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

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

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

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

1.2 Trace and determinant

We remind you about the following relations

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

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

$$A_{mn} = \langle m|\hat{A}|n\rangle \tag{4}$$

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

$$\mathrm{Tr}\,\hat{A} = \mathrm{Tr}\,A\,, \quad \det\hat{A} = \det A \tag{5}$$

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 $a_n, n = 1, 2, ...$ Explain why the trace and determinant can be expressed in terms of the eigenvalues as

$$\mathrm{Tr}\,\hat{A} = \sum_n a_n \quad \det\hat{A} = \prod_n a_n \tag{6}$$

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

$$\hat{A} = \sum_n a_n |n\rangle\langle n| \tag{7}$$

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

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

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

$$\det\, e^{\hat{A}} = e^{\mathrm{Tr}\,\hat{A}} \tag{9}$$

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

$$\langle\psi|\phi\rangle = \mathrm{Tr}(|\phi\rangle\langle\psi|) \tag{10}$$

1.3 Dirac's delta function

The basic relation defining the delta functions is the following

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

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

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

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

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

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

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

$$g(x_0) = 0 \tag{15}$$

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

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

(Hint, make change of variable $x \to g$ 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

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

1.4 Position and momentum eigenstates

The position and momentum eigenstates are given by the relations

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

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

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 give by

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

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:

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

a) Show the following relation

$$\frac{d\hat{F}}{d\lambda} = \left[\hat{A}, \hat{F}\right] \tag{22}$$

and use it to derive the expansion

$$\hat{F}(\lambda) = \hat{B} + \lambda\left[\hat{A}, \hat{B}\right] + \frac{\lambda^2}{2}\left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] ... \tag{23}$$

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

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

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

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

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

c) When $\left[\hat{A}, \hat{B}\right]$ 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

$$\hat{\mathbf{S}} = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{26}$$

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)

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

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

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

b) Show, by using the operator identity

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

the following relation

$$e^{-\frac{i}{2}\alpha\sigma_z}\,\sigma_x\,e^{\frac{i}{2}\alpha\sigma_z} = \cos\alpha\,\sigma_x + \sin\alpha\,\sigma_y \tag{29}$$

Explain why this shows that the unitary matrix

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

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

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

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

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