Introduction to Quantum Mechanics – Solution to Problem sheet 3

1. The Dirac notation

(a) (i) $\langle\phi|\chi\rangle\langle\phi|$ is a bra vector. The adjoint (ket vector) is given by

$$\begin{aligned}(\langle\phi|\chi\rangle\langle\phi|)^\dagger &= |\phi\rangle\langle\phi|\chi\rangle^* \\ &= \langle\chi|\psi\rangle|\phi\rangle\,.\end{aligned}$$

(ii) $\langle\phi|\hat{A}|\chi\rangle\langle\phi|\,\hat{A}$ is a bra vector.
The adjoint (ket vector) is given by

$$\begin{aligned}(\langle\phi|\hat{A}|\chi\rangle\langle\phi|\,\hat{A})^\dagger &= \hat{A}^\dagger|\phi\rangle(\langle\phi|A|\chi\rangle)^\dagger \\ &= \langle\chi|A^\dagger|\phi\rangle\,\hat{A}^\dagger|\phi\rangle\,.\end{aligned}$$

(iii) $c\,\langle\chi|\phi\rangle$ is a scalar.
The adjoint is its complex conjugate

$$\begin{aligned}(c\,\langle\chi|\phi\rangle)^\dagger &= c^*\,\langle\chi|\phi\rangle^* \\ &= c^*\,\langle\phi|\chi\rangle\end{aligned}$$

(iv) $c\,|\phi\rangle\langle\chi|$ is an operator.
The adjoint operator is given by

$$(c\,|\phi\rangle\langle\chi|)^\dagger = c^*\,|\chi\rangle\langle\phi|$$

(v) $\langle\chi|\hat{A}^\dagger|\phi\rangle$ is a scalar.
The adjoint is given by the complex conjugate scalar

$$(\langle\chi|\hat{A}^\dagger|\phi\rangle)^\dagger = \langle\phi|\hat{A}|\chi\rangle$$

Here c denotes a scalar, and $\hat{A}$ is an operator.

(b) (i) We have $|\psi_1\rangle = \frac{1}{\sqrt{2}}(\mathrm{i}\,|\phi_1\rangle + |\phi_3\rangle)$ and $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle + \mathrm{i}\,|\phi_3\rangle)$

$$\begin{aligned}\langle\psi_1|\psi_2\rangle &= \frac{1}{2}\left(-\mathrm{i}\,\langle\phi_1| + \langle\phi_3|\right)\left(|\phi_1\rangle + \mathrm{i}\,|\phi_3\rangle\right) \\ &= \frac{1}{2}\left(-\mathrm{i}\,\langle\phi_1|\phi_1\rangle + \langle\phi_1|\phi_3\rangle + \langle\phi_3|\phi_1\rangle + \mathrm{i}\,\langle\phi_3|\phi_3\rangle\right) \\ &= \frac{1}{2}(-\mathrm{i}+\mathrm{i}) = 0\end{aligned}$$

$$\begin{aligned}\langle\psi_1|\psi_1\rangle &= \frac{1}{2}\left(-\mathrm{i}\,\langle\phi_1| + \langle\phi_3|\right)\left(\mathrm{i}\,|\phi_1\rangle + |\phi_3\rangle\right) \\ &= \frac{1}{2}\left(\langle\phi_1|\phi_1\rangle + \langle\phi_3|\phi_3\rangle\right) \\ &= \frac{1}{2}(1+1) = 1\end{aligned}$$

$$\begin{aligned}\langle\psi_2|\psi_2\rangle &= \frac{1}{2}\left(\langle\phi_1| - \mathrm{i}\,\langle\phi_3|\right)\left(|\phi_1\rangle + \mathrm{i}\,|\phi_3\rangle\right) \\ &= \frac{1}{2}\left(\langle\phi_1|\phi_1\rangle + \langle\phi_3|\phi_3\rangle\right) \\ &= \frac{1}{2}(1+1) = 1.\end{aligned}$$

A vector orthogonal to $|\psi_{1,2}\rangle$ would be

$$|\psi_3\rangle = |\phi_2\rangle\,.$$

If you do not see this directly you could make the ansatz $|\psi_3\rangle = a|\phi_1\rangle + b|\phi_2\rangle + c|\phi_3\rangle$ and calculate the inner product with $|\psi_1\rangle$ and $|\psi_2\rangle$ to deduce conditions on the coefficients a, b, c.

(ii) We know that $|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3| = \hat{I}$ as $\{|\phi_{1,2,3}\rangle\}$ is an orthonormal set. In Dirac notation we have

$$\begin{aligned}
|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3| &= \frac{1}{2}\left(\mathrm{i}\,|\phi_1\rangle + |\phi_3\rangle\right)\left(-\mathrm{i}\,\langle\phi_1|\,\langle\phi_3|\right) \\
&+ \frac{1}{2}\left(|\phi_1\rangle + \mathrm{i}\,|\phi_3\rangle\right)\left(\langle\phi_1| - \mathrm{i}\,\langle\phi_3|\right) \\
&+ |\phi_2\rangle\langle\phi_2| \\
&= \frac{1}{2}(|\phi_1\rangle\langle\phi_1| + \mathrm{i}\,|\phi_1\rangle\langle\phi_3| - \mathrm{i}\,|\phi_3\rangle\langle\phi_1| + |\phi_3\rangle\langle\phi_3|) \\
&+ \frac{1}{2}(|\phi_1\rangle\langle\phi_1| - \mathrm{i}\,|\phi_1\rangle\langle\phi_3| + \mathrm{i}\,|\phi_3\rangle\langle\phi_1| + |\phi_3\rangle\langle\phi_3|) \\
&+ |\phi_2\rangle\langle\phi_2| \\
&= |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3| = \hat{I}.
\end{aligned}$$

In vector notation we have

$$\psi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}\mathrm{i}\\0\\1\end{pmatrix}, \qquad \psi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\\mathrm{i}\end{pmatrix}, \qquad \psi_3 = \begin{pmatrix}0\\1\\0\end{pmatrix}$$

Therefore, the matrix representation of $|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3|$ is

$$\begin{aligned}
\psi_1\psi_1^\dagger + \psi_2\psi_2^\dagger + \psi_3\psi_3^\dagger &= \frac{1}{2}\left(\begin{pmatrix}\mathrm{i}\\0\\1\end{pmatrix}\begin{pmatrix}-\mathrm{i} & 0 & 1\end{pmatrix} + \begin{pmatrix}1\\0\\\mathrm{i}\end{pmatrix}\begin{pmatrix}1 & 0 & -\mathrm{i}\end{pmatrix}\right) + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix}1 & 0 & \mathrm{i}\\ 0 & 0 & 0\\ -\mathrm{i} & 0 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1 & 0 & -\mathrm{i}\\ 0 & 0 & 0\\ \mathrm{i} & 0 & 1\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix} \\
&= \begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}.
\end{aligned}$$

(iii) We have

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}(-\mathrm{i}\,|\psi_1\rangle + |\psi_2\rangle) \quad \text{and} \quad |\phi_2\rangle = |\psi_3\rangle\,,$$

therefore

$$\begin{aligned}
|\chi\rangle &= \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\,|\psi_1\rangle + \frac{\mathrm{i}}{\sqrt{2}}\,|\psi_2\rangle + |\psi_3\rangle\right) \\
&= \frac{1}{2}\,|\psi_1\rangle + \frac{\mathrm{i}}{2}\,|\psi_2\rangle + \frac{1}{\sqrt{2}}\,|\psi_3\rangle\,.
\end{aligned}$$

2. Basis invariance of the trace

(a) Since $\{|d_j\rangle\}$ is an orthonormal basis we have

$$\hat{I} = \sum_j |d_j\rangle \langle d_j| \, .$$

Inserting this into the expression for the trace evaluated in the basis $\{|b_i\rangle\}$ twice gives

$$\begin{aligned}
\sum_i \langle b_i|\hat{O}|b_i\rangle &= \sum_{i,j,k} \langle b_i \,|d_j\rangle \langle d_j|\, \hat{O}\, |d_k\rangle \langle d_k|\, b_i\rangle \\
&= \sum_{i,j,k} \langle d_k|b_i\rangle \langle b_i|d_j\rangle \langle d_j|\, \hat{O}\, |d_k\rangle \, .
\end{aligned}$$

We recognise the identity operator $\hat{I} = \sum_i |b_i\rangle \langle b_i|$ in the last line and obtain

$$\begin{aligned}
\sum_i \langle b_i|\hat{O}|b_i\rangle &= \sum_{j,k} \langle d_k|d_j\rangle \langle d_j|\, \hat{O}\, |d_k\rangle \\
&= \sum_{j,k} \delta_{kj} \langle d_j|\, \hat{O}\, |d_k\rangle \\
&= \sum_{j} \langle d_j|\, \hat{O}\, |d_j\rangle
\end{aligned}$$

Hence the trace is basis independent.

(b) We have

$$\mathsf{Tr}(\hat{A}\hat{B}\hat{C}) = \sum_i \langle b_i|\hat{A}\hat{B}\hat{C}|b_i\rangle$$

Inserting two identity operators gives

$$\begin{aligned}
\mathsf{Tr}(\hat{A}\hat{B}\hat{C}) &= \sum_{i,j,k} \langle b_i|\hat{A}\,|b_j\rangle \langle b_j|\, \hat{B}\, |b_k\rangle \langle b_k|\, \hat{C}|b_i\rangle \\
&= \sum_{i,j,k} \langle b_k|\hat{C}|b_i\rangle \langle b_i|\hat{A}|b_j\rangle \langle b_j|\, \hat{B}\, |b_k\rangle \\
&= \sum_k \langle b_k|\hat{C}\hat{A}\hat{B}|b_k\rangle \\
&= \mathsf{Tr}(\hat{C}\hat{A}\hat{B}).
\end{aligned}$$

As required. The proof for $\mathsf{Tr}(\hat{C}\hat{A}\hat{B}) = \mathsf{Tr}(\hat{B}\hat{C}\hat{A})$ is the same.

(c) We have

$$\begin{aligned}
\mathsf{Tr}([\hat{A},\hat{B}]) &= \mathsf{Tr}(\hat{A}\hat{B}) - \mathsf{Tr}(\hat{B}\hat{A}) \\
&= 0,
\end{aligned}$$

due to the cyclic property of the trace. On the other hand we also have

$$\mathsf{Tr}(c\hat{I}_N) = cN \neq 0$$

for an N dimensional space. Hence no matrices may satisfy

$$[\hat{A},\hat{B}] = c\hat{I}_N,$$

for a non-zero c.

3. The spectral theorem

(a) The (m, n)-element of matrix A is given by $\langle m|\hat{A}|n\rangle$ substituting the definition from the question we obtain

$$\begin{aligned}\langle m|\hat{A}|n\rangle &= \sum_{jk} \langle m|(A_{jk} |j\rangle \langle k|)|n\rangle \\ &= \sum_{jk} A_{jk} \langle m|j\rangle \langle k|n\rangle \\ &= \sum_{jk} A_{jk}\delta_{mj}\delta_{kn} \\ &= A_{mn}\end{aligned}$$

Hence we may express $\hat{A}$ as $\hat{A} = \sum_{jk} A_{jk}|j\rangle\langle k|$

(b) We have

$$|\phi_n\rangle = \lambda_n |\phi_n\rangle$$

Since $\hat{A}$ is Hermitian we have a complete set of orthonormal eigenstates $\{|\phi_n\rangle\}$
Using these eigenstates to construct the identity operator we write

$$\begin{aligned}\hat{A} &= \hat{I}\hat{A}\hat{I} \\ &= \sum_{nm} |\phi_m\rangle \langle\phi_m| \hat{A} |\phi_n\rangle \langle\phi_n| \\ &= \sum_{nm} \lambda_n |\phi_m\rangle \langle\phi_m|\phi_n\rangle \langle\phi_n| \\ &= \sum_{nm} \lambda_n\delta_{mn} |\phi_m\rangle \langle\phi_n| \\ &= \sum_{n} \lambda_n |\phi_n\rangle \langle\phi_n|\end{aligned}$$

as required.

4. Hermiticity in L^2

If $\hat{K}$ is Hermitian we have

$$(\phi(x), \hat{K}\chi(x)) = (\hat{K}\phi(x), \chi(x)).$$

Applying the inner product in $L^2(\mathbb{R})$ and integrating by parts twice we obtain

$$\begin{aligned}(\phi(x), \hat{K}\chi(x)) &= -\int_{-\infty}^{+\infty} \phi^*(x)\frac{d^2}{dx^2}\chi(x)dx \\ &= -\left[\phi^*(x)\frac{d\chi}{dx}(x)\right]_{-\infty}^{\infty} + \int_{-\infty}^{+\infty} \frac{d\phi^*}{dx}(x)\frac{d\chi}{dx}(x)dx \\ &= -\left[\phi^*(x)\frac{d\chi}{dx}(x)\right]_{-\infty}^{\infty} + \left[\frac{d\phi^*}{dx}(x)\chi(x)\right]_{-\infty}^{\infty} - \int_{-\infty}^{+\infty} \frac{d^2\phi^*}{dx^2}(x)\chi(x)dx.\end{aligned}$$

Since we have $\phi(x), \chi(x) \to 0$ as $x \to \pm\infty$, we have

$$\begin{aligned}(\phi(x), \hat{K}\chi(x)) &= -\int_{-\infty}^{+\infty} \phi^*(x)\frac{d^2}{dx^2}\chi(x)dx \\ &= -\int_{-\infty}^{+\infty} \frac{d^2\phi^*}{dx^2}(x)\chi(x)dx \\ &= (\hat{K}\phi(x), \chi(x))\end{aligned}$$