

Ammonia masa example

QM 2.11, 2.12, 2.14, 2.16, 2.19(a)(b), 2.22, 2.23, 2.49

2.11 Show: if  $\hat{A}$  is a projection operator,  $1 - \hat{A}$  is too.

Def: Projection operator

$$P^T = P$$

$$P^2 = P$$

Therefore  $\hat{A}^T = \hat{A}$  and  $\hat{A}^2 = \hat{A}$

$$(\mathbb{1} - \hat{A})^T = \mathbb{1}^T - \hat{A}^T = \mathbb{1} - \hat{A}$$

$$\begin{aligned}(\mathbb{1} - \hat{A})^2 &= (\mathbb{1} - \hat{A})(\mathbb{1} - \hat{A}) \\ &= (\mathbb{1} - \hat{A})\mathbb{1} + (\mathbb{1} - \hat{A})(-\hat{A}) \\ &= (\mathbb{1} - \hat{A}) + \mathbb{1}(-\hat{A}) + (\hat{A})(-\hat{A}) \\ &= \mathbb{1} - \hat{A} - \hat{A} + \hat{A}^2 \\ &= \mathbb{1} - \hat{A} - \hat{A} + \hat{A} \\ &= \mathbb{1} - \hat{A}\end{aligned}$$

Therefore

$1 - \hat{A}$  is also a projection operator

(2.12)

show  $\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$  is a projection operator

regardless whether  $|\psi\rangle$  is normalized.

$$\left(\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}\right)^\dagger = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$$

since  $|\psi\rangle^\dagger = \langle\psi|$

and  $\langle\phi|\psi\rangle^\dagger = \langle\psi|\phi\rangle$ , so the first property is satisfied.

$$\begin{aligned} \left(\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}\right)^2 &= \frac{|\psi\rangle\langle\psi|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle^2} \quad \leftarrow \text{scalar} \\ &= \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \frac{\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \end{aligned}$$

2.14 Consider  $\hat{A}$  such that:

$$\hat{A} |\phi_1\rangle = |\phi_1\rangle$$

$$\hat{A} |\phi_2\rangle = -|\phi_2\rangle$$

$|\phi_1\rangle, |\phi_2\rangle$  orthonormal

a) Do the states form a basis? Note  $|\phi_1\rangle, |\phi_2\rangle$  are eigenvectors of  $\hat{A}$ . One approach is to check if  $\hat{A}$  is Hermitian. If so, Theorem 2.2 guarantees that its eigenvectors form a complete basis. So:

$$\hat{A} = \begin{matrix} & \begin{matrix} |\phi_1\rangle & |\phi_2\rangle \end{matrix} \\ \begin{matrix} \langle\phi_1| \\ \langle\phi_2| \end{matrix} & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{matrix} \quad \text{This is Hermitian, since } A = A^\dagger,$$

so  $\{|\phi\rangle\}$  is a basis by Thm 2.2.

b) Define  $\hat{B} = |\phi_1\rangle\langle\phi_2|$ . Is  $\hat{B}$  Hermitian?

$$B^\dagger = |\phi_2\rangle\langle\phi_1| \neq B \quad \text{so, } \boxed{\text{no}}$$

b)' Show  $\hat{B}^2 = 0$

$$\hat{B}^2 = \hat{B} \cdot \hat{B} = |\phi_1\rangle\langle\phi_2| \cdot |\phi_1\rangle\langle\phi_2| = |\phi_1\rangle\langle\phi_2| \underbrace{\langle\phi_2|\phi_1\rangle}_{=0} \langle\phi_2| = \boxed{0}$$

c) Show  $BB^\dagger$  and  $B^\dagger B$  are projection operators.

A projection operator must satisfy  $P^\dagger = P$  and  $P^2 = P$

$$\boxed{BB^\dagger = |\phi_1\rangle\langle\phi_2| \cdot |\phi_2\rangle\langle\phi_1| = |\phi_1\rangle\langle\phi_1|}$$

This is the form of a projection operator, as shown in class.

$$\text{Similarly } B^\dagger B = |\phi_2\rangle\langle\phi_1| \cdot |\phi_1\rangle\langle\phi_2| = \boxed{|\phi_2\rangle\langle\phi_2|}$$

$\boxed{\text{yes}}$

d) Show  $BB^\dagger - B^\dagger B$  is unitary.

We know from part (c) that

$$Q \equiv BB^\dagger - B^\dagger B = |\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|$$

Also, a unitary operator is defined as

$$\boxed{U^\dagger = U^{-1}} \text{ or } \boxed{UU^\dagger = \mathbb{1}}$$

$$\boxed{\text{Try } QQ^\dagger \stackrel{?}{=} \mathbb{1}}$$

$$Q^\dagger = Q$$

$$QQ^\dagger = (|\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|)(|\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|)$$

$$= |\phi_1\rangle\langle\phi_1|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\phi_2\rangle\langle\phi_2|$$

+ 0 + 0

from cross terms

$$= |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|$$

$$= \sum_i |\phi_i\rangle\langle\phi_i|$$

Hermitian  
operator

$$QQ^\dagger$$

$$= \mathbb{1}$$

So, yes, unitary

Note: You could also do this by writing the matrices

$$B = |\phi_1\rangle\langle\phi_2| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$B^\dagger = |\phi_2\rangle\langle\phi_1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$BB^\dagger = |\phi_1\rangle\langle\phi_1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$B^\dagger B = |\phi_2\rangle\langle\phi_2| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\text{Then } Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } Q^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

e) Consider  $\hat{C} = BB^\dagger + B^\dagger B$ . Show that  $\hat{C}|\phi_1\rangle = |\phi_1\rangle$   
 $\hat{C}|\phi_2\rangle = |\phi_2\rangle$

$$\hat{C} = |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|$$

$$= \mathbb{I} \text{ by Thm. 2.2}$$

Thus  $\hat{C}|\phi_1\rangle = |\phi_1\rangle$   
 $\hat{C}|\phi_2\rangle = |\phi_2\rangle$

2.16 a) Verify  $U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$  is unitary

By definition, a unitary operator satisfies

$$U^\dagger = U^{-1} \text{ or } U^\dagger U = \mathbb{I}$$

$$U^\dagger U \stackrel{?}{=} \mathbb{I} \Rightarrow \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \cos^2 + \sin^2 & 0 \\ 0 & \cos^2 + \sin^2 \end{pmatrix} = \mathbb{I}$$

So, yes,  $U$  is unitary

b) Find the eigenvalues and eigenvectors

$$0 = \begin{vmatrix} \cos\theta - \lambda & \sin\theta \\ \sin\theta & \cos\theta - \lambda \end{vmatrix} \Rightarrow (\cos\theta - \lambda)^2 + \sin^2\theta = 0$$

$$\cos^2\theta + \lambda^2 - 2\cos\theta\lambda + \sin^2\theta = 0$$

$$1 - 2\cos\theta\lambda + \lambda^2 = 0 \Rightarrow \lambda = \frac{2\cos\theta \pm \sqrt{(2\cos\theta)^2 - 4}}{2}$$

$$= \cos\theta \pm \sqrt{\cos^2\theta - 1}$$

$$= \cos\theta \pm i\sin\theta$$

$$\lambda = e^{\pm i\theta}$$

Find the eigenvectors

$$\lambda = e^{+i\theta}$$

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = e^{i\theta} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\cancel{\cos\theta}x - \sin\theta y = e^{i\theta}x = \cancel{\cos\theta}x + i\sin\theta x$$

$$-y = ix$$

Set  $x=1$ , then  $y=-i$

$$e^{i\theta} \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\lambda = e^{-i\theta}$$

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = e^{-i\theta} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\cancel{\cos\theta}x - \sin\theta y = \cancel{\cos\theta}x - i\sin\theta x$$

$$-y = -ix$$

Set  $x=1$ , then  $y=i$

$$e^{-i\theta} \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$2.19 (a) \quad \hat{A} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

$$\begin{vmatrix} -a & i \\ -i & -a \end{vmatrix} = 0 = a^2 - 1$$

$$a = \pm 1$$

$$\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = + \begin{pmatrix} x \\ y \end{pmatrix}$$

$$iy = x$$

$$x=1, y=-i \Rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \text{ eigenvector of } +1$$

$$x=1, y=+i \Rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ +i \end{pmatrix} \text{ eigenvector of } -1$$

(b) Is  $A^\dagger = A$ ?

$$\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \text{ so yes.}$$

Since  $A$  is Hermitian, its eigenvectors form a complete basis set, and are normal.

by Thm 2.2,

2.22

$$\hat{A} = \begin{pmatrix} 0 & 0 & -1+i \\ 0 & 3 & 0 \\ -1-i & 0 & 0 \end{pmatrix}$$

a) Find eigenvalues and eigenvectors

$$\det(\hat{A} - a\hat{I}) = \begin{vmatrix} -a & 0 & -1+i \\ 0 & 3-a & 0 \\ -1-i & 0 & -a \end{vmatrix} = 0$$

Expand by minors in terms of (3-a)

$$\det \hat{A} = (3-a)(-) \begin{vmatrix} -a & -1+i \\ -1-i & -a \end{vmatrix} = 0$$

$$(3-a) = 0 \quad \text{OR} \quad a^2 - (-)(1+i)(1-i) = 0$$

$$a^2 + 2 = 0$$

Therefore  $a = 3$   
OR  
 $a = \pm\sqrt{2}$

Eigenvectors

$a=3$	$a=+\sqrt{2}$	$a=-\sqrt{2}$
$\hat{A} \psi\rangle = a \psi\rangle$ $\downarrow \quad \downarrow$ $(-1+i)z = 3x \rightarrow z = \frac{3}{-1+i}x = \frac{3(-1-i)}{2}x$ $3y = 3y$ $(-1-i)x = 3z \rightarrow z = \frac{-1-i}{3}x$ $\downarrow \quad \downarrow$ true for any $y$ , so Set $y=1$ So $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$(-1+i)z = \sqrt{2}x$ $3y = \sqrt{2}y$ $(-1-i)x = \sqrt{2}z$ $\downarrow \quad \downarrow$ True if $y=0$ Pick $x=1$ then $z = -\frac{1}{\sqrt{2}}(1+i)$ So $\begin{pmatrix} 1 \\ 0 \\ -\frac{1}{\sqrt{2}}(1+i) \end{pmatrix}$	$(-1+i)z = -\sqrt{2}x$ $3y = -\sqrt{2}y$ $(-1-i)x = -\sqrt{2}z$ $\downarrow \quad \downarrow$ True if $y=0$ Pick $x=1$ then $z = \frac{1}{\sqrt{2}}(1+i)$ So $\begin{pmatrix} 1 \\ 0 \\ \frac{1}{\sqrt{2}}(1+i) \end{pmatrix}$
Normalized $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -\frac{1}{\sqrt{2}}(1+i) \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \frac{1}{\sqrt{2}}(1+i) \end{pmatrix}$

b) Show  $\langle a_1 | \langle a_2 | + \langle a_3 | \langle a_3 | = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ -\frac{1}{\sqrt{2}}(1+i) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{1}{\sqrt{2}}(1-i) \end{pmatrix}$

$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & 0 & -\frac{1}{\sqrt{2}}(1-i) \\ 0 & 0 & 0 \\ -\frac{1}{\sqrt{2}}(1+i) & 0 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}}(1+i) \\ 0 & 0 & 0 \\ \frac{1}{\sqrt{2}}(1-i) & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ \frac{1}{\sqrt{2}}(1+i) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{1}{\sqrt{2}}(1-i) \end{pmatrix}$$



Check the ~~testing~~ ~~that~~ eigenvectors to see if orthogonal

$$(0 \ 1 \ 0) \begin{pmatrix} 1 \\ 0 \\ \pm \frac{1}{2}(1+i) \end{pmatrix} = 0$$

$$(1, 0, -\frac{1}{\sqrt{2}}(1-i)) \begin{pmatrix} 1 \\ 0 \\ +\frac{1}{\sqrt{2}}(1+i) \end{pmatrix} = 1 + 0 - \frac{1}{\sqrt{2}}(2) = 0$$

c) Find  $P = |a_i\rangle\langle a_i|$

$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0 \ 1 \ 0) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Yes, by earlier problem

2.23

In a 3D vector space consider operator

$$\hat{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

on an orthonormal basis  $|1\rangle, |2\rangle, |3\rangle$

a) Is  $\hat{A}$  Hermitian?

Definition of Hermitian operator is

$$\hat{A}^\dagger = A = (A^T)^*$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \stackrel{?}{=} \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \text{ Yes!}$$

It is Hermitian.

a') calculate its eigenvalues and normalized eigen vectors.

$$\text{Apply } \det(\hat{A} - \lambda I) = 0$$

Expand  $\Rightarrow \begin{vmatrix} -\lambda & 0 & 1 \\ 0 & -1-\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = 0$

Here it is useful to "expand by minors." Identify the row or column with the most zeroes and expand.

$$0 + -(1+\lambda) \cdot \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} + 0 = 0$$

minor determinant

$$-(\lambda+1) \cdot (\lambda^2 - 1) = 0$$

$$(\lambda+1)(\lambda+1)(\lambda-1) = 0$$

↑ ↑ ↑

degenerate eigen values  $\lambda = -1$

$$\lambda = +1$$

Eigenvalues

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a) (continued) Now find the eigenvectors. Start w/ the non-degenerate one

$$\vec{A}|\phi\rangle = \lambda|\phi\rangle$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = + \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{matrix} z = x \\ -y = +y \Rightarrow y = 0 \\ x = z \end{matrix}$$

So we must have  $y=0$ ,  $x=z$ , so set  $x=1 \Rightarrow |\phi\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$

Normalizing:  $\langle\phi|\phi\rangle |a|^2 = |a|^2 \cdot (2) = 1 \Rightarrow |a| = \frac{1}{\sqrt{2}}$

$$\text{So } |\phi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \longleftrightarrow \lambda = +1$$

For the degenerate eigen value  $\lambda = -1$ :

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = -1 \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{matrix} z = -x \\ -y = -y \\ z = -x \end{matrix}$$

So  $y$  may be anything,  $z = -x$ . Choose  $y=0$ ,  $x=1$

$$\text{So } |\phi_2\rangle = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\text{Normalizing } |\phi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \longleftrightarrow \lambda = -1$$

The last eigenvector may be chosen orthogonal to the other two:

$$|\phi_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \longleftrightarrow \lambda = -1 \quad \leftarrow \text{degenerate}$$

a) Verify the eigenvectors are orthogonal:

~~degenerate~~  
nondegenerate

$$\langle\phi_2|\phi_1\rangle = \frac{1}{\sqrt{2}} (1 \ 0 \ 1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{2} (1 - 1) = 0 \quad \text{Yes!}$$

b) Calculate the matrices representing the projection operators for the two nondegenerate eigenvectors

Projection operators are of the form  $|\psi\rangle\langle\psi|$ , so

$$|\phi_1\rangle\langle\phi_1| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} (1 \ 0 \ 1) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$|\phi_2\rangle\langle\phi_2| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} (1 \ 0 \ -1) = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

2.49

Hamiltonian for a two state system

$$\hat{H} = E \begin{pmatrix} 1 & -i \\ +i & -1 \end{pmatrix}$$

a)  $\hat{H}^\dagger = E \begin{pmatrix} 1 & -i \\ +i & -1 \end{pmatrix} = \hat{H}$  so yes, it's Hermitian

$$\text{Tr} \hat{H} = 0$$

b)  $\begin{vmatrix} 1-a & -i \\ i & -1-a \end{vmatrix} = 0$

$$-(1-a)(1+a) - 1 = 0$$

$$a^2 - 1 - 1 = 0$$

$$a = \pm \sqrt{2}$$

Multiply by  $E$ , so

$$a = \pm \sqrt{2}E$$

$$\hat{H}|\psi\rangle = \sqrt{2}E|\psi\rangle$$

$$\begin{aligned} x - iy &= \sqrt{2}x \rightarrow -iy = (\sqrt{2}-1)x \rightarrow \frac{-i}{\sqrt{2}-1}y = x \rightarrow -i(\sqrt{2}+1)y = x \\ ix - y &= \sqrt{2}y \rightarrow (1+\sqrt{2})y = ix \rightarrow -i(1+\sqrt{2})y = x \end{aligned}$$

Set  $x=1$

$$y = (\sqrt{2}-1)i$$

Normalize  $(1 + (\sqrt{2}-1)^2)C^2 = 1$

$$C = \frac{1}{\sqrt{1+(\sqrt{2}-1)^2}}$$

$$\frac{1}{\sqrt{1+(\sqrt{2}-1)^2}} \begin{pmatrix} 1 \\ (\sqrt{2}-1)i \end{pmatrix}$$

The eigenvector for  $-\sqrt{2}$  is

$$\frac{1}{\sqrt{1+(\sqrt{2}-1)^2}} \begin{pmatrix} 1 \\ -(\sqrt{2}-1)i \end{pmatrix}$$