa XMa 0 YMa/2])
ylabel('Density \rho(x)')
ht=title(sprintf('Time t=%2d',t(1)));
subplot(3,1,2)
hab=plot(x(:),rhoab(t(1),x(:)));
axis([-XMa XMa 0 YMa/2])
ylabel('Density \rho(x)')
subplot(3,1,3)
hb=plot(x(:),rhob(t(1),x(:)));
```

```
axis([-XMa XMa 0 YMa])
xlabel('Position x')
ylabel('Density \rho(x)')
```

Write animation in file

```
FiNa='Gauss_Interference.gif';
n=1;
im=frame2im(getframe(gcf));
[A,map] = rgb2ind(im,16);
imwrite(A,map,FiNa,'gif','LoopCount',Inf,'DelayTime',0);
for n=2:size(t,2)
    ha.YData=rhoa(t(n),x(:));
    hab.YData=rhoab(t(n),x(:));
    hb.YData=rhob(t(n),x(:));
    ht.String=sprintf('Time t=%2.1f',t(n));
    im=frame2im(getframe(gcf));
    [A,map]=rgb2ind(im,16);
    imwrite(A,map,FiNa,'gif','WriteMode','append','DelayTime',0);
end
```