Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 2

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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Matrix-valued functions

Let us consider a function that attributes to every real number x a complex number $f(x)$. How does one generalize this function to matrices? If the function is analytic, this means that it equals its Taylor series (within some convergence radius, etc):

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x=0} x^n. \tag{1}$$

One may then define its value for some matrix M using the same Taylor series:

$$f(M) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x=0} M^n. \tag{2}$$

1. Use this definition to evaluate $\exp(zM) = \mathrm{e}^{zM}$ for

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{3}$$

   and for

$$M = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}. \tag{4}$$

   Here z is a complex number.

2. Now consider two different matrices M_1 and M_2 that commute, $[M_1, M_2] = M_1 M_2 - M_2 M_1 = 0$. Argue that the binomial formula still holds and show that $\exp(M_1 + M_2) = \exp(M_1) \exp(M_2)$.

An alternative definition can be introduced if the matrix M can be diagonalized. For an $N \times N$ matrix M, the eigen decomposition has the form:

$$M = \sum_{n=1}^{N} \lambda_n V_n V_n^\dagger, \tag{5}$$

where λ_n are the eigenvalues and V_n are the corresponding eigenvectors:

$$V_n = \begin{pmatrix} (V_n)_1 \\ (V_n)_2 \\ \vdots \\ (V_n)_N \end{pmatrix}, \qquad V_n^\dagger = \begin{pmatrix} (V_n)_1^* & (V_n)_2^* & \dots & (V_n)_N^* \end{pmatrix}. \tag{6}$$

The eigenvectors are are orthogonal, $V_n^\dagger V_m = 0$ when $n \neq m$, and normalized: $V_n^\dagger V_n = 1$.

3. Introduce the alternative definition of the matrix value of a function
$$\tilde{f}(M) = \sum_{n=1}^{N} f(\lambda_n) V_n V_n^\dagger. \tag{7}$$
Show that this definition is equivalent to the definition of Eq. (2), i.e., that $\tilde{f}(M) = f(M)$.

4. Now consider in particular the two matrices of part 1. Diagonalize them and explicitly show that $\tilde{f}(M) = f(M)$.

⋆ Problem 2 ⋆ Fun with commutators

The commutator of two operator $\hat{A}$ and $\hat{B}$ is defined as
$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$
Its two main properties are that it is linear in both of its arguments, $[\hat{A}_1 + \hat{A}_2, \hat{B}] = [\hat{A}_1, \hat{B}] + [\hat{A}_1, \hat{B}]$ and $[\hat{A}, \hat{B}_1 + \hat{B}_2] = [\hat{A}, \hat{B}_1] + [\hat{A}, \hat{B}_2]$, and that it is antisymmetric, $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$.

1. Another important general property is the Jacobi identity
$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0. \tag{8}$$
Prove it.

2. Show that
$$[\hat{A}, \hat{B}_1\hat{B}_2] = [\hat{A}, \hat{B}_1]\hat{B}_2 + \hat{B}_1[\hat{A}, \hat{B}_2], \tag{9}$$
and that in general
$$[\hat{A}, \hat{C}_1\hat{C}_2 \cdots \hat{C}_n] = [\hat{A}, \hat{C}_1]\hat{C}_2 \cdots \hat{C}_n + \hat{C}_1[\hat{A}, \hat{C}_2]\hat{C}_3 \cdots \hat{C}_n + \cdots + \hat{C}_1 \cdots \hat{C}_{n-1}[\hat{A}, \hat{C}_n]. \tag{10}$$
Tip: use induction.

3. Let us now consider the position $\hat{x}$ and momentum $\hat{p} = -\mathrm{i}\hbar\partial_x$ operators. Using the commutation relation $[\hat{p}, \hat{x}] = -\mathrm{i}\hbar$, show that
$$[\hat{p}, f(\hat{x})] = -\mathrm{i}\hbar f'(\hat{x}) \tag{11}$$
where f is an analytic function so $f(\hat{x})$ is defined via Eq. (2). (Matrices are the simplest examples of operators, and the definition (2) holds for more general operators like $\hat{x}$, $\hat{p}$, etc)

4. Now consider the Hamiltonian
$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{12}$$
Using the Ehrenfest relation, find $\partial_t \langle \hat{x} \rangle_t$ and $\partial_t \langle \hat{p} \rangle_t$. In the case of a harmonic well $V(x) = \frac{1}{2}m\omega_0^2 x^2$ solve the Ehrenfest relations to find $\langle \hat{x} \rangle_t$ and $\langle \hat{p} \rangle_t$ if initially at $t = 0$ they equal x_0 and p_0, respectively.

Problem 3 Fourier transform basics

1. The Dirac delta function $\delta(x)$ satisfies the identity
$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx}. \tag{13}$$
To make sense of this identity, regularize the integral on the right-hand side with a Gaussian weight e^{-ak^2} and in the end take the $a \to 0$ limit. Using the fact that the Gaussian integral $\int_{-\infty}^{\infty} dx\, \mathrm{e}^{-a(x-z)^2} = \sqrt{\pi/a}$ holds for an arbitrary complex z, but positive a, prove the above identity. You may invoke the results of Exercise Sheet 1.

2. Now consider an arbitrary function $f(x)$. Write it in terms of itself using a Dirac delta function. If the Fourier transform is defined with the convention

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx \, \mathrm{e}^{-\mathrm{i}kx} f(x), \tag{14}$$

what is the corresponding formula for $f(x)$ in terms of $\tilde{f}(k)$?

3. Define the scalar product of two functions f and g as

$$\langle f|g\rangle = \int_{-\infty}^{\infty} dx \, f^*(x) g(x). \tag{15}$$

Find the corresponding expression for $\langle f|g\rangle$ in terms of $\tilde{f}(k)$ and $\tilde{g}(k)$.

4. Now consider the momentum operator $\hat{p} = -\mathrm{i}\hbar\partial_x$. First show that $\langle f|\hat{p}g\rangle = \langle \hat{p}f|g\rangle$, i.e., that $\hat{p}$ is Hermitian. What must you assume about $f(x)$ and $g(x)$ for this to hold? Next, express $\langle f|\hat{p}g\rangle$ in terms of $\tilde{f}(k)$ and $\tilde{g}(k)$.