Homework 3

Problem 9

(a) Prove that if $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$ for all $|\psi\rangle$ then $\langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_1|\hat{B}|\psi_2\rangle$ for all $|\psi_1\rangle$ and $|\psi_2\rangle$.

Suggestion. Substitute $|\psi\rangle = |\psi_1\rangle + \lambda|\psi_2\rangle$ into $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$, then set $\lambda = 1$ and $\lambda = i$.

(b) By definition, $\hat{A} = \hat{B}$ if and only if $\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$ for all $|\psi\rangle$.

Use the result of part (a) to show that $\hat{A} = \hat{B}$ if and only if $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$ for all $|\psi\rangle$.

Solution

(a) Following the suggestion, we write

$$\langle\psi|\hat{A}|\psi\rangle - \langle\psi|\hat{B}|\psi\rangle = \underbrace{\langle\psi_1|\hat{A}|\psi_1\rangle - \langle\psi_1|\hat{B}|\psi_1\rangle}_{0} + |\lambda|^2\underbrace{\big[\langle\psi_2|\hat{A}|\psi_2\rangle - \langle\psi_2|\hat{B}|\psi_2\rangle\big]}_{0}$$
$$+ \lambda\big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_1|\hat{B}|\psi_2\rangle\big] + \lambda^*\big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_2|\hat{B}|\psi_1\rangle\big] = 0\,.$$

This equation must be satisfied for all complex λ, which is possible only if the expressions in the square brackets vanish. Indeed, substituting $\lambda = 1$ and $\lambda = i$, we obtain

$$\left.\begin{array}{l} \big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_1|\hat{B}|\psi_2\rangle\big] + \big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_2|\hat{B}|\psi_1\rangle\big] = 0 \\ \big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_1|\hat{B}|\psi_2\rangle\big] - \big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_2|\hat{B}|\psi_1\rangle\big] = 0 \end{array}\right\} \implies \langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_1|\hat{B}|\psi_2\rangle\,. \qquad \blacksquare$$

(b) It is obvious that $\hat{A} = \hat{B}$ implies $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$. To show that $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$ implies $\hat{A} = \hat{B}$, we pick an arbitrary orthonormal basis $\{|\phi_n\rangle\}$. By the result of part (a), components of vectors $\hat{A}|\psi\rangle$ and $\hat{B}|\psi\rangle$ in this basis coincide, $\langle\phi_n|\hat{A}|\psi\rangle = \langle\phi_n|\hat{B}|\psi\rangle$, hence these vectors are equal: $\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$ for all $|\psi\rangle$, i.e., $\hat{A} = \hat{B}$. $\blacksquare$

Problem 10

Show that if $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\psi\rangle^*$ for all $|\psi\rangle$ then $\langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_2|\hat{A}^\dagger|\psi_1\rangle^*$ for all $|\psi_1\rangle$ and $|\psi_2\rangle$.

Suggestion. Substitute $|\psi\rangle = |\psi_1\rangle + \lambda|\psi_2\rangle$ into $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\psi\rangle^*$ then set $\lambda = 1$ and $\lambda = i$ [cf. Problem 9(a)].

Solution

Proceeding as suggested, we obtain

$$\langle\psi|\hat{A}|\psi\rangle - \langle\psi|\hat{A}^\dagger|\psi\rangle^* = \underbrace{\langle\psi_1|\hat{A}|\psi_1\rangle - \langle\psi_1|\hat{A}^\dagger|\psi_1\rangle^*}_{0} + |\lambda|^2\underbrace{\big[\langle\psi_2|\hat{A}|\psi_2\rangle - \langle\psi_2|\hat{A}^\dagger|\psi_2\rangle^*\big]}_{0}$$
$$+ \lambda\big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_2|\hat{A}^\dagger|\psi_1\rangle^*\big] + \lambda^*\big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_1|\hat{A}^\dagger|\psi_2\rangle^*\big] = 0\,.$$

Substituting here $\lambda = 1$ and $\lambda = i$ as in Problem 10(a), we get

$$\left.\begin{array}{l} \big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_2|\hat{A}^\dagger|\psi_1\rangle^*\big] + \big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_1|\hat{A}^\dagger|\psi_2\rangle^*\big] = 0 \\ \big[\langle\psi_1|\hat{A}|\psi_2\rangle - \langle\psi_2|\hat{A}^\dagger|\psi_1\rangle^*\big] - \big[\langle\psi_2|\hat{A}|\psi_1\rangle - \langle\psi_1|\hat{A}^\dagger|\psi_2\rangle^*\big] = 0 \end{array}\right\} \implies \langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_2|\hat{A}^\dagger|\psi_1\rangle^*\,. \qquad \blacksquare$$

Problem 11

(a) Show that $\dfrac{d}{d\lambda}\big[e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}\big] = e^{\lambda\hat{A}}[\hat{A},\hat{B}]e^{-\lambda\hat{A}}$ for all $\hat{A}$ and $\hat{B}$.

(b) Derive the expansion $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \dfrac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dfrac{1}{3!}\Big[\hat{A},[\hat{A},[\hat{A},\hat{B}]]\Big] + \ldots$

Suggestion: expand $\hat{F}(\lambda) = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}$ in Taylor series about $\lambda = 0$, then set $\lambda = 1$.

Solution

(a) We have

$$\frac{d}{d\lambda}\big[e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}\big] = \big(\tfrac{d}{d\lambda}e^{\lambda\hat{A}}\big)\hat{B}e^{-\lambda\hat{A}} + e^{\lambda\hat{A}}\hat{B}\big(\tfrac{d}{d\lambda}e^{-\lambda\hat{A}}\big) = e^{\lambda\hat{A}}\hat{A}\hat{B}e^{-\lambda\hat{A}} - e^{\lambda\hat{A}}\hat{B}\hat{A}e^{-\lambda\hat{A}} = e^{\lambda\hat{A}}[\hat{A},\hat{B}]e^{-\lambda\hat{A}}. \qquad \blacksquare$$

(b) Applying repeatedly the formula derived in part (a), we find

$$\hat{F}(\lambda) = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}} \xrightarrow{\lambda\to 0} \hat{B},$$
$$\frac{d}{d\lambda}\hat{F}(\lambda) = e^{\lambda\hat{A}}[\hat{A},\hat{B}]e^{-\lambda\hat{A}} \xrightarrow{\lambda\to 0} [\hat{A},\hat{B}],$$
$$\frac{d^2}{d\lambda^2}\hat{F}(\lambda) = e^{\lambda\hat{A}}\big[\hat{A},[\hat{A},\hat{B}]\big]e^{-\lambda\hat{A}} \xrightarrow{\lambda\to 0} \big[\hat{A},[\hat{A},\hat{B}]\big],$$

and so on. Obviously, $(n+1)$-th order derivative of $\hat{F}(\lambda)$ at $\lambda = 0$ is given by the commutator of $\hat{A}$ with n-th order derivative. Taylor expansion of $\hat{F}(\lambda)$ about $\lambda = 0$ then reads

$$\hat{F}(\lambda) = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}} = \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\hat{F}^{(n)}(0) = \hat{B} + \lambda[\hat{A},\hat{B}] + \frac{\lambda^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{\lambda^3}{3!}\Big[\hat{A},[\hat{A},[\hat{A},\hat{B}]]\Big] + \ldots$$

Setting here $\lambda = 1$, we arrive at $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \dfrac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dfrac{1}{3!}\Big[\hat{A},[\hat{A},[\hat{A},\hat{B}]]\Big] + \ldots \qquad \blacksquare$

Problem 12

Operators $\hat{A}$ and $\hat{B}$ commute with their commutator: $\big[\hat{A},[\hat{A},\hat{B}]\big] = \big[\hat{B},[\hat{A},\hat{B}]\big] = \hat{0}$.

(a) Show that $\big[\hat{A},e^{\lambda\hat{B}}\big] = \lambda e^{\lambda\hat{B}}[\hat{A},\hat{B}]$. *Suggestion*: use the expansion derived in Problem 11(b).

(b) Show that $\hat{F}(\lambda) = e^{\lambda\hat{A}}e^{\lambda\hat{B}}e^{-\lambda(\hat{A}+\hat{B})}$ obeys the differential equation $\dfrac{d}{d\lambda}\hat{F}(\lambda) = \lambda[\hat{A},\hat{B}]\hat{F}(\lambda)$.

(c) By solving the equation derived in part (b), obtain the Baker-Hausdorff formula $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{\frac{1}{2}[\hat{A},\hat{B}]}$.

Solution

(a) Because $\hat{A}$ commutes with $[\hat{A},\hat{B}]$, the expansion of $e^{-\lambda\hat{B}}\hat{A}e^{\lambda\hat{B}}$ [see Problem 11(b)] terminates at linear in λ term. Taking into account that $e^{\lambda\hat{B}}e^{-\lambda\hat{B}} = \hat{1}$, we obtain

$$\hat{A}e^{\lambda\hat{B}} = e^{\lambda\hat{B}}\big(e^{-\lambda\hat{B}}\hat{A}e^{\lambda\hat{B}}\big) = e^{\lambda\hat{B}}\big(\hat{A} + \lambda[\hat{A},\hat{B}]\big) = e^{\lambda\hat{B}}\hat{A} + \lambda e^{\lambda\hat{B}}[\hat{A},\hat{B}] \quad\Longrightarrow\quad \big[\hat{A},e^{\lambda\hat{B}}\big] = \lambda e^{\lambda\hat{B}}[\hat{A},\hat{B}]. \qquad \blacksquare$$

(b) We have

$$\frac{d}{d\lambda}\hat F(\lambda) = \big(\tfrac{d}{d\lambda}e^{\lambda\hat A}\big)e^{\lambda\hat B}e^{-\lambda(\hat A+\hat B)} + e^{\lambda\hat A}\big(\tfrac{d}{d\lambda}e^{\lambda\hat B}\big)e^{-\lambda(\hat A+\hat B)} + e^{\lambda\hat A}e^{\lambda\hat B}\big(\tfrac{d}{d\lambda}e^{-\lambda(\hat A+\hat B)}\big)$$

$$= e^{\lambda\hat A}\Big\{\hat A e^{\lambda\hat B} + e^{\lambda\hat B}\hat B - e^{\lambda\hat B}(\hat A+\hat B)\Big\}e^{-\lambda(\hat A+\hat B)} = e^{\lambda\hat A}\big[\hat A, e^{\lambda\hat B}\big]e^{-\lambda(\hat A+\hat B)}.$$

Substituting here $\big[\hat A, e^{\lambda\hat B}\big] = \lambda e^{\lambda\hat B}[\hat A,\hat B]$ [see part (a)] and taking into account that $[\hat A,\hat B]$ commutes with both $e^{\lambda\hat A}$ and $e^{\lambda\hat B}$, we obtain

$$\frac{d}{d\lambda}\hat F(\lambda) = e^{\lambda\hat A}\lambda e^{\lambda\hat B}[\hat A,\hat B]e^{-\lambda(\hat A+\hat B)} = \lambda[\hat A,\hat B]e^{\lambda\hat A}e^{\lambda\hat B}e^{-\lambda(\hat A+\hat B)} = \lambda[\hat A,\hat B]\hat F(\lambda). \qquad \blacksquare$$

(c) Introducing new variable $t=\lambda^2/2$, we rewrite the differential equation derived in part (b) as

$$\frac{d}{dt}\hat F(t) = [\hat A,\hat B]\hat F(t).$$

Solution of this equation subject to the condition $\hat F(0)=\hat{\mathbb{1}}$ is unique and reads $\hat F(t) = e^{t[\hat A,\hat B]}$. Restoring the original variable λ, we get

$$\hat F(\lambda) = e^{\lambda\hat A}e^{\lambda\hat B}e^{-\lambda(\hat A+\hat B)} = e^{(\lambda^2/2)[\hat A,\hat B]}.$$

Setting here $\lambda=1$, multiplying both sides of the resulting equation by $e^{\hat A+\hat B}$, and taking into account that because the operators $[\hat A,\hat B]$ and $\hat A+\hat B$ commute, so do their exponents, we arrive at the Baker-Hausdorff formula:

$$e^{\hat A}e^{\hat B}e^{-(\hat A+\hat B)} = e^{\frac12[\hat A,\hat B]} \quad\Longrightarrow\quad e^{\hat A}e^{\hat B} = e^{\frac12[\hat A,\hat B]}e^{\hat A+\hat B} = e^{\hat A+\hat B}e^{\frac12[\hat A,\hat B]}. \qquad \blacksquare$$

Problem 13

By definition, *trace* of a linear operator acting in a finite-dimensional Hilbert space is the sum of its diagonal matrix elements: $\mathrm{tr}\hat A = \sum_n \langle\phi_n|\hat A|\phi_n\rangle$, where $\{|\phi_n\rangle\}$ is an orthonormal basis. (In an infinitely-dimensional space the sum in $\mathrm{tr}\hat A$ turns to an infinite series, which does not have to converge, let alone converge absolutely; equating two such divergent series would be meaningless.)

(a) Show that $\mathrm{tr}\hat A$ is independent of the choice of an orthonormal basis.

That is, show that $\sum_n\langle\phi_n|\hat A|\phi_n\rangle = \sum_n\langle\varphi_n|\hat A|\varphi_n\rangle$, where $\{|\phi_n\rangle\}$ and $\{|\varphi_n\rangle\}$ are two orthonormal basis sets.

(b) Show that $\mathrm{tr}(\hat A\hat B) = \mathrm{tr}(\hat B\hat A)$.

(c) Find $\mathrm{tr}\hat A$ for $\hat A = |\varphi\rangle\langle\psi|$, where $|\varphi\rangle$ and $|\psi\rangle$ are arbitrary vectors.

Solution

(a)

$$\mathrm{tr}\hat A = \sum_n\langle\phi_n|\hat A|\phi_n\rangle = \sum_n\langle\phi_n|\hat{\mathbb{1}}\hat A\hat{\mathbb{1}}|\phi_n\rangle = \sum_{n,m,k}\langle\phi_n|\varphi_m\rangle\langle\varphi_m|\hat A|\varphi_k\rangle\langle\varphi_k|\phi_n\rangle$$

$$= \sum_{m,k}\langle\varphi_m|\hat A|\varphi_k\rangle\sum_n\langle\varphi_k|\phi_n\rangle\langle\phi_n|\varphi_m\rangle = \sum_{m,k}\langle\varphi_m|\hat A|\varphi_k\rangle\underbrace{\langle\varphi_k|\hat{\mathbb{1}}|\varphi_m\rangle}_{\delta_{k,m}} = \sum_m\langle\varphi_m|\hat A|\varphi_m\rangle. \qquad \blacksquare$$

(b)

$$\mathrm{tr}(\hat A\hat B) = \sum_n\langle\phi_n|\hat A\hat B|\phi_n\rangle = \sum_n\langle\phi_n|\hat A\hat{\mathbb{1}}\hat B|\phi_n\rangle = \sum_{n,m}\langle\phi_n|\hat A|\phi_m\rangle\langle\phi_m|\hat B|\phi_n\rangle$$

$$= \sum_{n,m}\langle\phi_m|\hat B|\phi_n\rangle\langle\phi_n|\hat A|\phi_m\rangle = \sum_m\langle\phi_m|\hat B\hat{\mathbb{1}}\hat A|\phi_m\rangle = \sum_m\langle\phi_m|\hat B\hat A|\phi_m\rangle = \mathrm{tr}(\hat B\hat A). \qquad \blacksquare$$

(c)

$$\mathrm{tr}\,(|\varphi\rangle\langle\psi|) = \sum_n\langle\phi_n|\varphi\rangle\langle\psi|\phi_n\rangle = \sum_n\langle\psi|\phi_n\rangle\langle\phi_n|\varphi\rangle = \langle\psi|\hat{\mathbb{1}}|\varphi\rangle = \langle\psi|\varphi\rangle.$$