Quantum Dynamics, NWI-SM295, exercises week 5

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Question 1: Flux of a plane wave

A plane wave with wave vector $\boldsymbol{k}$ is given by

$$\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = Ne^{i\boldsymbol{k}\cdot\boldsymbol{r}}.$$

The expression for the flux-operator in 3D is

$$\boldsymbol{j} = \frac{\hbar}{\mu}\mathrm{Im}\Psi^*(\boldsymbol{r})\boldsymbol{\nabla}\Psi(\boldsymbol{r}).$$

1a. Determine the flux of wave function Ψ in an arbitrary point $\boldsymbol{r}$.

Answer: *See week 3, question* **2b**

$$\boldsymbol{j} = |N|^2\frac{\hbar}{\mu}\boldsymbol{k}. \tag{1}$$

Question 2: Spherical waves

Cartesian vector $\boldsymbol{r}$ can be expressed in spherical polar coordinates through

$$\begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} = r\begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{2}$$

2a. Write down the Hamiltonian of a free particle in spherical polar coordinates (r, θ, ϕ)

Answer: *See week 4, question 1:*

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{l}^2}{2\mu r^2} \tag{3}$$

2b. Show that spherical waves are eigenfunctions of the free particle Hamiltonian and calculate the energy

$$\Psi(r, \theta, \phi) = N\frac{e^{ikr}}{r}$$

Answer: *The $\hat{l}^2$ operator only acts on the angles, so we only need the radial part of the Hamtilonian:*

$$\begin{aligned} \hat{H}\Psi(r,\theta,\phi) &= -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r\,N\frac{e^{ikr}}{r} && (4)\\ &= -\frac{\hbar^2}{2\mu}N\frac{1}{r}\frac{\partial^2}{\partial r^2}e^{ikr} && (5)\\ &= \frac{\hbar^2k^2}{2\mu}N\frac{e^{ikr}}{r}, && (6)\\ &= \frac{\hbar^2k^2}{2\mu}\Psi(r,\theta,\phi), && (7) \end{aligned}$$

so the energy is $\frac{\hbar^2k^2}{2\mu}$.

Question 3: Flux operator in spherical polar coordinates

The gradient operator $\boldsymbol{\nabla}$, can be rewritten in arbitrary curvilinear $\{u_1(\boldsymbol{r}), \ldots, u_n(\boldsymbol{r})\}$ coordinates using

$$\boldsymbol{\nabla} = \begin{pmatrix} \frac{\partial}{\partial r_1} \\ \vdots \\ \frac{\partial}{\partial r_n} \end{pmatrix} = \boldsymbol{J}(\boldsymbol{J}^T\boldsymbol{J})^{-1}\begin{pmatrix} \frac{\partial}{\partial u_1} \\ \vdots \\ \frac{\partial}{\partial u_n} \end{pmatrix}$$

where $\boldsymbol{J}$ is the Jacobian matrix with elements

$$\boldsymbol{J}_{i,j} = \frac{\partial r_i}{\partial u_j}.$$

3a. Derive the expression for the gradient in spherical polar coordinates.

Answer: *The Jacobian is*

$$\boldsymbol{J} = \begin{pmatrix} \frac{\partial \boldsymbol{r}}{\partial r} & \frac{\partial \boldsymbol{r}}{\partial \theta} & \frac{\partial \boldsymbol{r}}{\partial \phi} \end{pmatrix} \tag{8}$$

$$= \begin{pmatrix} \cos\phi\sin\theta & r\cos\phi\cos\theta & -r\sin\phi\sin\theta \\ \sin\phi\sin\theta & r\sin\phi\cos\theta & r\cos\phi\sin\theta \\ \cos\theta & -r\sin\theta & 0 \end{pmatrix} \tag{9}$$

$$\equiv (\hat{\boldsymbol{r}} \;\; r\boldsymbol{e}_\theta \;\; r\sin\theta\boldsymbol{e}_\phi)\,. \tag{10}$$

Since the columns of the Jacobian are orthogonal to eachother, $\boldsymbol{J}^T\boldsymbol{J}$ *is diagonal*

$$\boldsymbol{J}^T\boldsymbol{J} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & \sin\theta^2 r^2 \end{pmatrix} \tag{11}$$

and so

$$\boldsymbol{J}(\boldsymbol{J}^T\boldsymbol{J})^{-1} = (\hat{\boldsymbol{r}} \;\; r\boldsymbol{e}_\theta \;\; r\sin\theta\boldsymbol{e}_\phi) \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^{-2} & 0 \\ 0 & 0 & r^{-2}\sin^{-2}\theta \end{pmatrix} = \begin{pmatrix} \hat{r} & \frac{\boldsymbol{e}_\theta}{r} & \frac{\boldsymbol{e}_\phi}{r\sin\theta} \end{pmatrix} \tag{12}$$

and

$$\boldsymbol{\nabla} = \hat{\boldsymbol{r}}\frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}. \tag{13}$$

Question 4: Flux of spherical waves

4a. Use the previous results to compute the flux of a spherical wave.

Answer:

$$\boldsymbol{j} = \frac{\hbar}{\mu}\mathrm{Im}\Psi^*(\boldsymbol{r})\boldsymbol{\nabla}\Psi(\boldsymbol{r}) \tag{14}$$

$$= \hat{\boldsymbol{r}}\frac{\hbar}{\mu}\mathrm{Im}\Psi^*(\boldsymbol{r})\frac{\partial}{\partial r}\Psi(\boldsymbol{r}) \tag{15}$$

$$= \hat{\boldsymbol{r}}\frac{\hbar}{\mu}|N|^2\mathrm{Im}\frac{e^{-ikr}}{r}\frac{\partial}{\partial r}\frac{e^{ikr}}{r} \tag{16}$$

$$= \hat{\boldsymbol{r}}\frac{\hbar}{\mu}|N|^2\mathrm{Im}\frac{e^{-ikr}}{r}\left(\frac{-1}{r^2} + \frac{ik}{r}\right)e^{ikr} \tag{17}$$

$$= \frac{\hat{\boldsymbol{r}}}{r^2}\frac{\hbar k}{\mu}|N|^2 \tag{18}$$

$$\boldsymbol{j} = \hat{\boldsymbol{r}}v\rho. \tag{19}$$

In the last step we defined the velocity $v = p/\mu$*, where the momentum is* $p = \hbar k$*, and the density* $\rho = |\Psi|^2 = |N|^2/r^2$.