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Problem 4.1: Linear algebra basics **[Written] (6 pts.)**

↪ ID: ex_linear_algebra_basics:qm2122

Learning objective

In this exercise we study the properties of Hermitian and unitary operators, which play a fundamental role in the description of quantum mechanics.

Let $\mathcal{H}$ be a finite-dimensional Hilbert space whose elements are denoted by $|\psi\rangle$, $|\phi\rangle$, ... Further, we consider linear operators A, B on that Hilbert space.

a) The *Hermitian conjugate* (or *adjoint*) of A (also denoted $A^\dagger$) is defined as

$$\langle\psi|A^\dagger\phi\rangle = \langle A\psi|\phi\rangle = \langle\phi|A\psi\rangle^* \,. \tag{1}$$

Show that $(AB)^\dagger = B^\dagger A^\dagger$.

b) An operator satisfying $A = A^\dagger$ is called *Hermitian* or *self-adjoint*. Show that the eigenvalues of Hermitian operators are real and the corresponding eigenvectors of two different eigenvalues are orthogonal. (*Remark*: You can assume that there are no degenerate eigenvalues.)

c) A (linear) operator that satisfies $UU^\dagger = U^\dagger U = I$ with I the identity, or equivalently $U^{-1} = U^\dagger$, is called a *unitary* operator. Show that unitary operators leave the norm of a vector unchanged. Show that the eigenvalues λ_n of a unitary operator have modulus unity, i.e. $\lambda_n = e^{i\phi_n}$ with $\phi_n \in \mathbb{R}$, and that eigenvectors corresponding to different eigenvalues are orthogonal.

d) Let A be a Hermitian operator. Show that the operator $U = e^{i\alpha A}$, $\alpha \in \mathbb{R}$, is unitary.

e) Consider an orthonormal basis set $\{|n\rangle\}$ and another basis set $\{|n'\rangle\}$ with $|n'\rangle = U\,|n\rangle$, where U is a unitary operator. Show that $\{|n'\rangle\}$ is also orthonormal. If we denote the matrix elements of an operator A by $A_{mn} = \langle m|A|n\rangle$, how do the matrix elements A_{mn} relate to the matrix elements in the basis $\{|n'\rangle\}$?

f) Let A and B be Hermitian operators with $[A, B] = 0$. Show that A and B can be diagonalized simultaneously. (*Remark:* Neglect the case of degenerate eigenvalues.)

Problem 4.2: Continuity and unitarity **[Written] (2 pts.)**

↪ ID: ex_continuity_unitarity:qm2122

Learning objective

This exercise verifies that the wave function gives rise to a consistent probability density. For one-dimensional scattering problems we can use the probability interpretation to proof a fundamental relation for the scattering parameters.

a) Show, that the probability density $\rho(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|^2$ obeys the continuity equation

$$\partial_t \rho(\boldsymbol{r},t) = -\nabla \boldsymbol{j}(\boldsymbol{r},t),$$

where $\boldsymbol{j}$ is the probability current

$$\boldsymbol{j}(\boldsymbol{r},t) = -\frac{i\hbar}{2m}\left[\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)\nabla\psi^*(\boldsymbol{r},t)\right]. \tag{2}$$

Prove that the total probability, $\int d\boldsymbol{r}\, |\psi(\boldsymbol{r},t)|^2$, is conserved.

b) Consider the scattering at a one-dimensional potential barrier with the reflection and transmission coefficients $r(k)$ and $t(k)$. Use the probability density current to show $|r(k)|^2 + |t(k)|^2 = 1$.

Problem 4.3: Wave packet at a potential barrier [Oral] (4 pts.)

↪ ID: ex_wave_packet_potential_barrier:qm2122

> **Learning objective**
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> In this exercise you will study a prototypical example of scattering in one dimension. Most scattering problems cannot be solved analytically, so you will learn how to find the solution numerically and derive an approximation which is valid in some parameter regimes.

Consider the following 1-dimensional potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq a \\ 0 & x > a \end{cases} \tag{3}$$

with $V_0 > 0$, and the solution of stationary Schrödinger equation

$$\psi_k(x) = \begin{cases} e^{ikx} + r(k)e^{-ikx} & x < 0 \\ B(k)e^{-\bar{k}x} + B'(k)e^{\bar{k}x} & 0 \leq x \leq a \\ t(k)e^{ikx} & x > a \end{cases} \tag{4}$$

with $k = \sqrt{2mE}/\hbar > 0$ and $\bar{k}^2 = 2mV_0/\hbar^2 - k^2$.

Suppose that at time t_0 one has a wave packet $\psi(x, t_0)$ centered at $-L$ and far from the barrier $L \gg a$ with $\sigma \ll L$

$$\psi(x, t_0) = \frac{1}{(2\pi\sigma)^{\frac{1}{4}}} e^{ik_0 x} e^{-\frac{(x+L)^2}{4\sigma}}. \tag{5}$$

with $k_0 \gg 1/\sqrt{\sigma}$.

a) Determine the reflection and transmission coefficients $r(k)$ and $t(k)$.

b) Decompose the wave packet $\psi(x, t_0)$ into eigenstates of the Hamiltonian.

   Hint: Assume that the functions $\psi_k(x)$ with $k > 0$ generate the initial state $\psi(x, t_0)$.

c) Suppose that the coefficients $t(k)$, $r(k)$, $B(k)$, $B'(k)$ are k-independent. Calculate the time evolution of the wave packet $\psi(x, t)$ and show that, after reaching the barrier, it splits into two wave packets: reflected and transmitted.

d) Numerically solve the time evolution of the wave packet in the general case with $t(k)$, $r(k)$, $B(k)$, $B'(k)$ explicitly k-dependent. Compare this exact solution to your approximations from task c).