Problem 2

Solution 2.(a)

The elements of our set - which we will check if they form a group - are given by,

$$\mathcal{G} = \{D_z(0), D_z(\pi/2), D_z(\pi), D_z(3\pi/2)\} \tag{46}$$

By definition of D_z rotations, we know that,

$$D_z(a)D_z(b) = D_z(a+b) \tag{47}$$

Using this property, we can form a multiplication table,

*	0	1	2	3
0	$D_z(0)$	$D_z(1)$	$D_z(2)$	$D_z(3)$
1	$D_z(1)$	$D_z(2)$	$D_z(3)$	$D_z(0)$
2	$D_z(2)$	$D_z(3)$	$D_z(0)$	$D_z(1)$
3	$D_z(3)$	$D_z(0)$	$D_z(1)$	$D_z(2)$

Table 1: $\mathcal{G}$ multiplication table

where $D_z(N)$ for $N \in 0, 1, 2, 3$ corresponds to,

$$D_z\left(\frac{n\pi}{2}\right) \tag{48}$$

- From the first row and column, we can see that D_0 forms the identity element on $\mathcal{G}$ with respect to $*$
- All the elements in the multiplication table belong in $\mathcal{G}$, proving closure on $\mathcal{G}$ with respect to $*$ operation
- There is an inverse for each of the element given by,

$$D_z(N) = D_z\left(|N-4|\right) \tag{49}$$

- Associative nature of the set $\mathcal{G}$ under $*$ can be proved,

$$\begin{aligned}
D\left(F\frac{\pi}{2}\right)\left(D\left(G\frac{\pi}{2}\right)D\left(H\frac{\pi}{2}\right)\right) &= D\left(F\frac{\pi}{2}\right)\left(D\left((G+H)\frac{\pi}{2}\right)\right) &(50)\\
&= D\left((F+G+H)\frac{\pi}{2}\right) &(51)\\
&= D\left(((F+G)+H)\frac{\pi}{2}\right) &(52)\\
&= \left(D\left(F\frac{\pi}{2}\right)D\left(G\frac{\pi}{2}\right)\right)D\left(H\frac{\pi}{2}\right) &(53)
\end{aligned}$$

Hence, we can conclude that $\mathcal{G}$ forms a group under $*$.

Solution 2.(b)

Yes, the group is abelian. You can determine this by seeing that the multiplication table is symmetric with respect to the diagonal.

Solution 2.(c)

The group has a subgroup,

$$\mathbb{Z}_2 = \{D_0, D_2\} \tag{54}$$

which can be seen from the multiplication table,

*	0	2
0	$D_z(0)$	$D_z(2)$
2	$D_z(2)$	$D_z(0)$

Table 2: $\mathbb{Z}_2$ multiplication table

where the associativity and identity are followed from the group $\mathcal{G}$.
The inverse for each of the element in this $\mathbb{Z}_2$ group is given by $D_z(2)$.

Solution 2.(d)

We want to find the eigenvalues σ_x for the mirror operator M_x.
The mirror operator takes (x, y) to $(-x, y)$.

$$M_x \left|x, y\right\rangle = \left|-x, y\right\rangle \tag{55}$$

Applying the M_x operator twice,

$$M_x(M_x \left|x, y\right\rangle) = M_x \left|-x, y\right\rangle \tag{56}$$
$$= \left|x, y\right\rangle \tag{57}$$
$$M_x^2 = \lambda^2 \left|x, y\right\rangle \tag{58}$$

Giving us, $\lambda^2 = 1$, hence the eigenvalues can be ± 1

Solution 2.(e)

The eigenvalues of $D_z(n\frac{\pi}{2})$ depends on n.

- For $n = 0$, we need to apply $D_z(0)$ once on a state to get back to the original state, which in turn means gives us the eigenvalue equation. Giving us,

$$\lambda_z(D_z(0)) = +1 \tag{59}$$

- For $n = 1$, we need to apply $D_z(1)$ four times on a state before we get back to the original state. Giving us,

$$\lambda_z(D_z(1)) = \pm 1, \pm i \tag{60}$$

  We get this by solving,

$$(\lambda_z(D_z(1)))^4 - 1 = 0 \tag{61}$$

- For $n = 2$, we need to apply $D_z(2)$ two times on a state before we get back to the original state. Giving us,

$$\lambda_z(D_z(2)) = \pm 1 \tag{62}$$

- For $n = 3$, we need to apply $D_z(3)$ four times on a state before we get back to the original state. Giving us,

$$\lambda_z(D_z(2)) = \pm 1, \pm i \tag{63}$$

Solution 2.(f)

To show that, in general the rotation operator and the mirror operator do not commute, we can use a counter-example,
Let us denote the state in which the atom is in by

$$\left|1\right\rangle, \quad \left|2\right\rangle, \quad \left|3\right\rangle, \quad \left|4\right\rangle \tag{64}$$

where 1,2,3,4 corresponds to the state in that particular quadrant.

$$M_x D_z(1) \left|1\right\rangle = M_x \left|2\right\rangle \tag{65}$$
$$= \left|1\right\rangle \tag{66}$$

$$D_z(1) M_x \left|1\right\rangle = D_z(1) \left|2\right\rangle \tag{67}$$
$$= \left|3\right\rangle \tag{68}$$

As $|1\rangle \neq |3\rangle$, we can conclude that, in general the rotation operator and the mirror symmetry operator do not commute.

Solution 2.(g)

We can show that M_x and $D_z(2)$ commute. We can arrange the 4 atoms in a set $\{0, 1, 2, 3\}$ corresponding to a permutation $\{1, 2, 3, 4\}$

$$\begin{aligned} D_z(2) M_x \{1, 2, 3, 4\} &= D_z(2)\{2, 1, 4, 3\} && (69) \\ &= \{4, 3, 2, 1\} && (70) \end{aligned}$$

and

$$\begin{aligned} M_x D_z(2) \{1, 2, 3, 4\} &= M_x\{3, 4, 1, 2\} && (71) \\ &= \{4, 3, 2, 1\} && (72) \end{aligned}$$

which show us that these operators commute for our given scenario where the atoms are allowed to be in those 4 particular positions. This means they can have simultaneous eigenstates

We did this by using the operation of these two operators on an arbitrary permutation given by,

$$\begin{aligned} M_x\{a, b, c, d\} &= \{b, a, d, c\} && (73) \\ D_z(2)\{a, b, c, d\} &= \{c, d, a, b\} && (74) \end{aligned}$$

Solution 2.(h)

Let us first check the action of our two operators on the potential,

$$\begin{aligned} M_x V &= M_x a X Y && (75) \\ &= -aXY && (76) \end{aligned}$$

which means M_x anticommutes with V, and

$$\begin{aligned} D_z(2) V &= D_z(2) a X Y && (77) \\ &= aXY && (78) \end{aligned}$$

giving us $D_z(2)$ to commute with V

All states where $\epsilon = \epsilon'$ will be zero due to orthogonality. After assuming $\epsilon = \epsilon'$ (and dropping the label from the Dirac notation as we are assuming the same ϵ), let us check which other states will be zero too.

$$\begin{aligned} \langle +, + | \, V \, | +, + \rangle &= \frac{1}{1^2} \langle +, + | \, D_z(2) M_x \; V \; M_x D_z(2) \, | +, + \rangle && (79) \\ &= -1 \langle +, + | \, D_z(2) V \underbrace{M_x M_x}_{\mathbb{1}} D_z(2) \, | +, + \rangle && (80) \\ &= -1 \langle +, + | \, V \, | ++ \rangle && (81) \\ &= 0 && (82) \end{aligned}$$

This means when the state has an even parity with respect to our operators $D_z(2), M_x$ go to zero.

By symmetry of the problem, a computation with $|-, -\rangle$ state will also give us the same result, where the state has an odd parity.

Let us check a state where the parities are mixed, i.e. even with $D_z(2)$ and odd with M_x,

$$\begin{aligned} \langle +, - | \, V \, | +, - \rangle &= - \langle +, - | \, M_x D_z(2) \; V \; D_z(2) M_x \, | +, - \rangle && (83) \\ &= \langle +, - | \, D_z(2) \; V D_z(2) \underbrace{M_x M_x}_{\mathbb{1}} | +, - \rangle && (84) \\ &= \langle +, - | \, V \, | +, - \rangle && (85) \end{aligned}$$

giving us something that is not necessarily zero. If we invert the parities, i.e. odd with $D_z(2)$ and even with M_x we will get a similar result by the symmetry of the problem.