

PHYS 606 – Spring 2017 – Homework II – Solution

[1](a) We need the Fourier transf.

$$\phi(k) = \hat{\psi}(x, 0) = \frac{1}{\sqrt{2\pi}\sigma} \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{ik_0 x} e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi}\sigma} e^{-i(k-k_0)x_0} e^{-\frac{(k-k_0)^2}{4\hat{\sigma}^2}} \quad \text{where } \hat{\sigma} = \frac{1}{2\sigma}$$

cf. HW I, [3](c) with $k \rightarrow k-k_0$.

Time dependence of a mode k is $e^{-i\omega(k)t}$, FT back with that at arbitrary t

(formula from I.4.3)

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi} \frac{1}{2\sigma}} \int_{\mathbb{R}} e^{-\sigma^2(k-k_0)^2} e^{-i(k-k_0)x_0} e^{i(kx - \omega(k)t)} dk$$

$$\left. \begin{array}{l} u = k - k_0 \\ \omega = \frac{\hbar}{2m} (k_0^2 + 2k_0 u + u^2) \end{array} \right\} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi} \frac{1}{2\sigma}} e^{i(k_0 x - \frac{\hbar k_0^2}{2m} t)} \int_{\mathbb{R}} e^{-\sigma^2 u^2} e^{-i u x_0} e^{i u x} e^{-i \frac{\hbar}{2m} k_0 u t} e^{-i \frac{\hbar}{2m} u^2 t} du$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi} \frac{1}{2\sigma}} e^{i k_0 (x - v_{ph} t)} \int_{\mathbb{R}} e^{-[u^2 (\sigma^2 + i \frac{\hbar}{2m} t) - i u (x - x_0 - v_{gr} t)]} du$$

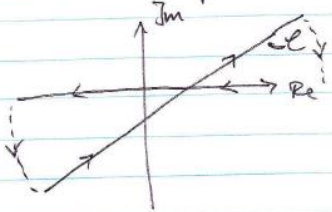
$$\left. \begin{array}{l} v_{ph} = \frac{\omega(k_0)}{k_0} = \frac{\hbar k_0}{2m} \\ v_{gr} = \frac{\partial \omega}{\partial k} \Big|_{k_0} = \frac{\hbar k_0}{m} \end{array} \right\}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi} \frac{1}{2\sigma}} e^{i k_0 (x - v_{ph} t)} \int_{\mathbb{R}} e^{-[\sqrt{\sigma^2 + i \frac{\hbar}{2m} t} u - \frac{i(x - x_0 - v_{gr} t)}{2\sqrt{\sigma^2 + i \frac{\hbar}{2m} t}}]^2} e^{-\frac{(x - x_0 - v_{gr} t)^2}{4(\sigma^2 + i \frac{\hbar}{2m} t)}} du$$

$$= \frac{1}{\sqrt{2\pi}} \frac{\sigma}{\sqrt{\pi}} e^{i k_0 (x - v_{ph} t)} e^{-\frac{(x - x_0 - v_{gr} t)^2}{4(\sigma^2 + i \frac{\hbar}{2m} t)}} \int_{\mathcal{C}} e^{-z^2} \left(\frac{dz}{du}\right)^{-1} dz$$

\mathcal{C} is an integration contour in \mathbb{C} , tilted away from the real axis and shifted

due to the transformation $z = u \sqrt{\sigma^2 + i \frac{\hbar}{2m} t} - \frac{i(x - x_0 - v_{gr} t)}{2\sqrt{\sigma^2 + i \frac{\hbar}{2m} t}}$



We can close the contour via sections at radius $\rightarrow \infty$ and the real line as shown $\oint_{\mathcal{C}} e^{-z^2} dz = 0$

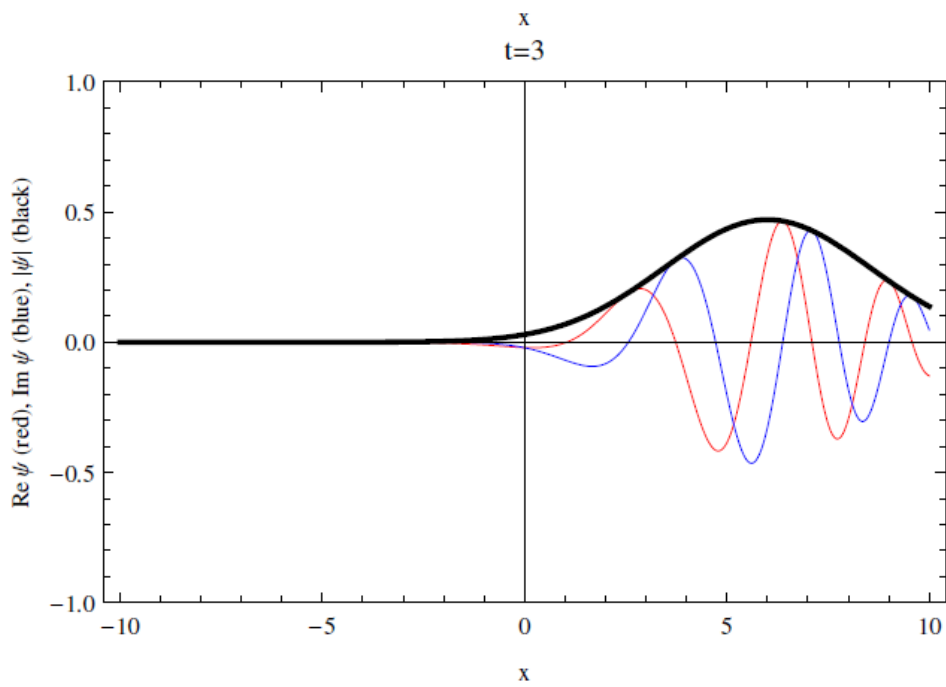
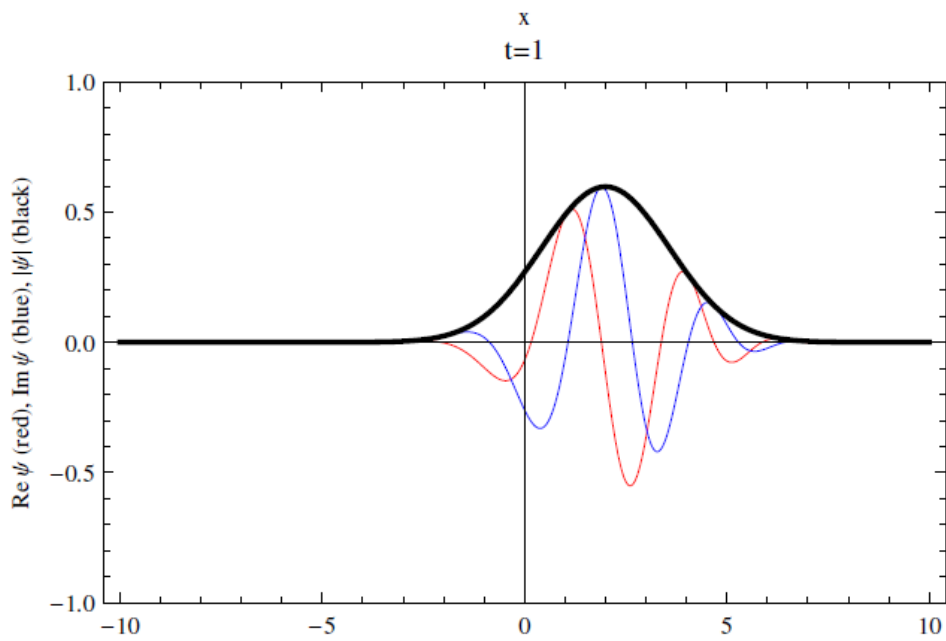
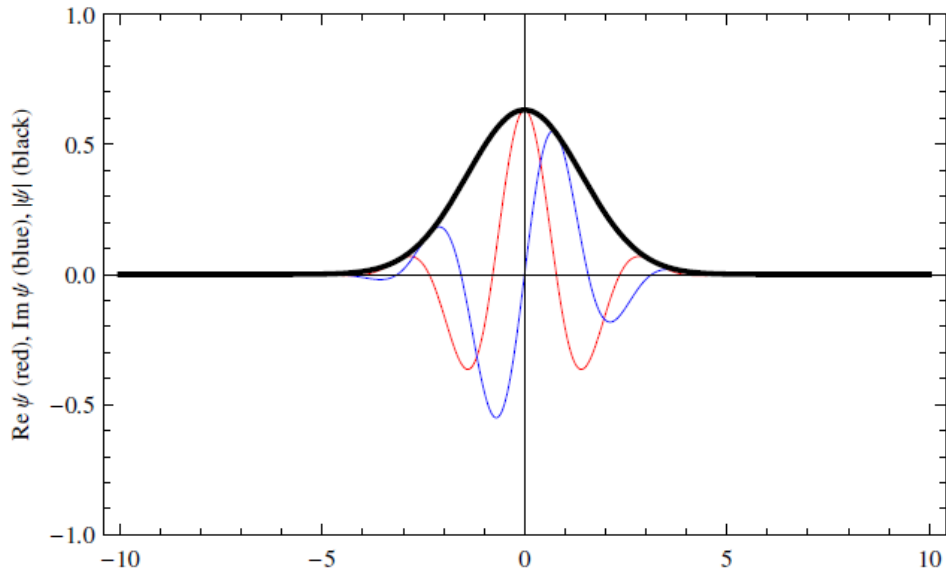
$$\text{Thus } \int_{\mathbb{R}} e^{-z^2} dz = \int_{\mathcal{C}} e^{-z^2} dz = \sqrt{\pi}$$

$$\frac{dz}{du} = \sqrt{\sigma^2 + i \frac{\hbar}{2m} t}$$

$$\Rightarrow \psi(x, t) = \frac{1}{\sqrt{2\pi}} \frac{\sigma}{\sqrt{\sigma^2 + i \frac{\hbar}{2m} t}} e^{i k_0 (x - v_{ph} t)} e^{-\frac{(x - x_0 - v_{gr} t)^2}{4(\sigma^2 + i \frac{\hbar}{2m} t)}}$$

(b)

$t=0, x_0=0, m=1, k_0=2, \sigma=1, \hbar=1$



Problem [2]

We have $i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi(\vec{r}, t) + V(\vec{r}) \psi(\vec{r}, t)$

Using the Fourier transformation $\psi(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \phi(\vec{p}, t) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p$

we get

$$\frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \left[i\hbar \frac{\partial}{\partial t} \phi(\vec{p}, t) \right] e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \phi(\vec{p}, t) \left[\underbrace{\left(-\frac{\hbar^2}{2m} \Delta\right) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}}_{= \frac{p^2}{2m} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}} + \underbrace{V(\vec{r}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}}_{V(-\frac{i}{\hbar} \nabla_p) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}} \right] d^3 p$$

partial integration in the last term: $\int \phi \nabla_p e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p =$

after repeated application to the power series expansion of V : $= \int (-\nabla_p \phi) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p + \text{boundary term } (\rightarrow 0)$

from a power series
 $\int_{\mathbb{R}^3} \frac{\partial^k}{\partial p_j^k} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p = \left(-\frac{i}{\hbar} \frac{\partial}{\partial p_j}\right)^k \int_{\mathbb{R}^3} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p$
 $k=1,2,3; \text{ not } \mathbb{N}$

$$\frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \left[i\hbar \frac{\partial}{\partial t} \phi(\vec{p}, t) - \frac{p^2}{2m} \phi(\vec{p}, t) - V\left(\frac{i}{\hbar} \nabla_p\right) \phi(\vec{p}, t) \right] e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p = 0$$

\Rightarrow Expression in bracket $[...] = 0$ (apply inverse FT!)

Problem [3]

(a) $\frac{d}{dt} \int_{V(t)} \rho d^3r = 0$ where V is a volume moving with the particles.

Choose ΔV so small that effectively $\int_{V(t)} \rho d^3r \approx \rho \Delta V$; for simplicity let it be a cuboid.

$$\Rightarrow \frac{d}{dt} \int_{\Delta V} \rho d^3r = \frac{\partial \rho}{\partial t} \Delta V + (\nabla \rho) \cdot \underbrace{\frac{d\vec{x}}{dt}}_{=\vec{v} \text{ velocity}} \Delta V + \rho \frac{d(\Delta V)}{dt}$$

$$= \frac{\partial \rho}{\partial t} \Delta V + (\nabla \rho) \cdot \vec{v} \Delta V + \rho \left[\frac{d(\Delta x)}{dt} \Delta y \Delta z + \Delta x \frac{d(\Delta y)}{dt} \Delta z + \Delta x \Delta y \frac{d(\Delta z)}{dt} \right]$$

$\frac{d(x_2 - x_1)}{dt} = v_2 - v_1$ where x_2, x_1 are positions of the front and back faces of ΔV , $x_2 - x_1 = \Delta x$
 $v_2 = v(x_2, t)$, $v_1 = v(x_1, t)$

$$= \frac{\partial \rho}{\partial t} \Delta V + (\nabla \rho) \cdot \vec{v} \Delta V$$

$$+ \rho \left[\frac{v_2(x_2) - v_1(x_1)}{\Delta x} + \frac{v_y(y_2) - v_y(y_1)}{\Delta y} + \frac{v_z(z_2) - v_z(z_1)}{\Delta z} \right] \Delta V$$

$$= \left[\frac{\partial \rho}{\partial t} + (\nabla \rho) \cdot \vec{v} + \rho (\nabla \cdot \vec{v}) \right] \Delta V \stackrel{!}{=} 0$$

(b) $\frac{\partial}{\partial t} (\psi_1 \psi_2^*) = \frac{\partial \psi_1}{\partial t} \psi_2^* + \psi_1 \frac{\partial \psi_2^*}{\partial t} = \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \Delta \psi_1 \right) \psi_2^* + \frac{1}{-i\hbar} \left(-\frac{\hbar^2}{2m} \Delta \psi_2^* \right) \psi_1$

$+ \frac{1}{i\hbar} \psi_1 V \psi_2^* + \frac{1}{-i\hbar} \psi_1 V^* \psi_2^* = 0$ for V real

$$= \frac{\hbar}{2mi} \left[\underbrace{\psi_1 \Delta \psi_2^* + \nabla \psi_1 \cdot \nabla \psi_2^*}_{\nabla \cdot (\psi_1 \nabla \psi_2^*)} - \underbrace{\nabla \psi_1 \cdot \nabla \psi_2^* + \Delta \psi_1 \psi_2^*}_{\nabla \cdot (\nabla \psi_1) \psi_2^*} \right] = -\nabla \cdot \vec{j}_{12}$$

with $\vec{j}_{12} = \frac{\hbar}{2mi} [\psi_2^* \nabla \psi_1 - \nabla \psi_2^* \psi_1]$

(c) For $\rho = |\psi|^2$ the cont. equation holds for $\vec{j} = \frac{\hbar}{2mi} [\psi^* \nabla \psi - \nabla \psi^* \psi]$

Use $\psi = A e^{i\hbar^{-1} S}$ as ansatz with A, S real

$$\begin{aligned} \nabla \psi &= \frac{\nabla A}{A} \psi + \frac{i}{\hbar} \nabla S \psi \Rightarrow \vec{j} = \frac{\hbar}{2mi} \left[\psi^* \left(\frac{\nabla A}{A} + \frac{i}{\hbar} \nabla S \right) \psi - \psi^* \left(\frac{\nabla A}{A} - \frac{i}{\hbar} \nabla S \right) \psi \right] \\ &= \frac{\nabla S}{m} \psi^* \psi = \frac{\nabla S}{m} \rho \end{aligned}$$

In the classical limit $\nabla S \rightarrow \vec{p}$ i.e. $\vec{j} \rightarrow \frac{\vec{p}}{m} \rho = \vec{v} \rho$

Problem [4]

Choose a volume V that encloses part of the surface (the plane $z=0$). Concretely, let us choose a cuboid with two sides of area A each that are parallel to the plane $z=0$. Those sides shall be at symmetric around $z=0$ at coordinates $z=-\varepsilon/2$ and $z=+\varepsilon/2$. The volume of the cuboid is then $V=A\varepsilon$ and the surface $z=0$ divides it into two equal parts. Now we integrate the continuity equation over the volume V and apply Gauss' Law.

$$0 = \int_V \frac{\partial}{\partial t} \rho \, dV + \int_V \nabla \cdot \vec{j} \, dV = \frac{d}{dt} \int_V \rho \, dV + \int_{\text{surface of } V} \vec{j} \cdot \hat{n}_s \, dS$$

↑
Gauss Law

$\hat{n}_s =$ normal unit vector to the outside, on each face of the cuboid.

Now take the limit $\varepsilon \rightarrow 0$ (areas A move closer to the surface). Then $V \rightarrow 0$ and the contribution of the four sides not parallel to the surface to \int_{surface} go to zero

$$\Rightarrow 0 \approx \lim_{\varepsilon \rightarrow 0^+} \vec{j}(\vec{S} + \varepsilon \hat{n}) \cdot \hat{n} A + \lim_{\varepsilon \rightarrow 0^-} \vec{j}(\vec{S} + \varepsilon \hat{n}) \cdot (-\hat{n}) A \quad (\square)$$

for points \vec{S} on the surface inside the cuboid; \hat{n} is now normal unit vector on surface in \vec{S}

I.e. the normal component of the current is continuous at the surface.

Since $\vec{j} = \frac{1}{2mi} [\psi^* \nabla \psi - \nabla \psi^* \psi]$ equation (\square) is obviously fulfilled if both ψ and the normal component of $\nabla \psi$ are continuous at the surface,