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

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

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 $\boldsymbol{r}$.

Question 2: Spherical waves

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

$$\begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} = r \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{1}$$

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

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

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

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.

Question 4: Flux of spherical waves

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