Group Theory

Solutions to Problem Set 8 December 7, 2001

1. A matrix A is said to be orthogonal if its matrix elements a_{ij} satisfy the following relations:

$$\sum_i a_{ij}a_{ik} = \delta_{j,k}, \qquad \sum_j a_{ij}a_{kj} = \delta_{ij}\ , \tag{1}$$

i.e., the rows and columns are orthogonal vectors. This ensures that $A^{\rm t}A = AA^{\rm t} = I$.

The direct product C of two matrices A and B, denoted by $C = A \otimes B$, is given in terms of matrix elements by

$$c_{ik;jl} = a_{ij}a_{kl}\ .$$

If A and B are orthogonal matrices, then we can show that C is also an orthogonal matrix by verifying the relations in Eq. (1). The first of these relations is

$$\sum_{ik} c_{ik;jl}c_{ik;j'l'}$$

$$= \sum_{ik} a_{ij}a_{kl}a_{ij'}a_{kl'} = \Big(\sum_i a_{ij}a_{ij'}\Big)\Big(\sum_k a_{kl}a_{kl'}\Big) = \delta_{j,j'}\delta_{l,l'}\ ,$$

where the last step follows from the first of Eqs. (1). The second orthogonality relation is

$$\sum_{jl} c_{ik;jl}c_{i'k';jl}$$

$$= \sum_{jl} a_{ij}a_{kl}a_{i'j}a_{k'l} = \Big(\sum_j a_{ij}a_{i'j}\Big)\Big(\sum_l a_{kl}a_{k'l}\Big) = \delta_{i,i'}\delta_{k,k'}$$

where the last step follows from the second of Eqs. (1). Thus, we have shown that the direct product of two orthogonal matrices is also an orthogonal matrix.

2. The direct product of two matrices A and B with matrix elements a_{ij} and b_{ij} is

$$c_{ik,jl} = a_{ij} b_{kl} \,.$$

The trace of the direct product $A \otimes B$ is obtained by setting $j = i$ and $l = k$ and summing over i and k:

$$\mathrm{tr}(A \otimes B) = \sum_{ik} c_{ik,ik} = \sum_{ik} a_{ii} b_{kk} = \sum_i a_{ii} \sum_k b_{kk} = \mathrm{tr}(A)\,\mathrm{tr}(B)\,,$$

which is the product of the traces of A and B.

3. We have two groups G_a and G_b with elements

$$G_a = \{e_a, a_2, a_3, \ldots, a_{|G_a|}\}$$

and

$$G_b = \{e_b, b_2, b_3, \ldots, b_{|G_b|}\}\,,$$

such that $a_i b_j = b_j a_i$ for all i and j. We are using a notation where it is understood that $a_1 = e_a$ and $b_1 = e_b$. The direct product $G_a \otimes G_b$ of these groups is the set obtained by forming the product of every element of G_a with every element of G_b:

$$G_a \otimes G_b = \{e, a_2, a_3, \ldots, a_{n_a}, b_2, b_3, \ldots, b_{n_b}, \ldots, a_i b_j, \ldots\}\,.$$

To show that $G_a \otimes G_b$ is a group, we must demonstrate that these elements fulfill each of the four requirements in Sec. 2.1.

Closure. The product of two elements $a_i b_j$ and $a_{i'} b_{j'}$ is given by

$$(a_i b_j)(a_{i'} b_{j'}) = (a_i a_{i'})(b_j b_{j'}) = a_k b_l\,,$$

where the first step follows from the commutativity of elements between the two groups and the second step from the group property of G_a and G_b.

Associativity. The associativity of the composition law follows from

$$\begin{aligned}(a_i b_{i'} a_j b_{j'}) a_k b_{k'} &= \Big[(a_i a_j) a_k\Big]\Big[(b_{i'} b_{j'}) b_{k'}\Big] \\ &= \Big[a_i (a_j a_k)\Big]\Big[b_{i'} (b_{j'} b_{k'})\Big] \\ &= a_i b_{i'} (a_j b_{j'} a_k b_{k'})\,,\end{aligned}$$

since associativity holds for G_a and G_b separately.

Unit Element. The unit element e for the direct product group is $e_a e_b = e_b e_a$, since

$$(a_i b_j)(e_a e_b) = (a_i e_a)(b_j e_b) = (e_a a_i)(e_b b_j) = (e_a e_b)(a_i b_j)\,.$$

Inverse. Finally, the inverse of each element $a_i b_j$ is $a_i^{-1} b_j^{-1}$ because

$$(a_i b_j)(a_i^{-1} b_j^{-1}) = (a_i a_i^{-1})(b_j b_j^{-1}) = e_a e_b$$

and

$$(a_i^{-1} b_j^{-1})(a_i b_j) = (a_i^{-1} a_i)(b_j^{-1} b_j) = e_a e_b\,.$$

Thus, we have shown that the direct product of two groups is itself a group. Since the elements of this group are obtained by taking all products of elements from G_a and G_b, the order of this group is $|G_a||G_b|$.

4. Suppose we have an irreducible representation for each of two groups G_a and G_b. We denote these representations, which may be of different dimensions, by $A(a_i)$ and $A(b_j)$, and their matrix elements by $A(a_i)_{ij}$ and $A(b_j)_{ij}$. Since these representations are irreducible, they satisfy the Great Orthogonality Theorem:

$$\sum_{a_i} A(a_i)^*_{ij} A(a_i)_{i'j'} = \frac{|G_a|}{d_a} \delta_{i,i'} \delta_{j,j'}\,,$$

$$\sum_{b_j} A(b_j)^*_{ij} A(b_j)_{i'j'} = \frac{|G_b|}{d_b} \delta_{i,i'} \delta_{j,j'}\,,$$

where d_a and d_b are the dimensions of the irreducible representations of G_a and G_b, respectively. A representation of the direct product of two groups, denoted by $A(a_i b_j)$, is obtained from the direct product of representations of each group:

$$A(a_i b_j)_{ik;jl} = A(a_i)_{ij} A(b_j)_{kl} \,.$$

The sum in the Great Orthogonality Theorem for the direct product representation is

$$\begin{aligned}
&\sum_{a_i}\sum_{b_j} A(a_i b_j)^*_{ik;jl} A(a_i b_j)_{i'k';j'l'} \\
&= \sum_{a_i}\sum_{b_j} A(a_i)^*_{ij} A(b_j)^*_{kl} A(a_i)_{i'j'} A(b_j)_{k'l'} \\
&= \underbrace{\Bigg[\sum_{a_i} A(a_i)^*_{ij} A(a_i)_{i'j'}\Bigg]}_{\displaystyle \frac{|G_a|}{d_a}\delta_{i,i'}\delta_{j,j'}} \underbrace{\Bigg[\sum_{b_j} A(b_j)^*_{kl} A(b_j)_{k'l'}\Bigg]}_{\displaystyle \frac{|G_b|}{d_b}\delta_{k,k'}\delta_{l,l'}} \\
&= \left(\frac{|G_a||G_b|}{d_a d_b}\right)\delta_{i,i'}\delta_{k,k'}\delta_{j,j'}\delta_{l,l'} \,.
\end{aligned}$$

This shows that this direct product representation is, in fact, irreducible. It has dimensionality $d_a d_b$ and the order of the direct product is, of course, $|G_a| \times |G_b|$.

5. If the φ_i are orthonormal, and if this property is required to be preserved by the group of the Hamiltonian (as it must, to conserve probability), then, in Dirac notation, we have

$$\begin{aligned}
(i,j) \equiv \int \varphi_i(x)^* \varphi_j(x)\,\mathrm{d}x &= \int [R\varphi_i(x)]^* R\varphi_j(x)\,\mathrm{d}x \\
&= (i|R^\dagger R|j) = \delta_{i,j} \,.
\end{aligned}$$

Therefore,

$$
\begin{aligned}
(i|R^\dagger R|j) &= \sum_{k,l}(k,l)\Gamma(R)^*_{ki}\Gamma(R)_{lj} \\
&= \sum_k \Gamma(R)^*_{ki}\Gamma(R)_{kj} \\
&= \sum_k \left[\Gamma(R)^\dagger\right]_{ik}\Gamma(R)_{kj} \\
&= \left[\Gamma(R)^\dagger\Gamma(R)\right]_{ij},
\end{aligned}
$$

i.e., when written in matrix notation,

$$\Gamma(R)^\dagger\Gamma(R) = I\,.$$

Thus, the matrix representation is unitary.

6. We again use Dirac notation to signify basis functions φ_i and φ_j corresponding to irreducible representations n and n', respectively: $|n,i)$ and $|n',j)$. Then, the operations R in the group of the Hamiltonian applied to these functions yield

$$
\begin{aligned}
R|n,i) &= \sum_k \Gamma^{(n)}(R)_{ki}|n,k)\,, \\
R|n',j) &= \sum_l \Gamma^{(n')}(R)_{lj}|n',l)\,.
\end{aligned}
$$

Since the operators and their representations are unitary,

$$(n',j|R^\dagger = (n',j|R^{-1} = \sum_l \Gamma^{(n')}(R)^*_{lj}(n',l|\,,$$

we have

$$
\begin{aligned}
(n',j|R^{-1}R|n,i) &= (n',j|n,i) \\
&= \sum_{kl}\Gamma^{(n')}(R)^*_{kj}\Gamma^{(n)}(R)_{li}(n',k|n,l)\,.
\end{aligned}
$$

If we now sum both sides of this equation over the elements of the group of the Hamiltonian, and invoke the Great Orthogonality Theorem, we obtain

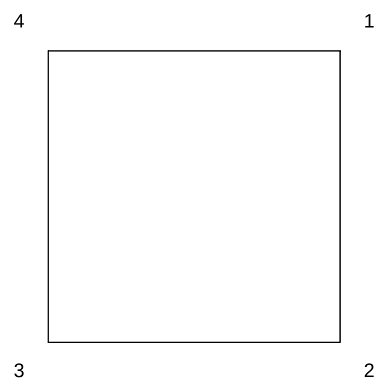
$$\begin{aligned}\sum_R (n',j|n,i) &= |G|(n',j|n,i)\\ &= \sum_{kl}\underbrace{\Big[\sum_R \Gamma^{(n')}(R)^*_{kj}\Gamma^{(n)}(R)_{li}\Big]}_{\frac{|G|}{d_n}\delta_{n,n'}\delta_{k,l}\delta_{i,j}}(n',k|n,l)\\ &= |G|\delta_{n,n'}\delta_{i,j}(n',k|n,k)\,,\end{aligned}$$

where $|G|$ is the order of the group of the Hamiltonian and d_n is the dimension of the nth irreducible representation. Therefore,

$$(n',j|n,i) = \delta_{n,n'}\delta_{i,j}\,,$$

since $(n,k|n,k) = 1$.

7. (a) A square is shown below:



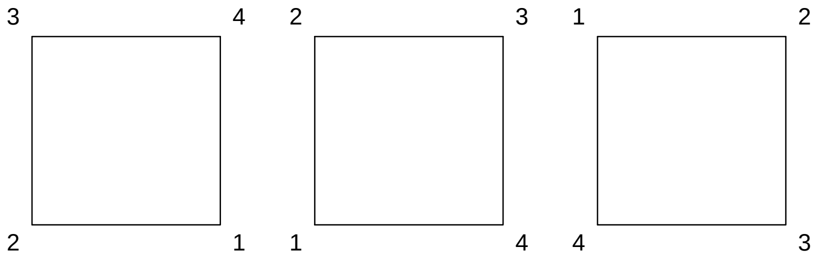
In analogy with the procedure described in Problem Set 7, we will use the following notation for the symmetry operations of this hexagon:

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ a_1 & a_2 & a_3 & a_4 \end{pmatrix},$$

where the a_i denote the number at the ith vertex after the transformation of the hexagon given in the indicated reference order. Thus, the identity operation, which identifies the reference order of the vertices, corresponds to

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{pmatrix}.$$

The symmetry operations on this square consist of the identity, rotations by angles of $\frac{1}{2}n\pi$ radians, for $n = 1, 2, 3$, two mirror planes which pass through opposite *faces* of the square, and two mirror planes which pass through opposite *vertices* of the square. For the rotations, the effect on the square is



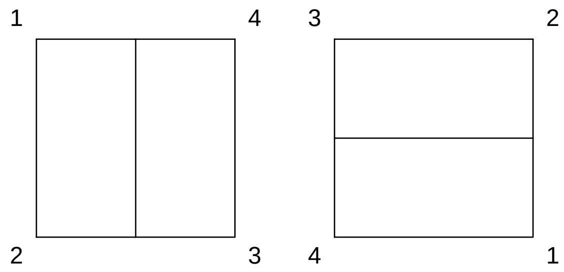
These operations correspond to

$$C_4 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 1 & 2 & 3 \end{pmatrix},$$

$$C_4^2 = C_2 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \end{pmatrix},$$

$$C_4^3 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix}.$$

The two mirror planes which pass through opposite *faces* of the square are

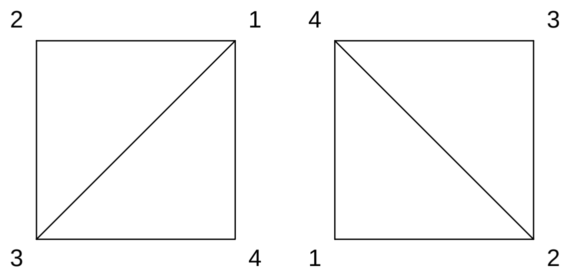


which correspond to

$$\sigma_{v,1} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \end{pmatrix},$$

$$\sigma_{v,2} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{pmatrix}.$$

Finally, the two mirror planes which pass through opposite *vertices* of the square are



These operations correspond to

$$\sigma'_{v,1} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 3 & 2 \end{pmatrix},$$

$$\sigma'_{v,2} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 2 & 1 & 4 \end{pmatrix}.$$

Elements in the same equivalence class must have the same order and correspond to the same "type" of operation. Thus, there are *five* equivalence classes of this group:

$$\{E\}, \quad \{C_2 = C_4^2\}, \quad \{2C_4\}, \quad \{2\sigma_v\}, \quad \{2\sigma_v'\}\,.$$

Note that, as in the case of the regular hexagon (Problem Set 7), all of the rotations need not belong to the same class, despite being the same "type" of operation because they must also have the same order.

(b) The order of this group is 8 and there are 5 equivalence classes. Thus, there must be five irreducible representations whose dimensionalities must satisfy

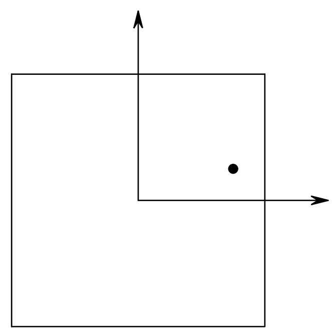
$$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 = 8\,.$$

The *only* solution of this equation (with positive integer values for the d_k) is

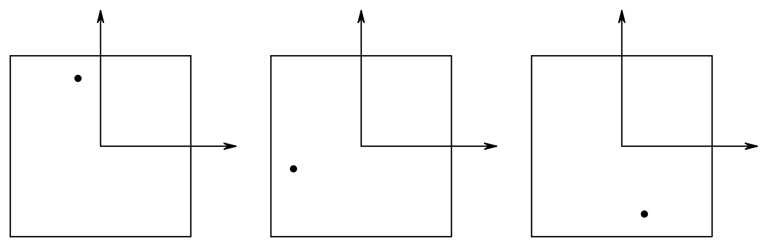
$$d_1 = 1, \quad d_2 = 1, \quad d_3 = 1, \quad d_4 = 1, \quad d_5 = 2\,.$$

These dimensionalities imply that the energy levels for a Hamiltonian with this symmetry are either nondegenerate or are two-fold degenerate. From the expression given for the energy eigenvalues, we see immediately that the energy eigenvalues with $p = q$ are non-degenerate, and those with $p \neq q$ are two-fold degenerate (but see below). Thus, the dimensions of the irreducible representations are consistent with these degeneracies.

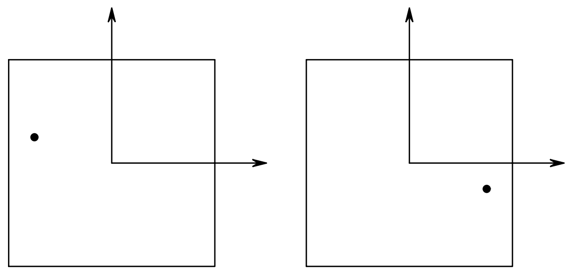
(c) The simplest way to obtain a two-dimensional representation of this group is to consider the action of each group element on some generic point (x, y). Then the action on this point of each of the operations given above can be determined by inspection. We begin with the figure below:



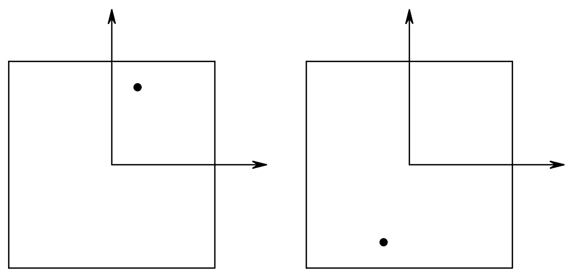
From the diagrammatic representation of each symmetry operation, we will be able to determine the corresponding representation, simply by inspection. The action on this point by the three rotations acn be represented as



These rotations are thus seen to transform the point (x, y) into $(-y, x)$, $(-x, -y)$, and $(y, -x)$, respectively. The two reflections that pass through the center of faces are



so they transform the (x, y) into $(-x, y)$ and $(x, -y)$, respectively. Finally, for the two reflection planes which pass through vertices,



which transform the point (x, y) into (y, x) and $(-y, -x)$, respectively. These transformations enable us to construct the characters corresponding to the "coordinate" representation. Then, together with the identical and parity representations, we have the following entries of the character table for this group:

	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_v'$
Γ_1	1	1	1	1	1
Γ_1'	1	1	1	-1	-1
Γ_1''	1				
Γ_1'''	1				
Γ_2	2	-2	0	0	0

The group multiplication table and the orthogonality of *columns* allows us to immediately complete the entries for the classes $\{C_2\}$ and $\{2C_4\}$:

	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_v'$
Γ_1	1	1	1	1	1
Γ_1'	1	1	1	-1	-1
Γ_1''	1	1	-1		
Γ_1'''	1	1	-1		
Γ_2	2	-2	0	0	0

The remaining four entries can be determined from the orthogonality of either rows or columns and again invoking the group multiplication table:

	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma'_v$
Γ_1	1	1	1	1	1
Γ'_1	1	1	1	-1	-1
Γ''_1	1	1	-1	1	-1
Γ'''_1	1	1	-1	-1	1
Γ_2	2	-2	0	0	0

(e) The eigenfunctions $\varphi_{1,1}(x,y)$ and $\varphi_{2,2}(x,y)$ are given by

$$\varphi_{1,1}(x,y) \propto \cos(\tfrac{1}{2}\pi x)\cos(\tfrac{1}{2}\pi y)$$

and

$$\varphi_{2,2}(x,y) \propto \sin(\pi x)\sin(\pi y)\,.$$

Since $\varphi_{1,1}(x,y)$ is invariant under the interchange of x and y and under changes in their signs, it transforms according to the **identical** representation. However, although $\varphi_{2,2}(x,y)$ is invariant under the interchange of x and y, each sine factor changes sign if their argument changes sign. Thus, this eigenfunction transforms according to the **parity** representation.

(f) The (degenerate) eigenfunctions $\varphi_{1,2}(x,y)$ and $\varphi_{2,1}(x,y)$ are

$$\begin{pmatrix}\varphi_{1,2}\\ \varphi_{2,1}\end{pmatrix} \propto \begin{bmatrix}\cos(\tfrac{1}{2}\pi x)\sin(\pi y)\\ \sin(\pi x)\cos(\tfrac{1}{2}\pi y)\end{bmatrix}.$$

The transformation properties of these eigenfunctions can be determined from the results of part (c). This yields the following matrix representation of each symmetry operation:

$$E = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \qquad C_4 = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}, \qquad C_4^2 = \begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix},$$

$$C_4^3 = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \qquad \sigma_{v,1} = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \sigma_{v,2} = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},$$

$$\sigma'_{v,1} = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \sigma'_{v,2} = \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}.$$

This produces the following characters:

$$\{E\} = 2, \quad \{C_2\} = -2, \quad \{2C_4\} = 0, \quad \{2\sigma_v\} = 0, \quad \{2\sigma_v'\} = 0\,,$$

which are the characters of the two-dimensional irreducible representation Γ_2, which is the "coordinate" irreducible representation.

(g) We have that the energies $E_{6,7}$ and $E_{2,9}$ are given by

$$E_{6,7} = E_{7,6} = \frac{\hbar^2\pi^2}{8m}(6^2 + 7^2) = 85\frac{\hbar^2\pi^2}{8m}$$

and

$$E_{2,9} = E_{9,2} = \frac{\hbar^2\pi^2}{8m}(2^2 + 9^2) = 85\frac{\hbar^2\pi^2}{8m}\,,$$

so this energy is *fourfold* degenerate. However, since the group operations have the effect of interchanging x and y with possible changes of sign, the eigenfunctions $\varphi_{6,7}$ and $\varphi_{7,6}$ are transformed only between one another, and the eigenfunctions $\varphi_{2,9}$ and $\varphi_{9,2}$ are transformed only between one another. In other words, this fourfold degeneracy is **accidental**, resulting only from the numerical coincidence of the energies of two twofold-degenerate states.

(h) We have already determined that $\varphi_{p,p}$ with p even transforms according to the identical representation, while if p is odd, $\varphi_{p,p}$ transforms according to the parity representation. Moreover, the pair of eigenfunctions $\varphi_{p,q}$ where p is even and q is odd transforms according to the coordinate representation.

Consider now the case where the eigenfunctions are of the form $\varphi_{p,q}$ where *both* p and q are even. The matrices corresponding to the symmetry operations are

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad C_4 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad C_4^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$C_4^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_{v,1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_{v,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\sigma'_{v,1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma'_{v,2} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The corresponding characters are

$$\{E\} = 2, \quad \{C_2\} = 2, \quad \{2C_4\} = 0, \quad \{2\sigma_v\} = 2, \quad \{2\sigma'_v\} = 0\,.$$

This representation must be *reducible*, since its characters do not correspond to those of any of the irreducible representations in the table determined in Part (d). A straightforward application of the Decomposition Theorem (or simple inspection) shows that this representation is the direct sum of the Γ_1 and Γ''_1 irreducible representations. This means that there is a linear combination of these eigenfunctions that diagonalizes the matrices corresponding to each symmetry operation of this group.

For the eigenfunctions of the form $\varphi_{p,q}$ where *both* p and q are odd, the matrices corresponding to the symmetry operations are

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad C_4 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad C_4^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$C_4^3 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_{v,1} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_{v,2} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\sigma'_{v,1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma'_{v,2} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The characters are now

$$\{E\} = 2, \quad \{C_2\} = 2, \quad \{2C_4\} = 0, \quad \{2\sigma_v\} = -2, \quad \{2\sigma'_v\} = 0\,.$$

which correspond to a *reducible* representation composed of the direct sum of the Γ_1' and Γ_1''' irreducible representations. Thus, *all* of the irreducible representations occur in the eigenfunctions of the two-dimensional square well.

8. The character table of the regular hexagon is reproduced below:

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1	-1	1	-1	1	-1
Γ_1'''	1	-1	1	-1	-1	1
Γ_2	2	1	-1	-2	0	0
Γ_2'	2	-1	1	2	0	0

A transformation properties of a vector perturbation can be deduced in a manner analogous to that for the equilateral triangle (Section 6.6.2). Applying each symmetry operation to $\boldsymbol{r} = (x, y, z)$ produces a *reducible* representation because these operations are either rotations or reflections through vertical planes. Thus, the z axis is invariant under every symmetry operation of this group which. Together with the fact that an (x, y) basis generates the two-dimensional irreducible representation Γ_2 [Problem 5(b), Problem Set 7], yields

$$\Gamma' = \Gamma_1 \oplus \Gamma_2 \,.$$

The corresponding characters are

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
$\Gamma_1 \oplus \Gamma_2$	3	2	0	-1	1	1

to determine the selection rule for an initial state that transforms according to the parity representation (Γ_1', we must calculated

$$\Gamma_1' \otimes \Gamma' = \Gamma_1' \otimes (\Gamma_1 \oplus \Gamma_2) \,.$$

The characters associated with this operation are

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
$\Gamma_1' \otimes (\Gamma_1 \oplus \Gamma_2)$	3	2	0	-1	-1	-1

Finally, either by inspection, or by applying the decomposition theorem, we find that

$$\Gamma_1' \otimes (\Gamma_1 \oplus \Gamma_2) = \Gamma_1' \oplus \Gamma_2 \, ,$$

so transitions between states that transform according to the parity representation and any states other than those that transform as the parity or coordinate representations are forbidden by symmetry.