

Problem set 1

We begin the weekly sets with some problems concerning basic and useful mathematical relations.

1.1 Commutators and anti-commutators

We use the standard notation for commutators and anticommutators

$$[A, B] = AB - BA \quad \{A, B\} = AB + BA \quad (1)$$

where A and B are two operators or matrices. Show the following identities,

$$\begin{aligned} [A, BC] &= [A, B]C + B[A, C] \\ [A, BC] &= \{A, B\}C - B\{A, C\} \end{aligned} \quad (2)$$

1.2 Trace and determinant

We remind you about the following relations

$$\text{Tr}(AB) = \text{Tr}(BA), \quad \det(AB) = \det A \det B \quad (3)$$

- a) Assume \hat{A} to be the operator for a quantum observable and A to be the matrix representation of this operator in an orthonormalized basis $\{|n\rangle\}$, which means

$$A_{mn} = \langle m|\hat{A}|n\rangle \quad (4)$$

We define the trace and determinant of the (abstract) operator as

$$\text{Tr } \hat{A} = \text{Tr } A, \quad \det \hat{A} = \det A \quad (5)$$

Show that if we change to a new basis $\{|n'\rangle\}$, which is related to the first by a unitary transformation, that will not change the values of the trace and determinant.

- b) Assume \hat{A} is a hermitian operator with eigenvalues $a_n, n = 1, 2, \dots$. Explain why the trace and determinant can be expressed in terms of the eigenvalues as

$$\text{Tr } \hat{A} = \sum_n a_n \quad \det \hat{A} = \prod_n a_n \quad (6)$$

- c) The *spectral decomposition* of an hermitian operator \hat{A} is a sum of the form

$$\hat{A} = \sum_n a_n |n\rangle\langle n| \quad (7)$$

where a_n are the eigenvalues and $|n\rangle$ are the corresponding eigenvectors of the operator. A function $f(a)$ defines an *operator function* $\hat{f} \equiv f(\hat{A})$ of \hat{A} by the related decomposition

$$\hat{f} \equiv \sum_n f(a_n) |n\rangle\langle n| \quad (8)$$

Use this definition and the results of problem b) to show that we have the following relation

$$\det e^{\hat{A}} = e^{\text{Tr} \hat{A}} \quad (9)$$

We assume the trace of \hat{A} to be well defined and finite (which may not necessarily be the case in an infinite dimensional Hilbert space).

d) Show that for general state vectors $|\psi\rangle$ and $|\phi\rangle$ we have the relation

$$\langle\psi|\phi\rangle = \text{Tr}(|\phi\rangle\langle\psi|) \quad (10)$$

1.3 Dirac's delta function

The basic relation defining the delta functions is the following

$$f(x) = \int_{-\infty}^{\infty} dx' \delta(x - x') f(x') \quad (11)$$

with $f(x)$ as any chosen function. Clearly $\delta(x)$ is not a function in the usual sense, and in particular it has the property that $\delta(x) = 0$ for $x \neq 0$ and $\delta(0) = \infty$. Nevertheless it is possible (with some care) to treat it as a function, and as we know from the wavefunction description of quantum physics it is in many cases a very useful concept.

We remind you about the formulas for Fourier transformation in one dimension

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \tilde{f}(k) e^{ikx} \quad (12)$$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx} \quad (13)$$

a) Show that the delta function has the following Fourier expansion

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} \quad (14)$$

b) Assume $g(x)$ is a differentiable function with zero at one point x_0 ,

$$g(x_0) = 0 \quad (15)$$

Assume also that the derivative does not vanish at this point, $g'(x_0) \neq 0$. Show by use of the definition (11), and by studying the integral $\int dx \delta(g(x)) f(x)$, that we have the following relation

$$\delta(g(x)) = \frac{1}{|g'(x_0)|} \delta(x - x_0) \quad (16)$$

(Hint, make change of variable $x \rightarrow g$ in the integral.) Assume that the function $g(x)$ has several zeros, at the points $x = x_i$. Explain why this gives the generalized formula

$$\delta(g(x)) = \sum_i \frac{1}{|g'(x_i)|} \delta(x - x_i) \quad (17)$$

1.4 Position and momentum eigenstates

The position and momentum eigenstates are given by the relations

$$\hat{x}|x\rangle = x|x\rangle \quad \langle x|x'\rangle = \delta(x - x') \quad \int dx |x\rangle\langle x| = \mathbb{1} \quad (18)$$

$$\hat{p}|p\rangle = p|p\rangle \quad \langle p|p'\rangle = \delta(p - p') \quad \int dp |p\rangle\langle p| = \mathbb{1} \quad (19)$$

Furthermore, in the x-representation the momentum operator is given by $\hat{p} = -i\hbar \frac{d}{dx}$. Use these relations together with the Fourier expansion of the delta function to show that the scalar product of a momentum and a position state is given by

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}xp} \quad (20)$$

1.5 Some operator expansions

Assume \hat{A} and \hat{B} to be two operators, generally not commuting.

We define the following two composite operators:

$$\hat{F}(\lambda) = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}, \quad \hat{G}(\lambda) = e^{\lambda\hat{A}}e^{\lambda\hat{B}} \quad (21)$$

a) Show the following relation

$$\frac{d\hat{F}}{d\lambda} = [\hat{A}, \hat{F}] \quad (22)$$

and use it to derive the expansion

$$\hat{F}(\lambda) = \hat{B} + \lambda [\hat{A}, \hat{B}] + \frac{\lambda^2}{2} [\hat{A}, [\hat{A}, \hat{B}]] + \dots \quad (23)$$

b) Show the following relation between $\hat{G}(\lambda)$ and $\hat{F}(\lambda)$,

$$\frac{d\hat{G}}{d\lambda} = (\hat{A} + \hat{F})\hat{G} \quad (24)$$

and use this to demonstrate the following expansion (Campbell-Baker-Hausdorff)

$$\hat{G}(\lambda) = e^{\lambda\hat{A} + \lambda\hat{B} + \frac{\lambda^2}{2}[\hat{A}, \hat{B}] + \dots} \quad (25)$$

by calculating the exponent on the right-hand side to second order in λ .

c) When $[\hat{A}, \hat{B}]$ commutes with both \hat{A} and \hat{B} the expression (25) is exact without the higher order terms indicated by ... in (25). Verify this by use of (23) and (24), and by noting that the eigenvalues of \hat{G} satisfy a differential equation that can be integrated.

1.6 Spin operators and Pauli matrices

A spin half operator $\hat{\mathbf{S}}$ is defined in the standard way as

$$\hat{\mathbf{S}} = \frac{\hbar}{2} \boldsymbol{\sigma} \quad (26)$$

where $\boldsymbol{\sigma}$ is a vector with the three Pauli matrices $(\sigma_1, \sigma_2, \sigma_3)$ (or equivalently written as $(\sigma_x, \sigma_y, \sigma_z)$) as Cartesian components. We use the standard expressions for these 2x2 matrices, as given in the lecture notes. We also introduce the rotated Pauli matrix, defined by $\sigma_{\mathbf{n}} = \mathbf{n} \cdot \boldsymbol{\sigma}$, where \mathbf{n} is an unspecified three dimensional unit vector.

- a) Show that $\sigma_{\mathbf{n}}$ has eigenvalues ± 1 , and the eigenstate (in matrix form) corresponding to the eigenvalue $+1$ is (up to an arbitrary phase factor)

$$\Psi_{\mathbf{n}} = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix} \quad (27)$$

with (θ, ϕ) as the polar angles of the unit vector \mathbf{n} . Also show the relation

$$\Psi_{\mathbf{n}}^\dagger \boldsymbol{\sigma} \Psi_{\mathbf{n}} = \left(\Psi_{\mathbf{n}}^\dagger \sigma_x \Psi_{\mathbf{n}}, \Psi_{\mathbf{n}}^\dagger \sigma_y \Psi_{\mathbf{n}}, \Psi_{\mathbf{n}}^\dagger \sigma_z \Psi_{\mathbf{n}} \right) = \mathbf{n} \quad (28)$$

- b) Show, by using the operator identity

$$e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}} = \hat{B} + \lambda [\hat{A}, \hat{B}] + \frac{\lambda^2}{2} [\hat{A}, [\hat{A}, \hat{B}]] \dots,$$

the following relation

$$e^{-\frac{i}{2} \alpha \sigma_z} \sigma_x e^{\frac{i}{2} \alpha \sigma_z} = \cos \alpha \sigma_x + \sin \alpha \sigma_y \quad (29)$$

Explain why this shows that the unitary matrix

$$\hat{U} = e^{-\frac{i}{2} \alpha \sigma_{\mathbf{n}}} = e^{-\frac{i}{\hbar} \alpha \mathbf{n} \cdot \hat{\mathbf{S}}} \quad (30)$$

induces a spin rotation of angle α about the axis \mathbf{n} .

- c) Demonstrate, by expansion of the exponential function, the following identity

$$e^{-\frac{i}{2} \alpha \sigma_{\mathbf{n}}} = \cos \frac{\alpha}{2} \mathbb{1} - i \sin \frac{\alpha}{2} \sigma_{\mathbf{n}} \quad (31)$$

with $\mathbb{1}$ as the 2x2 identity matrix.