PHYS 606 – Spring 2014 – HW 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)

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

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

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

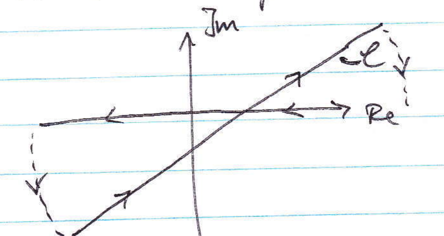
$$= \sqrt{\frac{\sigma}{\sqrt{2\pi^3}}}\, e^{ik_0(x-v_{ph}t)}\int_{\mathbb{R}} e^{-\left[u^2\left(\sigma^2+i\frac{\hbar}{2m}t\right) - iu(x-x_0-v_{gr}t)\right]}\, du$$

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

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

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

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

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

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

(b) See plots below. The change of width is determined by $\frac{\hbar}{2m}$.

[2] (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, $x_2 - x_1 = \Delta x$, $v_2 = v_x(x_2,t)$, $v_1 = v_x(x_1,t)$

$$= \frac{\partial\rho}{\partial t}\Delta V + (\nabla\rho)\cdot\vec{v}\,\Delta V + \rho\Bigg[\underbrace{\frac{v_x(x_2)-v_x(x_1)}{\Delta x} + \frac{v_y(y_2)-v_y(y_1)}{\Delta y} + \frac{v_z(z_2)-v_z(z_1)}{\Delta z}}_{\nabla\vec{v}}\Bigg]\Delta V$$

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

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

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

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

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. $\vec{j} \to \frac{\vec{p}}{m}\rho = \vec{v}\rho$

[3] Hamilton fct. $H(x,p) = \frac{p^2}{2m} - bx$

Hamilton–Jacobi: $\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - bx + \frac{\partial S}{\partial t} = 0$ with $p = \frac{\partial S}{\partial x}$

Since $\frac{\partial H}{\partial t} = 0$ time is separable: $S = W(x) - Et$

$$\Rightarrow \frac{1}{2m}\left(\frac{dW}{dx}\right)^2 = E + bx \quad \Rightarrow \quad \frac{dW}{dx} = \pm\sqrt{2m(E+bx)}$$

$$\Rightarrow W(x) = \pm\frac{1}{3mb}\left[2m(E+bx)\right]^{3/2} + \text{const.}$$

$$\Rightarrow S(x,t) = \pm\frac{1}{3mb}\left[2m(E+bx)\right]^{3/2} - Et + \text{const.}$$

E is constant of motion choose it a the variable after canonical transf.

$\Rightarrow$ Associated momentum $\beta = \frac{\partial S}{\partial \alpha} = \text{const.}$ and $\beta = \pm\frac{1}{b}\sqrt{2m(E+bx)} - t$

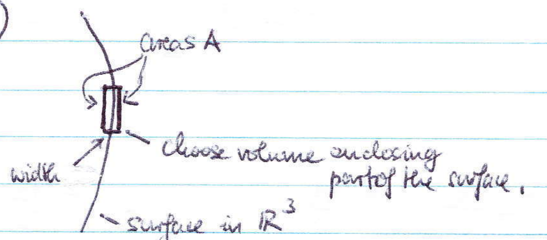
$$\Rightarrow x = \frac{b}{2m}(t+\beta)^2 - \frac{E}{b}$$

Initial conditions: $x(0) = \frac{b\beta^2}{2m} - \frac{E}{b} \stackrel{!}{=} x_0$ $\qquad \dot{x}(0) = \frac{b\beta}{m} \stackrel{!}{=} v_0$

$$\Rightarrow \beta = \frac{m}{b}v_0 \quad \text{and} \quad E = \frac{b^2}{2m}\frac{m^2}{b^2}v_0^2 - bx_0 = \frac{1}{2}mv_0^2 - bx_0$$

$$\Rightarrow x(t) = \frac{b}{2m}\left(t + \frac{m}{b}v_0\right)^2 - \frac{mv_0^2}{2b} + x_0$$

[4] (a)



Choose a volume $V = A\cdot\varepsilon$ in the form of a cuboid which encloses a part of the surface as shown. A should be small enough so that the curvature can be neglected and the two faces of area A are essentially parallel to the surface element, on both sides of it.

Integrate the continuity eqn. over this volume V:

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

$\hat{n}_s$ = 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, which are eqs. (5), (6).

(b) $\psi_{\vec{k}_1} = e^{i(\vec{k}_1\cdot\vec{r} - \omega t)}$ solves the S.E. for constant potential $V_1 < E$ and by plugging in we receive the dispersion relation $\underbrace{\hbar\omega}_{E} = \frac{\hbar^2 k_1^2}{2m} + V_1$.

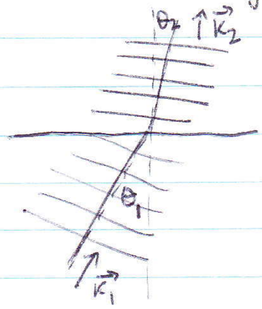
Similar for const. pot. energy V_2. $e^{i(\vec{k}_2\cdot\vec{r} - \omega t)} = \psi_{\vec{k}_2}$

Matching at $z=0$ using (5): $e^{i(k_1^x x + k_1^y y - \omega_1 t)} = e^{i(k_2^x x + k_2^y y - \omega_2 t)}$

This is only possible for all x, y and t simultaneously if $k_1^x = k_2^x$, $k_1^y = k_2^y$ and $\omega_1 = \omega_2$ (i.e. $E_1 = E_2 = E$)

From the frequencies: $\frac{\hbar k_1^2}{2m} + V_1 = \frac{\hbar k_2^2}{2m} + V_2 \Rightarrow {k_1^z}^2 - {k_2^z}^2 = \frac{2m}{\hbar}(V_2 - V_1)$

This can be brought into the form of Snell's Law of Refraction:



$$\sin\theta_1 = \frac{\sqrt{{k_1^x}^2 + {k_1^y}^2}}{k_1} \, , \quad \sin\theta_2 = \frac{\sqrt{{k_2^x}^2 + {k_2^y}^2}}{k_2}$$

$$\Rightarrow \frac{\sin\theta_2}{\sin\theta_1} = \frac{k_1}{k_2} = \frac{\sqrt{\frac{2m}{\hbar^2}(E - V_1)}}{\sqrt{\frac{2m}{\hbar^2}(E - V_2)}} = \sqrt{\frac{E - V_1}{E - V_2}} \text{ " } = \frac{n_1}{n_2} \text{ "}$$

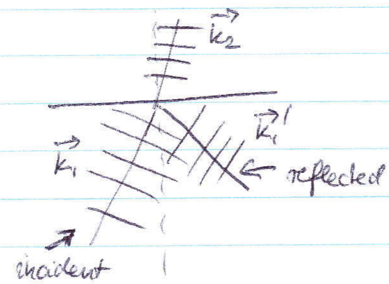
An index of refraction in a pot. energy V could be defined as $n = \sqrt{\frac{E-V}{E}}$

(c) Check boundary condition (6):

$$\frac{\partial}{\partial z}\psi_{\vec{k}_1}\Big|_{z=0} = i k_1^z \psi_{\vec{k}_1}\Big|_{z=0} \qquad \frac{\partial}{\partial z}\psi_{\vec{k}_2}\Big|_{z=0} = i k_2^z \psi_{\vec{k}_2}\Big|_{z=0}$$

Since $\psi_{\vec{k}_1}\big|_{z=0} = \psi_{\vec{k}_2}\big|_{z=0}$: $k_1^z = k_2^z$ in contradiction to (6)

Guidance from optics suggests to add a reflected wave $\psi_{\vec{k}_1'}$ with $\vec{k}_1' = (k_1^x, k_1^y, -k_1^z)$



Try $\quad \alpha\psi_{\vec{k}_1} + \beta\psi_{\vec{k}_1'}$ for $z < 0$

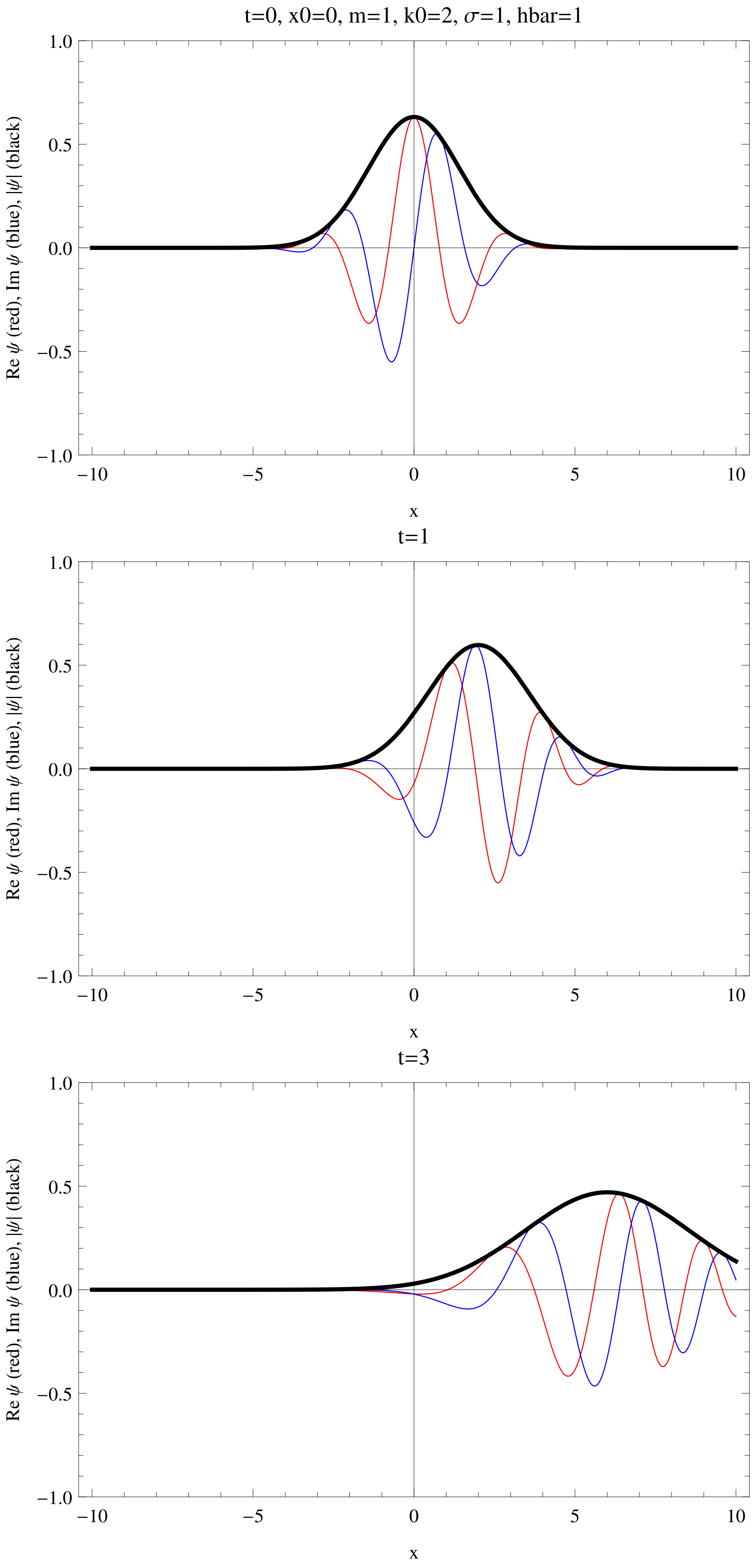
$\quad \gamma\psi_{\vec{k}_2}$ for $z > 0$

Boundary cond. (5) satisfied for $\alpha + \beta = \gamma$ (A)

(6): $\alpha i k_1^z + \beta i(-k_1^z) = \gamma i k_2^z \Rightarrow (\alpha - \beta) k_1^z = \gamma k_2^z$ (B)

There are solutions to eqs. (A) + (B)

This is not the only but the simplest solution to this problem.


t=0, x0=0, m=1, k0=2, σ=1, hbar=1
t=1
t=3
Re ψ (red), Im ψ (blue), |ψ| (black)
x
1.0
0.5
0.0
−0.5
−1.0
−10
−5
0
5
10