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 $\tilde{f}(M) = f(M)$.

Solution 1

1. The key property to observe is that for both matrices $M^2 = I$, where I is the 2×2 identity. Hence

$$\begin{aligned}\exp(zM) &= \sum_{n=0}^{\infty} \frac{z^n}{n!} M^n = \sum_{n=0}^{\infty} \frac{z^{2n}}{(2n)!} M^{2n} + \sum_{n=0}^{\infty} \frac{z^{2n+1}}{(2n+1)!} M^{2n+1} \\ &= I \sum_{n=0}^{\infty} \frac{z^{2n}}{(2n)!} + M \sum_{n=0}^{\infty} \frac{z^{2n+1}}{(2n+1)!} = I\cosh(z) + M\sinh(z).\end{aligned}$$

Hence

$$\begin{aligned}\exp z \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} &= \begin{pmatrix} \cosh z & \sinh z \\ \sinh z & \cosh z \end{pmatrix}, \\ \exp z \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} &= \begin{pmatrix} \cosh z & -\mathrm{i}\sinh z \\ \mathrm{i}\sinh z & \cosh z \end{pmatrix}.\end{aligned}$$

2. Binomial formulas still holds because $M_{1/2}$ algebraically behave like complex numbers (scalars) when they commute. Hence:

$$\begin{aligned}\exp(M_1 + M_2) &= \sum_{n=0}^{\infty} \frac{1}{n!}(M_1 + M_2)^n = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} M_1^k M_2^{n-k} \\ &= \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{1}{k!(n-k)!} M_1^k M_2^{n-k}\end{aligned}$$

Now we reparameterize the sum from (n, k) to (k, ℓ) with $\ell = n - k$. To cover all the same pairs as the (n, k) sum, the sums over (k, ℓ) must span all non-negative integers. Hence:

$$\exp(M_1 + M_2) = \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} \frac{1}{k!\ell!} M_1^k M_2^\ell = \exp(M_1)\exp(M_2).$$

3. The key property is that

$$M^n = \sum_{m=1}^{N} \lambda_m^n V_m V_m^\dagger,$$

which follows from the fact that V_m are orthonormal. Thus

$$\begin{aligned}f(M) &= \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} M^n = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} \sum_{m=1}^{N} \lambda_m^n V_m V_m^\dagger \\ &= \sum_{m=1}^{N} \left(\sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} \lambda_m^n \right) V_m V_m^\dagger = \sum_{m=1}^{N} f(\lambda_m) V_m V_m^\dagger = \tilde{f}(M).\end{aligned}$$

4. By diagonalizing the matrices in the usual way, one finds

$$z\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \longrightarrow \lambda_1 = z, V_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}, \lambda_2 = -z, V_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix},$$
$$z\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix} \longrightarrow \lambda_1 = z, V_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}, \lambda_2 = -z, V_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}.$$

So

$$\exp z\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\mathrm{e}^z + \mathrm{e}^{-z} & \mathrm{e}^z - \mathrm{e}^{-z}\\ \mathrm{e}^z - \mathrm{e}^{-z} & \mathrm{e}^z + \mathrm{e}^{-z}\end{pmatrix},$$
$$\exp z\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\mathrm{e}^z + \mathrm{e}^{-z} & -\mathrm{i}(\mathrm{e}^z - \mathrm{e}^{-z})\\ \mathrm{i}(\mathrm{e}^z - \mathrm{e}^{-z}) & \mathrm{e}^z + \mathrm{e}^{-z}\end{pmatrix},$$

which agrees with the previous.

⋆ 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 $V(x) = \frac{1}{2}m\omega_0^2x^2$ 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.

Solution 2

1. Since

$$[\hat{A}_1, [\hat{A}_2, \hat{A}_3]] = (\hat{A}_1\hat{A}_2\hat{A}_3 - \hat{A}_2\hat{A}_3\hat{A}_1) + (\hat{A}_3\hat{A}_2\hat{A}_1 - \hat{A}_1\hat{A}_3\hat{A}_2),$$

under a cyclic summation ($1,2,3 \to 2,3,1$ and $3,1,2$) the pairs of terms that we have grouped above vanish.

2. The $n = 2$ case is just a matter of a little algebra. To prove for general n, in the induction step one simply uses the $n = 2$ formula with $\hat{B}_1 = \hat{C}_1$ and $\hat{B}_2 = \hat{C}_2 \cdots \hat{C}_n$.

3. From part 2, one sees that $[\hat{p}, \hat{x}^n] = -\mathrm{i}\hbar n\hat{x}^{n-1}$. Thus

$$\begin{aligned}[\hat{p}, f(\hat{x})] &= \left[\hat{p}, \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} \hat{x}^n\right] = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} [\hat{p}, \hat{x}^n] \\ &= -\mathrm{i}\hbar \sum_{n=1}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} n\hat{x}^{n-1} = -\mathrm{i}\hbar f'(\hat{x}).\end{aligned}$$

4. The Ehrenfest relation

$$\partial_t \left\langle \hat{A} \right\rangle_t = -\frac{i}{\hbar} \left\langle [\hat{A}, \hat{H}] \right\rangle_t$$

gives

$$\begin{aligned}\partial_t \langle \hat{x} \rangle_t &= -\frac{i}{\hbar} \left\langle \left[\hat{x}, \frac{\hat{p}^2}{2m} + V(\hat{x})\right] \right\rangle_t = -\frac{i}{\hbar} \left\langle \frac{\hat{p}[\hat{x},\hat{p}] + [\hat{x},\hat{p}]\hat{p}}{2m} \right\rangle_t = \frac{\langle \hat{p} \rangle_t}{m}, \\ \partial_t \langle \hat{p} \rangle_t &= -\frac{i}{\hbar} \left\langle \left[\hat{p}, \frac{\hat{p}^2}{2m} + V(\hat{x})\right] \right\rangle_t = - \langle V'(\hat{x}) \rangle_t \,,\end{aligned}$$

where used the fact that the commutator is linear, and that operators commute with themselves. For a harmonic oscillators the above reduce to the equations of motion familiar from classical mechanics. Their solution is

$$\begin{aligned}\langle \hat{x} \rangle_t &= x_0 \cos(\omega_0 t) + \frac{p_0}{m\omega_0} \sin(\omega_0 t), \\ \langle \hat{p} \rangle_t &= p_0 \cos(\omega_0 t) - m\omega_0 x_0 \sin(\omega_0 t).\end{aligned}$$

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 $\tilde{g}(k)$.

Solution 3

1.

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx - ak^2} &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left[-a\left(k + \frac{\mathrm{i}x}{2a}\right)^2 - \frac{x^2}{4a}\right] \\
&= \frac{1}{2\pi}\sqrt{\frac{\pi}{a}}\mathrm{e}^{-x^2/(4a)} \longrightarrow \delta(x)
\end{aligned}$$

as $a \to 0$ since it's the same as in Excercise Sheet 1, Problem 1, with $\sigma = 2\sqrt{a}$.

2.

$$\begin{aligned}
f(x) &= \int_{-\infty}^{\infty} \mathrm{d}x'\, \delta(x - x')f(x') = \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}k(x-x')} f(x') \\
&= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx} \int_{-\infty}^{\infty} \mathrm{d}x' \mathrm{e}^{-\mathrm{i}kx'} f(x') = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx} \tilde{f}(k).
\end{aligned}$$

3. This is called Parseval's identity:

$$\begin{aligned}
\langle f|g\rangle &= \int_{-\infty}^{\infty} dx dx'\, f^*(x)\, \delta(x - x')g(x') = \int_{-\infty}^{\infty} dx dx' f^*(x)g(x') \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}k(x-x')} \\
&= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[\int_{-\infty}^{\infty} dx\, \mathrm{e}^{-\mathrm{i}kx} f(x)\right]^* \int_{-\infty}^{\infty} dx'\, \mathrm{e}^{-\mathrm{i}kx'} g(x') = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{f}^*(k)\tilde{g}(k).
\end{aligned}$$

4. By partially integrating one obtains

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} dx\, f^*(x)(-\mathrm{i}\hbar)\partial_x g(x) = -\mathrm{i}\hbar \int_{-\infty}^{\infty} dx \partial_x \left[f^*(x)g(x)\right] + \int_{-\infty}^{\infty} dx\, (\mathrm{i}\hbar)\partial_x f^*(x)g(x),$$

and thus

$$\langle f|\hat{p}g\rangle = \langle \hat{p}f|g\rangle - \mathrm{i}\hbar f^*(x)g(x)\big|_{-\infty}^{x=\infty}.$$

The assumption is therefore that $f(x)$ and $g(x)$ decay as $x \to \pm\infty$. Next

$$\hat{p}g(x) = -\mathrm{i}\hbar\partial_x \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx}\tilde{g}(k) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathrm{e}^{\mathrm{i}kx} \left[\hbar k \cdot \tilde{g}(k)\right],$$

so using Parseval's identity

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{f}^*(k)\hbar k\tilde{g}(k).$$