2.1

a)

The Hermitian conjugate of $\hat{H}$ is found by transposing and complex conjugation, and one immediately finds $\hat{H}^\dagger = \hat{H}$, i.e. $\hat{H}$ is Hermitean.

b)

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

so the eigenvalue is $\lambda_1 = 3/2$. Similarly, we find $\hat{H}\,|2\rangle = \frac{1}{2}\,|2\rangle$ and $\hat{H}\,|3\rangle = \frac{1}{2}\,|3\rangle$ so $\lambda_2 = \lambda_3 = 1/2$. So the last two eigenvalues are degenerate.

c)

We start by computing the inner products between the basis vectors. For example,

$$\langle 1|1\rangle = \frac{1}{2}(-i, 1, 0)\begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix}. \tag{1}$$

Similarly, $\langle 2|2\rangle = \langle 3|3\rangle = 1$ so all three are normalised. Moreover, $\langle 1|2\rangle = \langle 1|3\rangle = 0$ **but** $\langle 2|3\rangle - \frac{1}{\sqrt{3}}$. In other words, the eigenvectors corresponding to the two degenerate eigenvalues are not orthogonal. Therefore, the operator $\hat{H}$ will not be diagonal in this particular basis, as is seen from direct calculation of the matrix elements:

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

Here, we have used the eigenvalue relations from **b)** and the above inner products between the basis vectors. Thus,

$$\hat{H} \simeq \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2\sqrt{3}} \\ 0 & -\frac{1}{2\sqrt{3}} & \frac{1}{2} \end{pmatrix} \tag{2}$$

which is non-diagonal as anticipated.

d)

We use the Gram-Schmidt method to construct an orthonormal basis. Since $|1\rangle$ is already orthogonal to both $|2\rangle$ and $|3\rangle$, we keep it as it is. Similarly, we choose to keep $|2\rangle$ and modify the third basis vector, i.e.

$$\begin{aligned} |1'\rangle &= |1\rangle \\ |2'\rangle &= |2\rangle \\ |3'\rangle &\to |3\rangle - \langle 1|3\rangle |1\rangle - \langle 2|3\rangle |2\rangle = |3\rangle + \frac{1}{\sqrt{3}} |2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix}. \end{aligned} \tag{3}$$

Finally, we need to normalise $|3'\rangle$, so

$$|3'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix}. \tag{4}$$

Calculating the matrix elements of $\hat{H}$ in this new basis we find

$$\left(\langle i'| \hat{H} |j'\rangle \right) = \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{5}$$

which is indeed diagonal – as it should be in an orthonormal basis of eigenvectors.

2.2

In this problem we frequently use the definition of the Hermitian conjugate of an operator. In Griffiths' notation the Hermitian conjugate (or adjoint) of $\hat{Q}$ is defined via

$$\left\langle f|\hat{Q}g \right\rangle = \left\langle \hat{Q}^\dagger f|g \right\rangle \tag{6}$$

for all f and g.

a)

We solve this subproblem in coordinate basis, where Eq.(6) takes the explicit form

$$\int_{-\infty}^{\infty} f^*(x)(\hat{Q}g(x))dx = \int_{-\infty}^{\infty} (\hat{Q}^\dagger f(x))^* g(x)dx. \tag{7}$$

We will suppress the integration limits in what follows. Since

$$\int f^*(x)(ig(x))dx = \int (-if(x))^* g(x)dx, \tag{8}$$

we immediately see that $i^\dagger = -i$. Of course, since i is a constant, we could have shown this without resorting to the coordinate basis. Now for x^2:

$$\int f^*(x)(x^2 g(x))dx = \int (x^2 f(x))^* g(x)dx. \tag{9}$$

and so $(x^2)^\dagger = x^2$. Finally, consider the differential operator. To "move" it from g to f we perform an integration by parts,

$$\int f^*(x)(\frac{d}{dx}g(x))dx = |_{-\infty}^{\infty} f^*(x)g(x) - \int (\frac{d}{dx}f(x))^* g(x)dx. \tag{10}$$

The surface term must be zero in order for f and g to be normalizable wave functions (they must go to zero as $x \to \pm\infty$ in order for the normalization integral to be finite). This leaves us with

$$\int f^*(x)(\frac{d}{dx}g(x))dx = \int (-\frac{d}{dx}f(x))^* g(x)dx \tag{11}$$

and thus

$$\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}. \tag{12}$$

Note that $\frac{d}{dx}$ is *not* Hermitian. However, $i\frac{d}{dx}$ is, since the extra i provides the necessary minus sign upon conjugation (see the discussion in section 3.2). Thus only the latter can represent a physical observable. (It is, of course, essentially the momentum operator.)

b)

Here we consider $\langle f| \hat{K}\hat{L} |g\rangle$. By definition, we have the following identity for the composite operator $\hat{K}\hat{L}$ (again in Griffiths' notation),

$$\left\langle f|(\hat{K}\hat{L})g\right\rangle = \left\langle (\hat{K}\hat{L})^\dagger f|g\right\rangle. \tag{13}$$

But we can also consider the action of the two operators individually,

$$\langle f| \hat{K}\hat{L} |g\rangle = \langle f| \hat{K} \left|\hat{L}g\right\rangle = \left\langle (\hat{K}^\dagger f|(\hat{L}g)\right\rangle = \left\langle \hat{L}^\dagger \hat{K}^\dagger f|g\right\rangle. \tag{14}$$

This shows that

$$(\hat{K}\hat{L})^\dagger = L^\dagger \hat{K}^\dagger. \tag{15}$$

This is of course the expected result. As it stands, this is an operator identity. But we know that operators can be represented as matrices in a given basis, and that the same relation is true for the Hermitian conjugate of products of matrices.

c)

Consider

$$\langle\lambda| \hat{K}\hat{L} |g\rangle = \left\langle (\hat{K}^\dagger\lambda)\right| \hat{L} |g\rangle = \left\langle (\hat{K}\lambda)\right| \hat{L} |g\rangle = \lambda^* \langle\lambda| \hat{L} |g\rangle = \lambda \langle\lambda| \hat{L} |g\rangle \tag{16}$$

where we have used that $\hat{K}$ is Hermitian ($\hat{K}^\dagger = \hat{K}$) and thus has real eigenvalues, $\lambda^* = \lambda$.

2.3 (optional)

First of all, there is a 'trivial' set of eigenstates of $\hat{H}$, $|\gamma_n\rangle$, all with eigenvalue zero. The states $|\psi\rangle$ and $|\phi\rangle$ on the other hand are clearly not eigenstates, as $\hat{H}$ maps them into one another. This hints that we can find eigenstates as some linear combinations of the two. Thus we postulate an eigenstate as

$$|\lambda\rangle = |\psi\rangle + c\,|\phi\rangle \tag{17}$$

where c is a constant to be determined. (It is convenient, and ok, to set the constant in front of $|\psi\rangle$ to 1, since the state is anyway not (yet) normalized.) Demanding that $|\lambda\rangle$ is an eigenstate means that it must obey

$$\hat{H}\,|\lambda\rangle = \lambda\,|\lambda\rangle \tag{18}$$

where λ is the corresponding eigenvalue. From problem set 1 we recall that $\hat{H}\,|\psi\rangle = g\,|\phi\rangle$, and $\hat{H}\,|\phi\rangle = g^*\,|\psi\rangle$. Using this we get

$$g\,|\phi\rangle + cg^*\,|\psi\rangle = \lambda\left(|\psi\rangle + c\,|\phi\rangle\right). \tag{19}$$

Our goal is to determine possible values of λ (eigenvalues), and c (this specifies the linear combinations that are indeed eigenstates). The easiest way of solving this is by identifying coefficients (noting that $|\psi\rangle$ and $|\phi\rangle$ are linearly independent), i.e.

$$\begin{aligned} g &= c\lambda \qquad (20) \\ cg^* &= \lambda. \qquad (21) \end{aligned}$$

This immediately gives $\lambda^2 = g^*g = |g|^2$ with the two solutions

$$\lambda_\pm = \pm|g|. \tag{22}$$

Correspondingly one finds $c = \pm g/|g|$ so that the (unnormalized) eigenvectors are

$$|\lambda_\pm\rangle = |\psi\rangle \pm \frac{g}{|g|}\,|\phi\rangle\,. \tag{23}$$

Alternatively we could have multiplied (19) from the left by $\langle\phi|$ and $\langle\psi|$ respectively, giving

$$\begin{aligned} g + cg^*\,\langle\phi|\psi\rangle &= \lambda\left(\langle\phi|\psi\rangle + c\right) \qquad (24) \\ cg^* + g\,\langle\psi|\phi\rangle &= \lambda\left(c\,\langle\psi|\phi\rangle + 1\right) \qquad (25) \end{aligned}$$

These are simplified by introducing the condition $g\,\langle\psi|\phi\rangle = g^*\,\langle\phi|\psi\rangle$ found in problem set 1. Solving this set of equations for λ and c one finds the same solutions as above.