PHYS 606 – Spring 2015 – Homework II – Solution

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

$$\phi(k) = \hat{\psi}(x,0) = \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma}}\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} e^{-\frac{(x-x_0)^2}{4\sigma^2}}\, e^{ik_0x}\, e^{-ikx}\,dx$$

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

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

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

(formula from I.4.3)

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

$u = k-k_0$, $\omega = \frac{\hbar}{2m}\left(k_0^2+2k_0u+u^2\right)$

$$= \sqrt{\frac{\sigma}{\sqrt{2\pi^3}}}\, e^{i\left(k_0x-\frac{\hbar k_0^2}{2m}t\right)}\int_{\mathbb{R}} e^{-\sigma^2u^2}\, e^{-iux_0}\, e^{iux}\, e^{-i\frac{\hbar}{m}k_0ut}\, e^{-i\frac{\hbar}{2m}u^2t}\,du$$

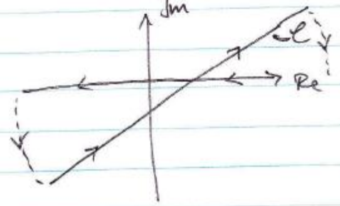
$$= \sqrt{\frac{\sigma}{\sqrt{2\pi^3}}}\, e^{ik_0(x-v_{ph}t)}\int_{\mathbb{R}} e^{-\left[u^2\left(\sigma^2+i\frac{\hbar}{2m}t\right)-iu(x-x_0-v_{gr}t)\right]}\,du$$

$v_{ph} := \frac{\omega(k_0)}{k_0} = \frac{\hbar k_0}{2m}$, $v_{gr} := \frac{\partial\omega}{\partial k}\Big|_{k_0} = \frac{\hbar k_0}{m}$

$$= \sqrt{\frac{\sigma}{\sqrt{2\pi^3}}}\, e^{ik_0(x-v_{ph}t)}\int_{\mathbb{R}} e^{-\left[u\sqrt{\sigma^2+i\frac{\hbar}{2m}t}-\frac{i(x-x_0-v_{gr}t)}{2\sqrt{\sigma^2+i\frac{\hbar}{2m}t}}\right]^2}\, e^{-\frac{(x-x_0-v_{gr}t)^2}{4\left(\sigma^2+i\frac{\hbar}{2m}t\right)}}\,du$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma}}\frac{\sigma}{\sqrt{\pi}}\, e^{ik_0(x-v_{ph}t)}\, e^{-\frac{(x-x_0-v_{gr}t)^2}{4\left(\sigma^2+i\frac{\hbar}{2m}t\right)}}\int_{\mathcal{C}} e^{-z^2}\left(\frac{dz}{du}\right)^{-1}dz$$

$\mathcal{C}$ is an integration contour in $\mathbb{C}$, tilted away from the real axis and shifted due to the transformation $z = u\sqrt{\sigma^2+i\frac{\hbar}{2m}t} - \frac{i(x-x_0-v_{gr}t)}{2\sqrt{\sigma^2+i\frac{\hbar}{2m}t}}$



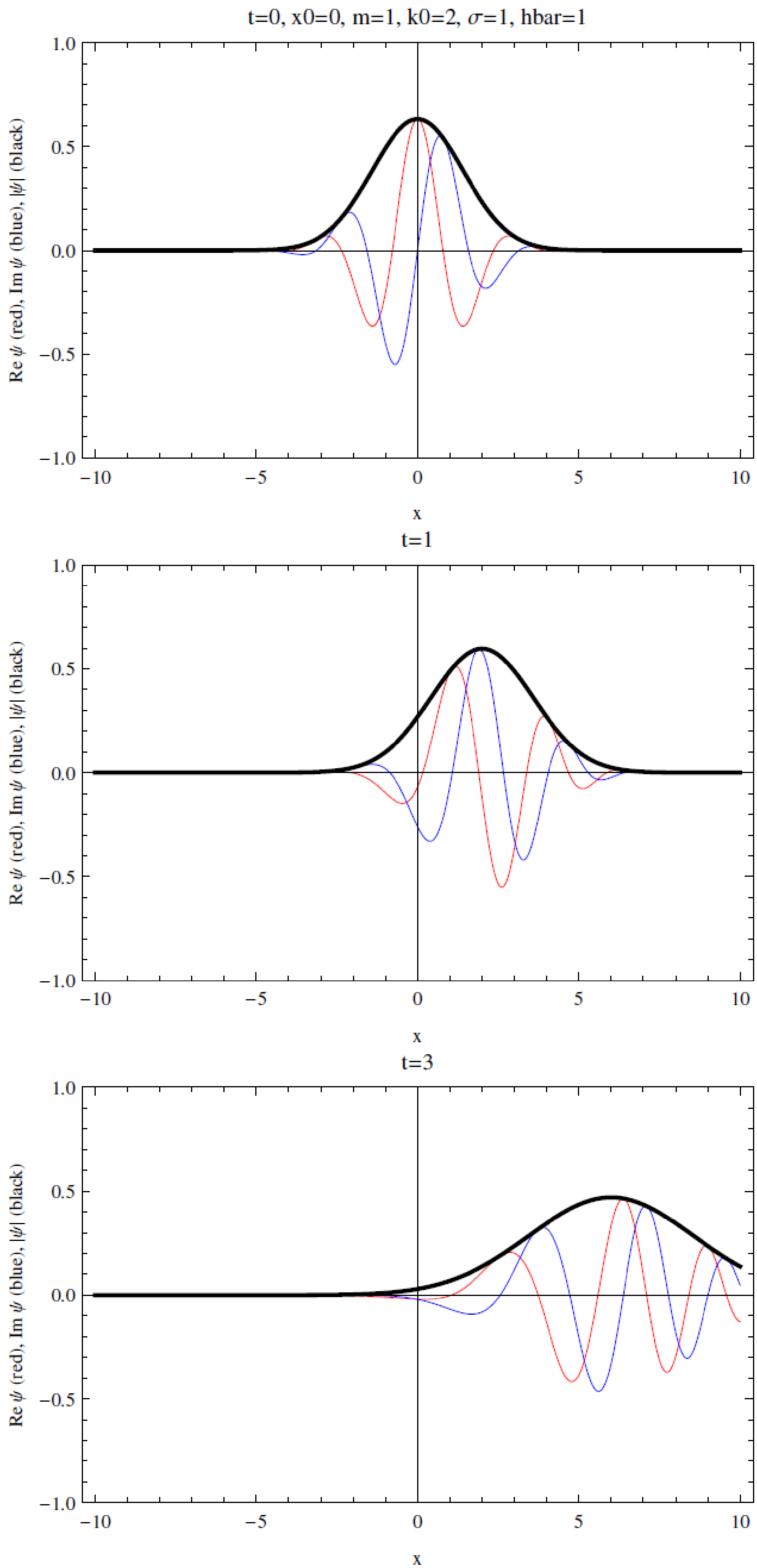
We can close the contour via sections at radius $\to \infty$ and the real line as shown $\oint e^{-z^2}dz = 0$

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

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

$$\Rightarrow \psi(x,t) = \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma}}\frac{\sigma}{\sqrt{\sigma^2+\frac{i\hbar}{2m}t}}\, e^{ik_0(x-v_{ph}t)}\, e^{-\frac{(x-x_0-v_{gr}t)^2}{4\left(\sigma^2+\frac{i\hbar}{2m}t\right)}}$$

(b)


t=0, x0=0, m=1, k0=2, σ=1, hbar=1
Re ψ (red), Im ψ (blue), $|\psi|$ (black)
x
t=1
Re ψ (red), Im ψ (blue), $|\psi|$ (black)
x
t=3
Re ψ (red), Im ψ (blue), $|\psi|$ (black)
x

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

we get

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

from a power series
$r_k^n e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} = \left(-\frac{i}{\hbar}\frac{\partial}{\partial p_k}\right)^n e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$
$k = 1,2,3;\ n \in \mathbb{N}$

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

$= \int (-\nabla_p \phi)\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\, d^3p$ + boundary term $(\to 0)$

after repeated application to the power series expansion of V:

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

$\Rightarrow$ Expression in bracket $[\ldots] = 0$ (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.

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

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

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

$v_2 = v_x(x_2,t)$, $v_1 = v_x(x_1,t)$

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

$$+ \rho\underbrace{\left[\frac{v_x(x_2)-v_x(x_1)}{\Delta x} + \frac{v_y(y_2)-v_y(y_1)}{\Delta y} + \frac{v_z(z_2)-v_z(z_1)}{\Delta z}\right]}_{\nabla\vec{v}}\Delta V$$

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

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

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

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

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

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

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

$$\nabla\psi = \frac{\nabla A}{A}\psi + \frac{i}{\hbar}\nabla S\,\psi \Rightarrow \vec{j} = \frac{\hbar}{2mi}\left[\psi^*\left(\frac{\nabla A}{A} + \frac{i}{\hbar}\nabla S\right)\psi - \psi^*\left(\frac{\nabla A}{A} - \frac{i}{\hbar}\nabla S\right)\psi\right]$$

$$= \frac{\nabla S}{m}\psi^*\psi = \frac{\nabla S}{m}\rho$$

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

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*=-ε/2 and *z*=+ε/2. The volume of the cuboid is then *V*=*A*ε and the surface *z*=0 divides it into to equal parts. Now we integrate the continuity equation over the volume *V* and apply Gauss' Law.

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

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

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

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

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