2.4 Gaussian wave packet

Setup

```
d_x = 1;
x_coord = -20:d_x:20;
d_k = 0.1;
k_coord = -5:d_k:5;
s_x = 5;
```

a) Normalization of wave packet

Using $\int_{-\infty}^{\infty} |\varphi(x)|^2 dx = 1$, one get

$$\frac{1}{\varphi_0^2} = \int_{-\infty}^{\infty} |\exp\left(-\frac{x^2}{4s_x}\right)|^2 dx = \sqrt{\frac{2\pi|s_x|^2}{\Re(s_x)}} \rightarrow \varphi_0 = \sqrt[4]{\frac{\Re(s_x)}{2\pi|s_x|^2}}.$$

This can be calculated analytically:

```
phi_0 = (2*pi*abs(s_x)^2/real(s_x))^(-0.25)
```

```
phi_0 = 0.4224
```

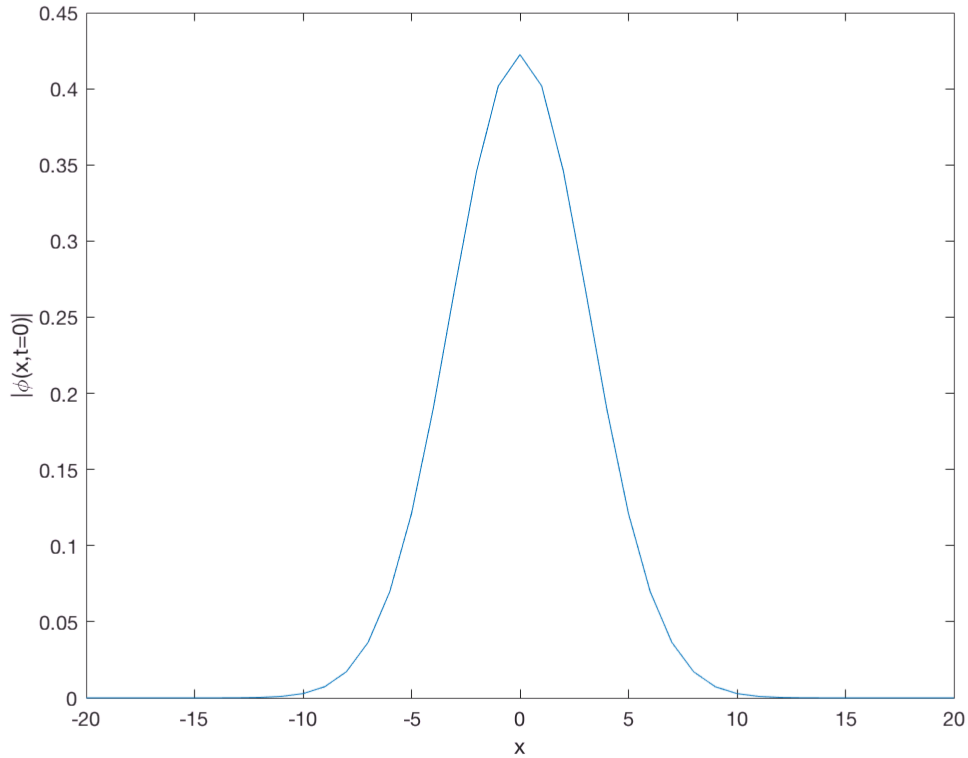
Or alternatively, summing up the terms:

```
phi_0_sq = 0;
for x = 1:length(x_coord)
    d_phi_sq = exp(-x_coord(x)^2/4/s_x)^2*d_x;
    phi_0_sq = phi_0_sq + d_phi_sq;
end
phi_0 = sqrt(1/phi_0_sq)
```

```
phi_0 = 0.4224
```

Plot $\varphi(x) = \varphi_0 \exp\left(-\frac{x^2}{4s_x}\right)$:

```
figure(1);
phi_x = phi_0*exp(-x_coord.^2/4/s_x);
plot(x_coord,abs(phi_x));

xlabel('x')
ylabel('|\phi(x,t=0)|')
```



b) Fourier transformation to k-space

The Fourier transformation of the Gaussian wave packet is

$$\Phi(k) = \Phi_0 \exp\left(-\frac{k^2}{4s_k}\right) = \sqrt{2s_x}\,\varphi_0 \exp\left(-s_x k^2\right)$$

with $s_k = \dfrac{1}{4s_x}$ and $\Phi_0 = \sqrt{2s_x}\,\varphi_0$.

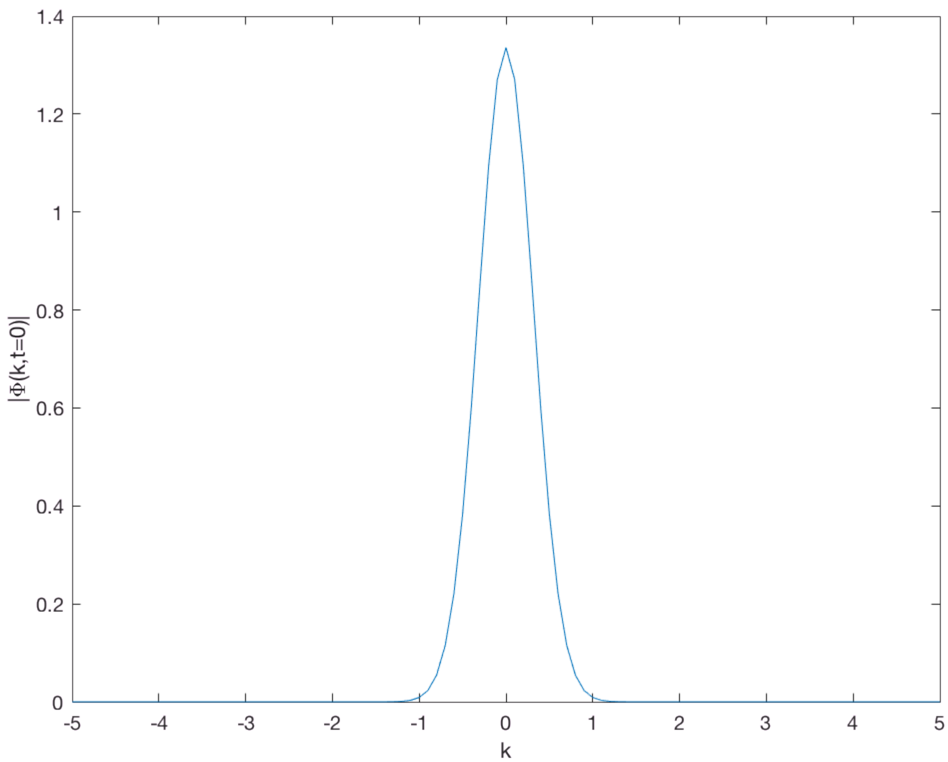
It can be shown that $\int_{-\infty}^{\infty} |\Phi(k)|^2 dk = 1$. This can be calculated numerically:

```
s_k = 1/4/s_x;
phi_0_k = sqrt(2*s_x)*phi_0;

phi_k_sq = 0;
for k = 1:length(k_coord)
    d_phi_k_sq = (phi_0_k*exp(-k_coord(k)^2/4/s_k))^2*d_k;
    phi_k_sq = phi_k_sq + d_phi_k_sq;
end
phi_k_sq
```

```
phi_k_sq = 1.0000
```

The wave packet in k-space can be plotted:

```
figure(2);
phi_k_t0 = phi_0_k*exp(-k_coord.^2/4/s_k);
plot(k_coord,abs(phi_k_t0));

xlabel('k')
ylabel('|\Phi(k,t=0)|')
```



The FWHM can be calculated by $\left| \exp\left(-\frac{k^2}{4 s_k} \right) \right|^2 = \frac{1}{2}$ and yield

$$FWHM = \sqrt{\frac{8 \ln(2) |s_k|^2}{\Re(s_k)}} = \sqrt{\frac{2 \ln(2)}{\Re(s_x)}}$$

in k-space. The value is:

```
fwhm_k = sqrt(2*log(2)/real(s_x))
```

```
fwhm_k = 0.5266
```

Again, this can be calculated numerically:

```
fwhm_k = 0;
for k = 1:length(k_coord)
    if exp(-k_coord(k)^2/4/s_k) > 0.5
        fwhm_k = fwhm_k + d_k;
    end
end
```

```
fwhm_k
```

```
fwhm_k = 0.7000
```

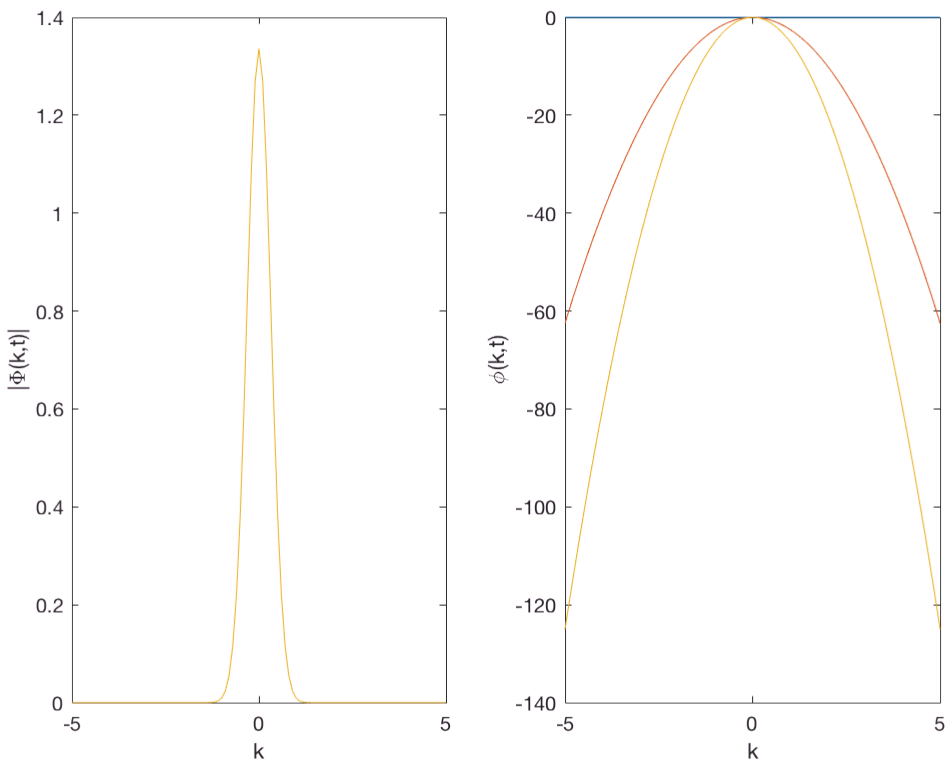
c) Time evolution in k-space

The time evolution of DeBroglie waves is given by

$$\Phi(k,t) = \Phi(k,t=0)\exp\left(-i\omega(k)t\right).$$

The dispersion relation is given by $\omega(k) = \frac{\hbar k^2}{2m}$ and the time evolution yield:

```
figure(3);

h_bar = 1;
m = 1;
omega = h_bar*k_coord.^2/2/m;

for t = [0 5 10]
    phi_k_t = phi_k_t0.*exp(-1i*omega*t);
    phase_t = -omega*t;
    subplot(1,2,1);
    plot(k_coord,abs(phi_k_t));
    hold on;
    subplot(1,2,2);
    plot(k_coord,phase_t);
    hold on;
end

subplot(1,2,1)
xlabel('k')
ylabel('|\Phi(k,t)|')
subplot(1,2,2)
xlabel('k')
ylabel('\phi(k,t)')
```



d) Inverse Fourier transformation to x-space

Plot

$$\varphi(x) = \frac{\widetilde{\varphi}_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{k^2}{4s_k}\right) \exp\left(-i\omega(k)t\right) \exp\left(ikx\right) dk$$

for different dispersion relations of $\omega(k)$:

```
figure(4);
clear fig;

omega = k_coord;                %linear dispersion
%omega = k_coord.^2;             %quadratic dispersion
%omega = k_coord + k_coord.^2;   %linear + quadratic dispersion

for t = [0 5 10]
    phi_x_ft = zeros(1,length(x_coord));
    for x = 1:length(x_coord)
        for k = 1:length(k_coord)
            phi_k = phi_0_k/sqrt(2*pi)*exp(-k_coord(k).^2/4/s_k);
            d_phi_k = phi_k*exp(-1i*omega(k)*t)*exp(1i*k_coord(k)*x_coord(x));
            phi_x_ft(x) = phi_x_ft(x) + d_phi_k;
        end
    end
    plot(x_coord,abs(phi_x_ft));
    hold on;
```

```
end

hold off;

legend({'t=T_0','t=T_1','t=T_2'})
xlabel('x')
ylabel('|\phi(x,t)|')
```