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Course: **8.321 - Quantum Theory I**
Problem set: **#2**

1. Let A be a skew-Hermitian operator, i.e., $A^\dagger = -A$.

(a) Let λ and $|\lambda\rangle$ be an eigenvalue and eigenvector of A, respectively. Then we have

$$A|\lambda\rangle = \lambda|\lambda\rangle \implies \lambda\langle\lambda|\lambda\rangle = \langle\lambda|A|\lambda\rangle = -\langle\lambda|A|\lambda\rangle = \langle\lambda|A^*|\lambda\rangle = \lambda^*\langle\lambda|\lambda\rangle \implies -\lambda = \lambda^*.$$

Since $\lambda \in \mathbb{C}$, the only solution is $\lambda = 0$. Thus, the only real eigenvalue of A (up to multiplicity/degeneracy) is 0.

(b) Let A, B be Hermitian operators. Then

$$[A,B] = AB - BA = A^\dagger B^\dagger - B^\dagger A^\dagger = (BA - AB)^\dagger = -(AB - BA)^\dagger = -[A,B]^\dagger.$$

Thus $[A,B]$ is skew-Hermitian.

2. Let H, K be Hermitian operators with non-negative eigenvalues and assume that that the trace defined throughout this problem. Since H, K are Hermitian operators we may assume that there exist complete orthonormal (eigen)bases $\{|h_i\rangle\}$ and $|k_i\rangle$ for H, K respectively with $H|h_i\rangle = h_i|h_i\rangle$ and $K|k_i\rangle = k_i|k_i\rangle$, and $h_i, k_i \geq 0$ for all i. Then we can spectral-decompose H, K in their product as follows

$$HK = \sum_n h_n |h_n\rangle\langle h_n| \sum_m k_m |k_m\rangle\langle k_m| = \sum_{n,m} h_n k_m |h_n\rangle\langle h_n|k_m\rangle\langle k_m|.$$

Since $\text{tr}(A) = \sum_i \langle\phi_i|A|\phi_i\rangle$ for any orthonormal basis $\{\phi_i\}$, we have

$$\begin{aligned}\text{tr}(HK) &= \sum_j \langle h_j| \left[\sum_{n,m} h_n k_m |h_n\rangle\langle h_n|k_m\rangle\langle k_m|\right] |h_j\rangle \\ &= \sum_{n,m} h_n k_m \langle h_n|k_m\rangle\langle k_m|h_n\rangle, \quad \text{by orthonormality} \\ &= \sum_{n,m} h_n k_m |\langle h_n|k_m\rangle|^2.\end{aligned}$$

Since $h_i, k_i \geq 0$ for all i, and the modulus square is always nonnegative, we see that $\text{tr}(HK) \geq 0$, as desired.

Suppose $\text{tr}(HK) = 0$, then by nonnegativity we must have $h_n k_m |\langle h_n|k_m\rangle|^2 = 0$ for all n, m, or equivalently $h_n k_m \langle h_n|k_m\rangle = 0$ for all n, m. In view of the first equation for HK, we see that $HK = 0$.

3. Let a Hermitian operator H be given with positive spectrum and a complete orthonormal basis.

(a) We want to prove that for any two vectors $|\alpha\rangle, |\beta\rangle$

$$|\langle\alpha|H|\beta\rangle|^2 \leq \langle\alpha|H|\alpha\rangle\langle\beta|H|\beta\rangle.$$

There are two ways to go about this proof, in which both approaches are actually the same and only differ by appearance. I will present the notationally "light" version first. This goes as follows: Since H is Hermitian with positive spectrum, we may find a complete orthonormal basis in which H is diagonal. The transformation between H and its diagonalization D is given by a unitary operator U as $H = U^\dagger D U$. Since D is diagonal with positive entries, we can define its square root $\sqrt{D}$. From here, we can also define the square root of H, denoted $\sqrt{H}$ by $U^\dagger\sqrt{D}U$. We can check:

$$\sqrt{H}\sqrt{H} = U^\dagger\sqrt{D}UU^\dagger\sqrt{D}U = U^\dagger\sqrt{D}\sqrt{D}U = U^\dagger D U = H.$$

It is easy to show that $\sqrt{H}$ is also Hermitian:

$$\sqrt{H}^\dagger = \left(U^\dagger \sqrt{D} U\right)^\dagger = U^\dagger \sqrt{D}^\dagger U = U^\dagger \sqrt{D} U = \sqrt{H},$$

where we have used the fact that $\sqrt{D}$ is strictly diagonal and positive, thus Hermitian. The rest of the proof is now a simple application of the Cauchy-Schwarz inequality for inner products:

$$\begin{aligned}
\left|\langle\alpha| H \left|\beta\right\rangle\right|^2 &= \left|\langle\alpha| \sqrt{H}\sqrt{H} \left|\beta\right\rangle\right|^2 = \left|\langle\alpha| \sqrt{H}^\dagger \sqrt{H} \left|\beta\right\rangle\right|^2 = \left|\left\langle \alpha\sqrt{H}^\dagger \middle| \sqrt{H}\beta\right\rangle\right|^2 \\
&\leq \left\langle \sqrt{H}\alpha \middle| \sqrt{H}\alpha\right\rangle \left\langle \sqrt{H}\beta \middle| \sqrt{H}\beta\right\rangle \\
&= \langle\alpha| \sqrt{H}^\dagger \sqrt{H} \left|\alpha\right\rangle \left\langle\beta\right| \sqrt{H}^\dagger \sqrt{H} \left|\beta\right\rangle = \langle\alpha| H \left|\alpha\right\rangle \left\langle\beta\right| H \left|\beta\right\rangle
\end{aligned}$$

as desired.

The more notationally heavy approach is to consider a complete orthonormal eigenbasis for H, which we may call $\{|\lambda_i\rangle\}$ where $\{\lambda_i\}$ are the eigenvalues of H. Under this basis, we have

$$|\alpha\rangle = \sum_i a_i |\lambda_i\rangle \qquad |\beta\rangle = \sum_i b_i |\lambda_i\rangle$$

and so

$$\left|\langle\alpha| H \left|\beta\right\rangle\right|^2 = \left|\sum_i a_i^* \langle\lambda_i| \lambda_j b_j \left|\lambda_j\right\rangle\right|^2 = \left|\sum_i a_i^* \lambda_i b_i\right|^2 = \left|\sum_i \left(a_i\sqrt{\lambda_i}\right)^\dagger \left(b_i\sqrt{\lambda_i}\right)\right|^2.$$

Note that $\sqrt{\lambda_i} \in \mathbb{R}^+$, which is possible because $\lambda_i > 0$. Now, call

$$|\alpha'\rangle = \sum_i a_i\sqrt{\lambda_i} |\lambda_i\rangle \qquad |\beta'\rangle = \sum_i b_i\sqrt{\lambda_i} |\lambda_i\rangle .$$

It is clear that

$$\left|\langle\alpha| H \left|\beta\right\rangle\right|^2 = \left|\left\langle\alpha'\middle|\beta'\right\rangle\right|^2.$$

On the other hand, we have

$$\begin{aligned}
\langle\alpha| H |\alpha\rangle &= \sum_{i,j} a_i^* a_j \lambda_j \left\langle\lambda_i\middle|\lambda_j\right\rangle = \sum_i |a_i|^2\lambda_i = \langle\alpha'|\alpha'\rangle \\
\left\langle\beta\right| H \left|\beta\right\rangle &= \sum_{i,j} b_i^* b_j \lambda_j \left\langle\lambda_i\middle|\lambda_j\right\rangle = \sum_i |b_i|^2\lambda_i = \left\langle\beta'\middle|\beta'\right\rangle .
\end{aligned}$$

Applying the Cauchy-Schwarz inequality,

$$\left|\langle\alpha| H \left|\beta\right\rangle\right|^2 = \left|\left\langle\alpha'\middle|\beta'\right\rangle\right|^2 \leq \langle\alpha'|\alpha'\rangle \left\langle\beta'\middle|\beta'\right\rangle = \langle\alpha| H |\alpha\rangle \left\langle\beta\right| H \left|\beta\right\rangle$$

we successfully proved the desired result.

(b) The trace of H is simply the sum of its eigenvalues, so $\mathrm{tr}(H) > 0$. To show explicitly, we use the orthonormal basis introduced in Part (a). Since $\lambda_i > 0$ for all i, we have

$$\mathrm{tr}(H) = \sum_i \langle\lambda_i| H |\lambda_i\rangle = \sum_i \lambda_i \langle\lambda_i|\lambda_i\rangle = \sum_i \lambda_i > 0.$$

4. Let a unitary operator U be given which satisfies the eigenvalue equation $U|\lambda\rangle = \lambda|\lambda\rangle$.

(a) Since $\langle\lambda|\lambda\rangle \neq 0$ (because $|\lambda\rangle$ is an eigenvector), we have

$$\langle\lambda|\lambda\rangle = \langle\lambda| U^\dagger U |\lambda\rangle = |\lambda|^2 \langle\lambda|\lambda\rangle \implies |\lambda|^2 = 1.$$

Since $\lambda \in \mathbb{C}$, it must be of the form $\lambda = e^{i\theta}$ where $\theta \in \mathbb{R}$.

(b) Let distinct eigenvectors $\left|\mu\right\rangle$ and $|\lambda\rangle$ be given with corresponding (distinct) eigenvalues $e^{i\theta_\mu}$ and $e^{i\theta_\lambda}$. We have

$$\left\langle\mu\middle|\lambda\right\rangle = \left\langle\mu\right| U^\dagger U |\lambda\rangle = e^{-i\theta_\mu} e^{i\theta_\lambda} \left\langle\mu\middle|\lambda\right\rangle.$$

Since the eigenvalues are not the same, we have that $e^{-i\theta_\mu} e^{i\theta_\lambda} \neq 1$ (i.e., that the complex conjugate of one is not the complex conjugate of the other). Thus, equality holds only if $\left\langle\mu\middle|\lambda\right\rangle = 0$.

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