Problem Set II

FYS3110

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Problem 2.1

An operator $\hat{H}$ is represented in a particular orthonormal basis as the matrix

$$\hat{H} \simeq \begin{pmatrix} 1 & \frac{i}{2} & 0 \\ -\frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{1}$$

a)

$\hat{H}$ is Hermitian if it is equal to its own transpose conjugate, $\hat{H} = \hat{H}^\dagger$.

$$\hat{H}^\dagger = (\hat{H}^*)^T = \begin{pmatrix} 1 & -\frac{i}{2} & 0 \\ \frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}^T = \begin{pmatrix} 1 & \frac{i}{2} & 0 \\ -\frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} = \hat{H} \tag{2}$$

b)

Three ket vectors are given

$$|1\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} \tag{3}$$

$$|2\rangle \simeq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4}$$

$$|3\rangle \simeq \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} \tag{5}$$

$|1\rangle$ is and eigenvector of $\hat{H}$ with eigenvalue $\frac{3}{2}$:

$$\hat{H}\,|1\rangle = \begin{pmatrix} 1 & \frac{i}{2} & 0 \\ -\frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{3i}{2} \\ \frac{3}{2} \\ 0 \end{pmatrix} = \frac{3}{2}\,|1\rangle \tag{6}$$

$|2\rangle$ is and eigenvector of $\hat{H}$ with eigenvalue $\frac{1}{2}$:

$$\hat{H}\,|2\rangle = \begin{pmatrix} 1 & \frac{i}{2} & 0 \\ -\frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} = \frac{1}{2}\,|2\rangle \tag{7}$$

$|3\rangle$ is and eigenvector of $\hat{H}$ with eigenvalue $\frac{1}{2}$:

$$\hat{H}\,|3\rangle = \begin{pmatrix} 1 & \frac{i}{2} & 0 \\ -\frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} -\frac{i}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} = \frac{1}{2}\,|3\rangle \tag{8}$$

c)

Computing the matrix elements of the linear operator

$$\langle 1|\,\hat{H}\,|1\rangle = \frac{3}{2}\,\langle 1|1\rangle = \frac{3}{2}\frac{1}{2}\begin{pmatrix} -i & 1 & 0 \end{pmatrix} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} = \frac{3}{2}\frac{1}{2}2 = \frac{3}{2} \tag{9}$$

$$\langle 1|\,\hat{H}\,|2\rangle = \frac{1}{2}\,\langle 1|2\rangle = \frac{1}{2}\frac{1}{\sqrt{2}}\begin{pmatrix} -i & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0 \tag{10}$$

$$\langle 1|\,\hat{H}\,|3\rangle = \frac{1}{2}\,\langle 1|3\rangle = \frac{1}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{3}}\begin{pmatrix} i & 1 & 0 \end{pmatrix} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{3}}0 = 0 \tag{11}$$

$$\langle 2|\,\hat{H}\,|1\rangle = \frac{3}{2}\,\langle 2|1\rangle = \frac{3}{2}\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} = 0 \tag{12}$$

$$\langle 2|\,\hat{H}\,|2\rangle = \frac{1}{2}\,\langle 2|2\rangle = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2} \tag{13}$$

$$\langle 2|\,\hat{H}\,|3\rangle = \frac{1}{2}\,\langle 2|3\rangle = \frac{1}{2}\frac{1}{\sqrt{3}}\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} = -\frac{1}{2\sqrt{3}} \tag{14}$$

$$\langle 3|\,\hat{H}\,|1\rangle = \frac{3}{2}\,\langle 3|1\rangle = \frac{3}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{3}}\begin{pmatrix} i & 1 & -1 \end{pmatrix} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} = \frac{3}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{3}}0 = 0 \tag{15}$$

$$\langle 3|\,\hat{H}\,|2\rangle = \frac{1}{2}\,\langle 3|2\rangle = \frac{1}{2}\frac{1}{\sqrt{3}}\begin{pmatrix} i & 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2}\frac{1}{\sqrt{3}}(-1) = -\frac{1}{2\sqrt{3}} \tag{16}$$

$$\langle 3|\,\hat{H}\,|3\rangle = \frac{1}{2}\,\langle 3|3\rangle = \frac{1}{2}\frac{1}{3}\begin{pmatrix} i & 1 & -1 \end{pmatrix} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2}\frac{1}{3}3 = \frac{1}{2} \tag{17}$$

Thus, the full matrix is

$$H_{ij} = \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2\sqrt{3}} \\ 0 & -\frac{1}{2\sqrt{3}} & \frac{1}{2} \end{pmatrix} \tag{18}$$

Evidently, the matrix H_{ij} is not diagonal, but is symmetric with the eigenvalues as main diagonal entries.

d)

From the results when H_{ij} was computed one can already gather that $|2\rangle$ and $|3\rangle$ are non-orthogonal. The Gram-Schmidt precedure can be employed to convert a linearly independent basis into an orthonormal one, but it is not necessary to do all the work. It is easy to see that the kets are already of unit length as $\sqrt{\langle i|i\rangle} = 1, i = 1, 2, 3$. A new orthonomral basis is computed as follows.

Everything is already fine with the first ket:

$$|1'\rangle = |1\rangle \tag{19}$$

The second vector in the new basis is the $|2\rangle$ minus the part pointing along the first vector.

$$|2'\rangle = |2\rangle - |1'\rangle \langle 1'|2\rangle = |2\rangle \tag{20}$$

The second ket in the new basis is also equal to its “predecessor”, because no part of it points along the first ket ($\langle 1'|2\rangle = 0$).

Finally, the third new basis vector is computed by subtracting both the part of it that points along the first and the second vector.

$$\left|\tilde{3}\right\rangle = |3\rangle - |1'\rangle \langle 1'|3\rangle - |2'\rangle \langle 2'|3\rangle = |3\rangle - |2'\rangle \langle 2'|3\rangle \tag{21}$$

$$= \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} - \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix} \tag{22}$$

Now this vector must be normalised

$$|3'\rangle = \frac{\left|\tilde{3}\right\rangle}{\sqrt{\langle\tilde{3}|\tilde{3}\rangle}} = \frac{\left|\tilde{3}\right\rangle}{\sqrt{\frac{1}{3}\begin{pmatrix} i & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}}} = \frac{\left|\tilde{3}\right\rangle}{\sqrt{\frac{2}{3}}} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix} \tag{23}$$

One should have been able to see that one coming from far away. It is easy to see that

$$\langle i'|j'\rangle = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \tag{24}$$

Therefore, $H_{i'j'}$ must be a diagonal matrix. The only unknown element is

$$\langle 3'|\,\hat{H}\,|3'\rangle = \frac{1}{2}\begin{pmatrix} i & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & \frac{i}{2} & 0 \\ \frac{i}{2} & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}\begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} i & 1 & 0 \end{pmatrix}\begin{pmatrix} -\frac{i}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} = \frac{1}{2} \tag{25}$$

Not surprisingly, the last eigenvalue is the same and the new matrix is

$$H_{i'j'} = \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{26}$$

2.2

a)

Find the Hermitian conugate of the following operators i, x and $\frac{d}{dx}$. Given an operator $\hat{O}$, its Hermitian conjugate $\hat{O}^\dagger$ satisfies the following property by definition.

$$\left\langle \phi \middle| \hat{O}\psi \right\rangle = \left\langle \hat{O}^\dagger\phi \middle| \psi \right\rangle \tag{27}$$

where $\langle\phi|$ and $|\psi\rangle$ are simply an arbitrary bra and ket, respectively. Given a (complex) number α the following properties are important.

$$\alpha\,|\psi\rangle = |\psi\rangle \tag{28}$$

$$\langle\alpha\phi| = \langle\phi|\,\alpha* \tag{29}$$

Therefore, in general an operator which is simply an complex number will haves its complex conjugate as Hermitian conjugate.

$$\langle(a-ib)\phi|\psi\rangle = \langle\phi|(a+ib)\psi\rangle \tag{30}$$