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 a quantum observable and A to be the matrix representation of the observable 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 Heisenberg's equation of motion

In the Heisenberg picture the state vectors are time independent, while the observables change with time. An observable $\hat{A}$ which has no *explicit* time dependence satisfies Heisenberg's equation of motion, in the form

$$\frac{d}{dt}\hat{A} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right] \tag{26}$$

with $\hat{H}$ as the Hamiltonian of the system.

Assume a particle of mass m moves in a one-dimensional potential $V(x)$. In the coordinate representation the position and momentum operators are given as

$$\hat{x} = x\,, \quad \hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{27}$$

Find the expressions for Heisenberg's equation of motion for $\hat{x}$ and $\hat{p}$ and show that these give for the position operator a differential equation with the same form as the classical equation of motion of a particle with mass m in the potential $V(x)$.

1.7 Time dependent unitary transform

Two unitarily equivalent descriptions of a quantum system are related by a *time dependent* unitary transformation $\hat{U}(t)$, which acts on state vectors as

$$|\psi(t)\rangle \quad \rightarrow \quad |\psi'(t)\rangle = \hat{U}(t)|\psi(t)\rangle \tag{28}$$

and on the observables as

$$\hat{A} \quad \rightarrow \quad \hat{A}'(t) = \hat{U}(t)\,\hat{A}\,\hat{U}(t)^{-1}\,. \tag{29}$$

Show that the Hamiltonian $\hat{H}'$, which determines the Schrödinger equation of the transformed state vector $|\psi'(t)\rangle$, includes an additional term which depends on the time derivative of $\hat{U}(t)$,

$$\hat{H} \rightarrow \hat{H}'(t) = \hat{U}(t)\,\hat{H}\,\hat{U}(t)^{-1} + i\hbar\frac{d\hat{U}}{dt}\hat{U}^{-1} \tag{30}$$

Discuss the meaning of the difference between the equations (29) and (30).