

# Group Theory in Quantum Mechanics

## Lecture 11 (2.21.17)

### Representations of cyclic groups $C_3 \subset C_6 \supset C_2$

(Quantum Theory for Computer Age - Ch. 6-9 of Unit 3 )

(Principles of Symmetry, Dynamics, and Spectroscopy - Sec. 3-7 of Ch. 2 )

*Review of  $C_2$  spectral resolution for 2D oscillator (Lecture 6 : p. 11, p. 17, and p. 11)*

*$C_3$   $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory*

*$C_3$   $\mathbf{H}$ -and- $\mathbf{r}^p$ -matrix representations and conjugation symmetry*

*$C_3$  Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations*

*$C_3$  character table and modular labeling*

*Ortho-completeness inversion for operators and states*

*Comparing wave function operator algebra to bra-ket algebra*

*Modular quantum number arithmetic*

*$C_3$ -group jargon and structure of various tables*

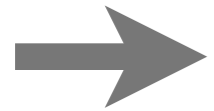
*$C_3$  Eigenvalues and wave dispersion functions*

*Standing waves vs Moving waves*

*WebApps used*

*WaveIt App*

*MolVibes*



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*$C_6$  Spectral resolution: 6<sup>th</sup> roots of unity and higher*

*Complete sets of coupling parameters and Fourier dispersion*

*Gauge shifts due to complex coupling*

# $C_2$ Symmetric two-dimensional harmonic oscillators (2DHO)

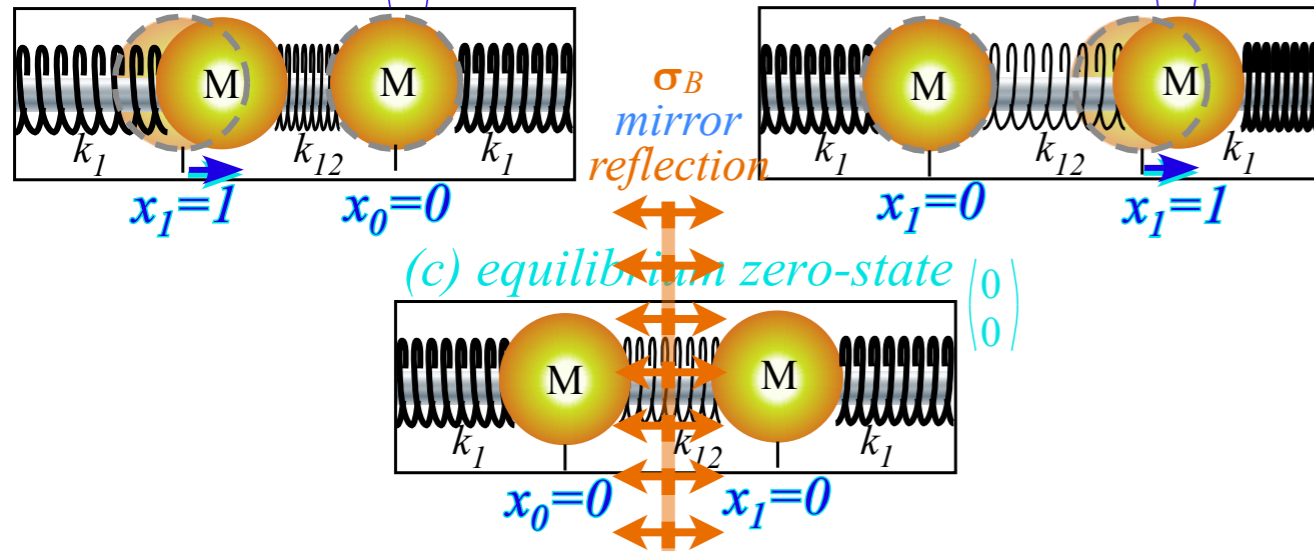
2D HO "binary" bases and coord.  $\{x_0, x_1\}$

(a) unit base state

$$|0\rangle = |x\rangle = |2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

(b) unit base state

$$|1\rangle = |y\rangle = |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



2D HO Matrix operator equations

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} = - \begin{pmatrix} \frac{k_1 + k_{12}}{M} & \frac{-k_{12}}{M} \\ \frac{-k_{12}}{M} & \frac{k_1 + k_{12}}{M} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$= - \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \text{More conventional coordinate notation}$$

$$|\ddot{\mathbf{x}}\rangle = - \mathbf{K} |\mathbf{x}\rangle \quad \{x_0, x_1\} \rightarrow \{x_1, x_2\}$$

$C_2$  (Bilateral  $\sigma_B$  reflection) symmetry conditions:

$$K_{11} \equiv K \equiv K_{22} \text{ and: } K_{12} \equiv k \equiv K_{21} = -k_{12} \quad (\text{Let: } M=1)$$

$$\begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} = \begin{pmatrix} K & k \\ k & K \end{pmatrix} = K \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + k \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{K} = K\mathbf{1} + k\sigma_B$$

$K$ -matrix is made of its symmetry operators in

group  $C_2 = \{\mathbf{1}, \sigma_B\}$  with product table:

$C_2$	$\mathbf{1}$	$\sigma_B$
$\mathbf{1}$	$\mathbf{1}$	$\sigma_B$
$\sigma_B$	$\sigma_B$	$\mathbf{1}$

Symmetry product table gives  $C_2$  group representations in group basis  $\{|0\rangle = \mathbf{1}|0\rangle \equiv |\mathbf{1}\rangle, |1\rangle = \sigma_B|0\rangle \equiv |\sigma_B\rangle\}$

$$\begin{pmatrix} \langle \mathbf{1} | \mathbf{1} | \mathbf{1} \rangle & \langle \mathbf{1} | \mathbf{1} | \sigma_B \rangle \\ \langle \sigma_B | \mathbf{1} | \mathbf{1} \rangle & \langle \sigma_B | \mathbf{1} | \sigma_B \rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} \langle \mathbf{1} | \sigma_B | \mathbf{1} \rangle & \langle \mathbf{1} | \sigma_B | \sigma_B \rangle \\ \langle \sigma_B | \sigma_B | \mathbf{1} \rangle & \langle \sigma_B | \sigma_B | \sigma_B \rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

# $C_2$ Symmetric two-dimensional harmonic oscillators (2DHO)

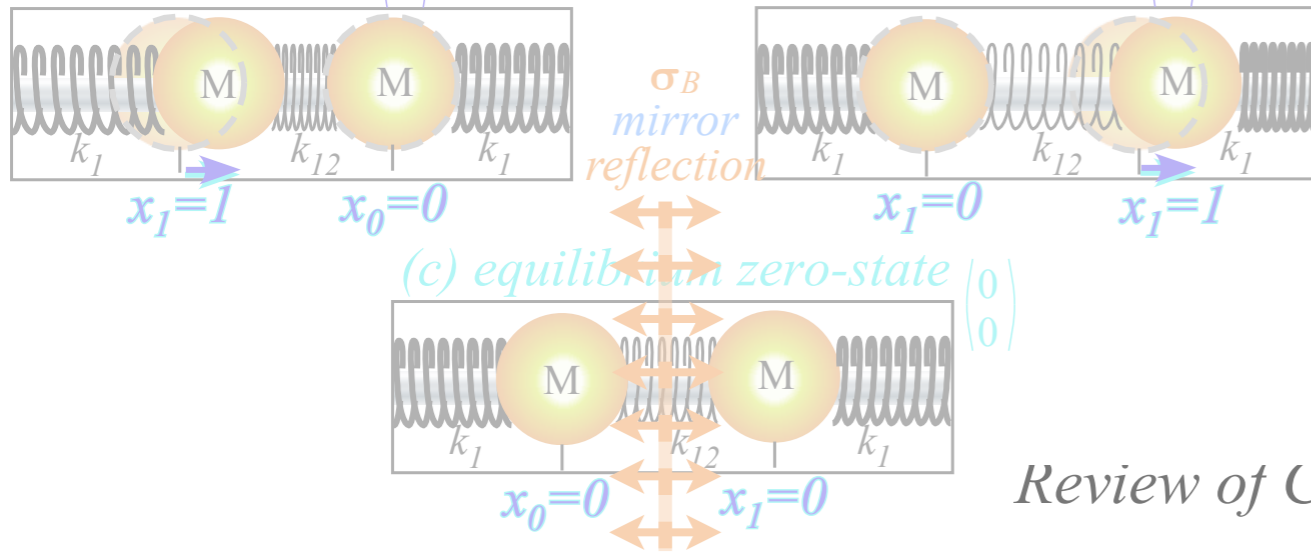
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Review of  $C_2$  spectral resolution for 2D oscillator Lecture 6 p.17

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group  $C_2 = \{\mathbf{1}, \sigma_B\}$  with product table:

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$$\begin{pmatrix} \langle \mathbf{1} | \mathbf{1} | \mathbf{1} \rangle & \langle \mathbf{1} | \mathbf{1} | \sigma_B \rangle \\ \langle \sigma_B | \mathbf{1} | \mathbf{1} \rangle & \langle \sigma_B | \mathbf{1} | \sigma_B \rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} \langle \mathbf{1} | \sigma_B | \mathbf{1} \rangle & \langle \mathbf{1} | \sigma_B | \sigma_B \rangle \\ \langle \sigma_B | \sigma_B | \mathbf{1} \rangle & \langle \sigma_B | \sigma_B | \sigma_B \rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$\mathbf{P}^\pm$ -projectors:

$$\mathbf{P}^+ = \frac{\mathbf{1} + \sigma_B}{2} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$\mathbf{P}^- = \frac{\mathbf{1} - \sigma_B}{2} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Minimal equation of  $\sigma_B$  is:  $\sigma_B^2 = 1$

$$\text{or: } \sigma_B^2 - 1 = 0 = (\sigma_B - 1)(\sigma_B + 1)$$

with eigenvalues:

$$\{\chi^+(\sigma_B) = +1, \chi^-(\sigma_B) = -1\}$$

Spectral decomposition of  $C_2(\sigma_B)$  into  $\{\mathbf{P}^+, \mathbf{P}^-\}$

$$\mathbf{1} = \mathbf{P}^+ + \mathbf{P}^-$$

$$\sigma_B = \mathbf{P}^+ - \mathbf{P}^-$$

# $C_2$ Symmetric 2DHO eigensolutions

$$\mathbf{K} = K\mathbf{1} - k_{12}\sigma_B$$

$K$ -matrix is made of its symmetry operators

$$K \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - k_{12} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} k_1 + k_{12} & -k_{12} \\ -k_{12} & k_1 + k_{12} \end{pmatrix}$$

in group  $C_2 = \{\mathbf{1}, \sigma_B\}$  with product table:

$C_2(\sigma_B)$  spectrally decomposed into  $\{\mathbf{P}^+, \mathbf{P}^-\}$  projectors:  $\mathbf{P}^+ = \frac{\mathbf{1} + \sigma_B}{2} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = |+\rangle\langle +|$

$$\mathbf{1} = \mathbf{P}^+ + \mathbf{P}^-$$

$$\sigma_B = \mathbf{P}^+ - \mathbf{P}^-$$

Eigenvalues of  $\sigma_B$ :

$$\{\chi^+(\sigma_B) = +1, \chi^-(\sigma_B) = -1\}$$

Eigenvalues of  $\mathbf{K} = K\mathbf{1} - k_{12}\sigma_B$ :

$$\begin{aligned} \varepsilon^+(\mathbf{K}) &= K - k_{12}, & \varepsilon^-(\mathbf{K}) &= K + k_{12} \\ &= k_1, & &= k_1 + 2k_{12} \end{aligned}$$

Even mode  $|+\rangle = |0_2\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} / \sqrt{2}$

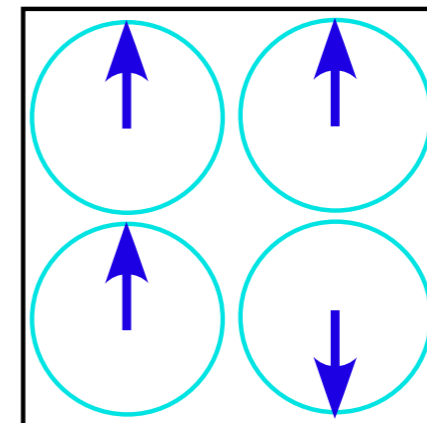
Diagonalizing transformation (D-tran) of  $K$ -matrix:

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} k_1 + k_{12} & -k_{12} \\ -k_{12} & k_1 + k_{12} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} k_1 & 0 \\ 0 & k_1 + 2k_{12} \end{pmatrix}$$

$C_2$  mode phase character tables

$p$  is position  
 $p=0$      $p=1$

$m=0$	1	1
$m=1$	1	-1



norm:  $1/\sqrt{2}$

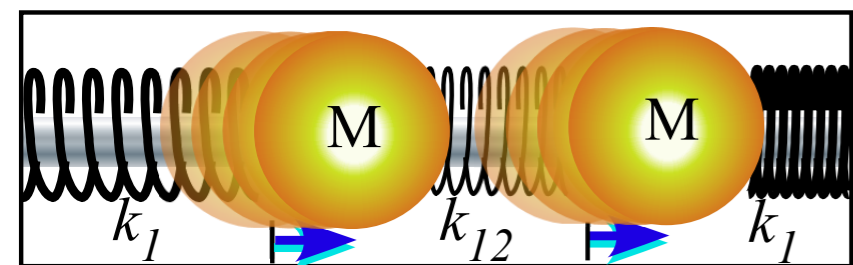
(D-tran)

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} =$$

$$\begin{pmatrix} \langle x_1 | + \rangle & \langle x_1 | - \rangle \\ \langle x_2 | + \rangle & \langle x_2 | - \rangle \end{pmatrix}$$

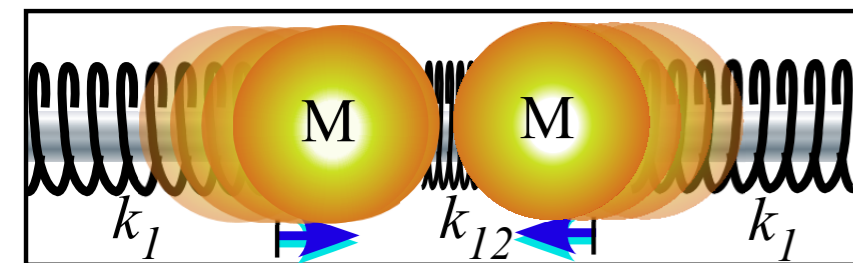
(D-tran is its own inverse in this case!)

$m$  is wave-number or "momentum"

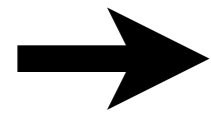


$$x_0 = 1/\sqrt{2} \quad x_1 = 1/\sqrt{2}$$

Odd mode  $|-\rangle = |1_2\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix} / \sqrt{2}$



$$x_0 = 1/\sqrt{2} \quad x_1 = -1/\sqrt{2}$$



*C<sub>3</sub> **g**<sup>†</sup>**g**-product-table and basic group representation theory*

*C<sub>3</sub> **H**-and-**r**<sup>p</sup>-matrix representations and conjugation symmetry*

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# $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory

$C_3$	$\mathbf{r}^0 = \mathbf{1}$	$\mathbf{r}^1 = \mathbf{r}^{-2}$	$\mathbf{r}^2 = \mathbf{r}^{-1}$
$\mathbf{r}^0 = \mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2 = \mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
$\mathbf{r}^1 = \mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{1}$

## $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table

Pairs each operator  $\mathbf{g}$  in the 1<sup>st</sup> row  
with its inverse  $\mathbf{g}^\dagger = \mathbf{g}^{-1}$  in the 1<sup>st</sup> column  
so all *unit*  $\mathbf{1} = \mathbf{g}^{-1} \mathbf{g}$  elements lie on diagonal.



# $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory

$C_3$	$\mathbf{r}^0 = \mathbf{1}$	$\mathbf{r}^1 = \mathbf{r}^{-2}$	$\mathbf{r}^2 = \mathbf{r}^{-1}$
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$\mathbf{r}^2 = \mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
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A  $C_3$   $\mathbf{H}$ -matrix is then constructed directly from the  $\mathbf{g}^\dagger \mathbf{g}$ -table and so is each  $\mathbf{r}^p$ -matrix representation.

$$\mathbf{H} = \begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + r_1 \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} + r_2 \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$= r_0 \cdot \mathbf{1} \quad + r_1 \cdot \mathbf{r}^1 \quad + r_2 \cdot \mathbf{r}^2$$



# $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory

$C_3$	$\mathbf{r}^0 = \mathbf{1}$	$\mathbf{r}^1 = \mathbf{r}^{-2}$	$\mathbf{r}^2 = \mathbf{r}^{-1}$
$\mathbf{r}^0 = \mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2 = \mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
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## $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table

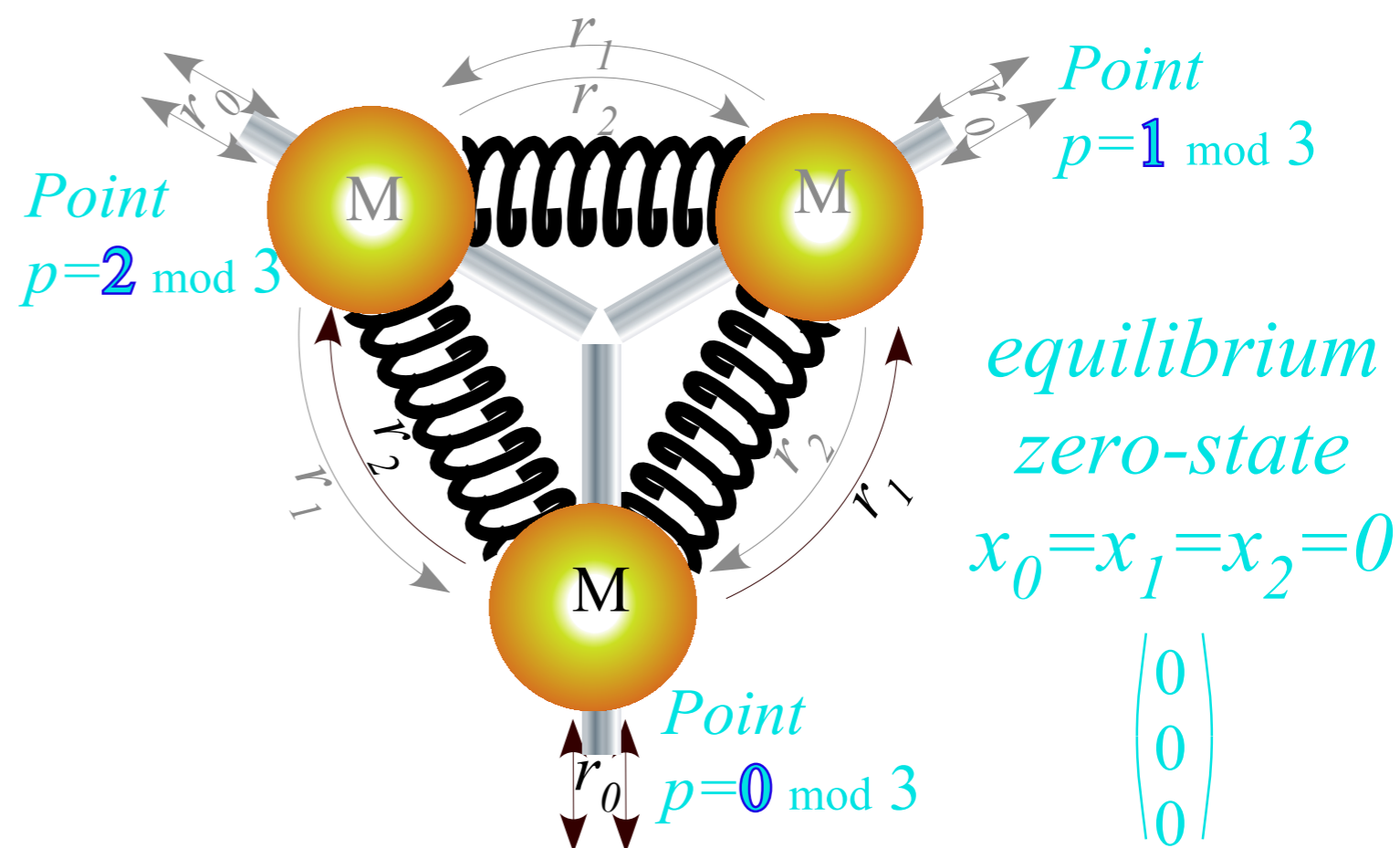
Pairs each operator  $\mathbf{g}$  in the 1<sup>st</sup> row with its inverse  $\mathbf{g}^\dagger = \mathbf{g}^{-1}$  in the 1<sup>st</sup> column so all *unit*  $\mathbf{1} = \mathbf{g}^{-1} \mathbf{g}$  elements lie on diagonal.

A  $C_3$   $\mathbf{H}$ -matrix is then constructed directly from the  $\mathbf{g}^\dagger \mathbf{g}$ -table and so is each  $\mathbf{r}^p$ -matrix representation.

$$\mathbf{H} = \begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + r_1 \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} + r_2 \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$= r_0 \cdot \mathbf{1} + r_1 \cdot \mathbf{r}^1 + r_2 \cdot \mathbf{r}^2$$

$\mathbf{H}$ -matrix coupling constants  $\{r_0, r_1, r_2\}$  relate to particular operators  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$  that transmit a particular force or current.



# $C_3$ $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory

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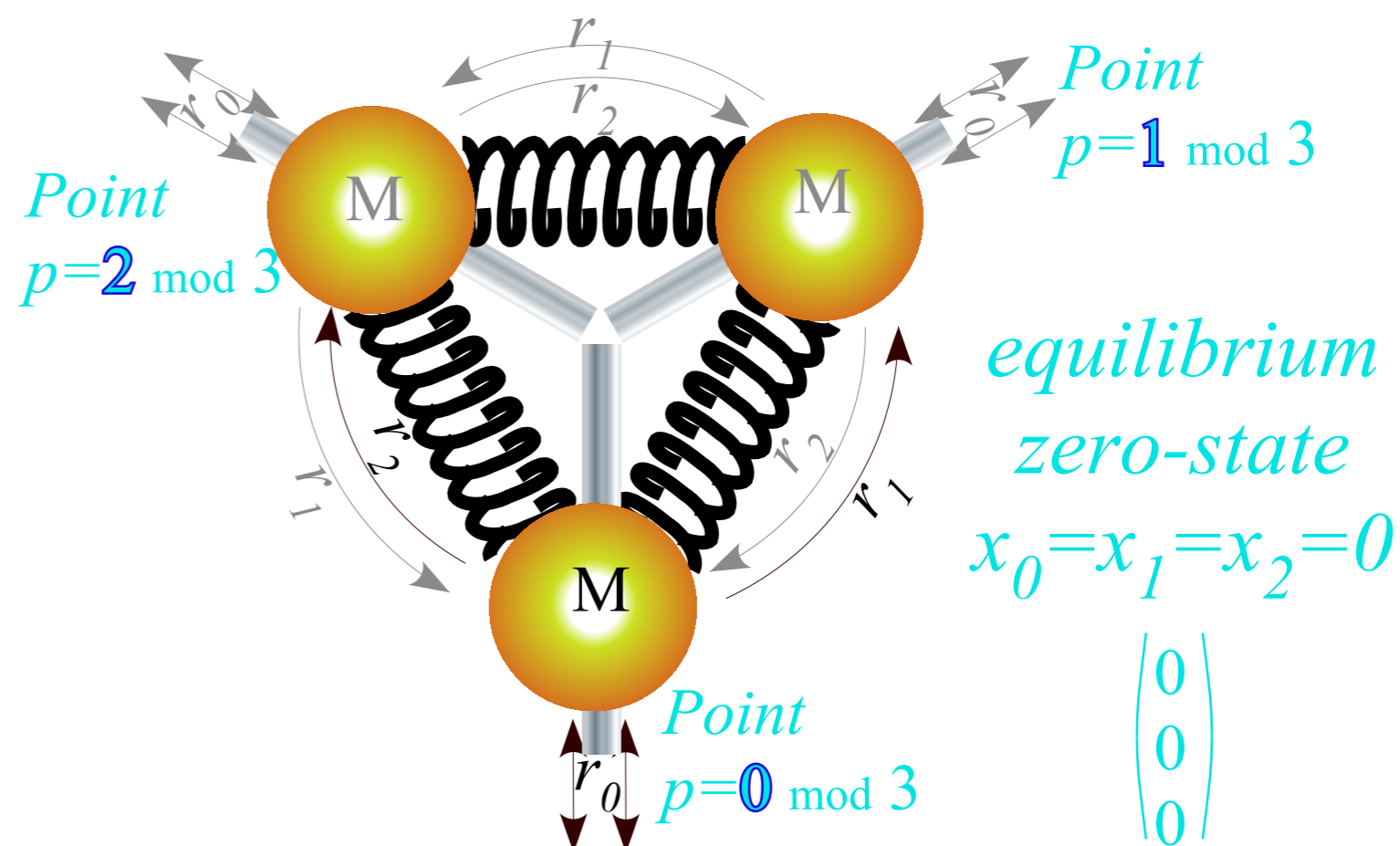
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Constants  $r_k$  that are *grayed-out* may change values if  $C_3$  symmetry is broken

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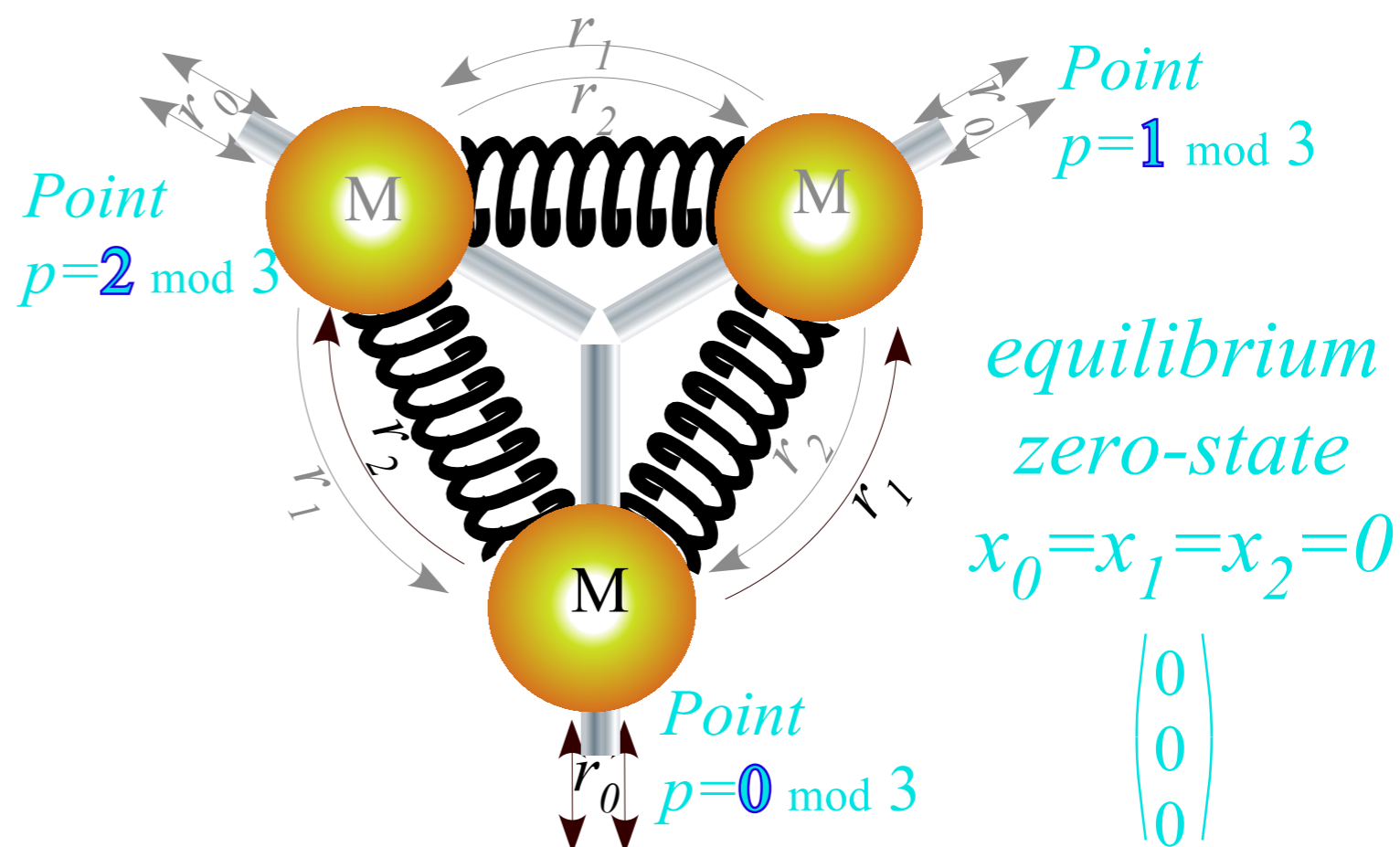
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### Conjugation symmetry

However, no matter how  $C_3$  is broken, a Hermitian-symmetric Hamiltonian ( $H_{jk}^* = H_{kj}$ ) requires that  $r_0^* = r_0$  and  $r_1^* = r_2$ .



$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

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$$= r_0 \cdot \mathbf{1} + r_1 \cdot \mathbf{r}^1 + r_2 \cdot \mathbf{r}^2$$

$\mathbf{H}$ -matrix coupling constants  $\{r_0, r_1, r_2\}$  relate to particular operators  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$  that transmit a particular force or current.

### Conjugation symmetry

Hermitian Hamiltonian ( $H_{jk}^* = H_{kj}$ ) requires  $r_0^* = r_0$  and  $r_1^* = r_2$ .

$C_3$  operators  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$

also label unit

base states:

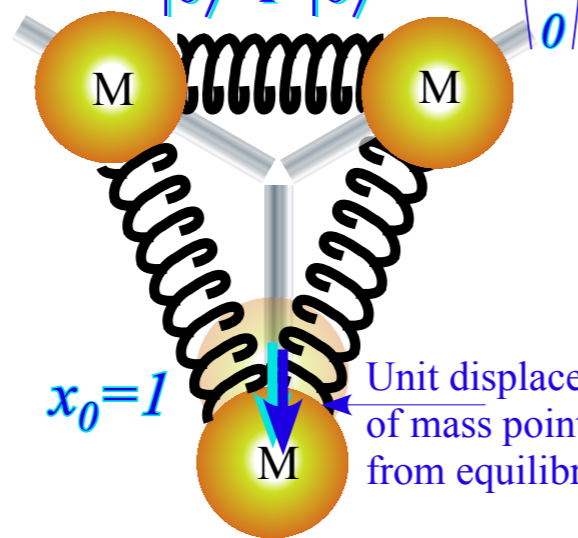
$$|0\rangle = \mathbf{r}^0 |0\rangle$$

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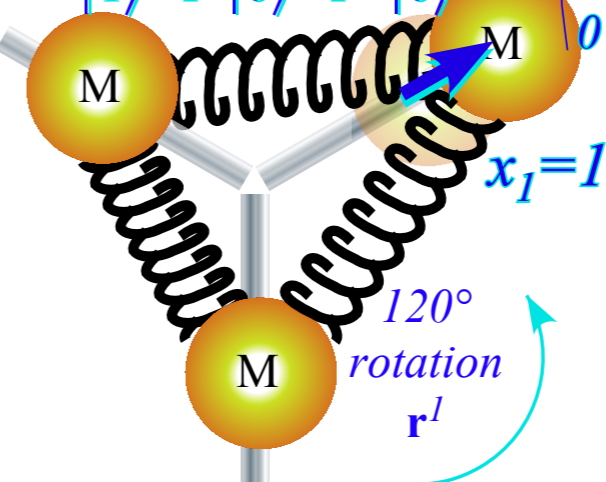
$$|2\rangle = \mathbf{r}^2 |0\rangle$$

modulo-3

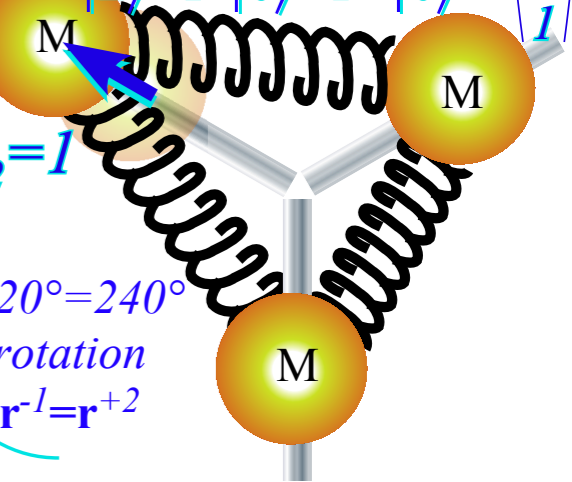
( $p=0$ ) unit base state  $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$   
 $|0\rangle = \mathbf{r}^0 |0\rangle$



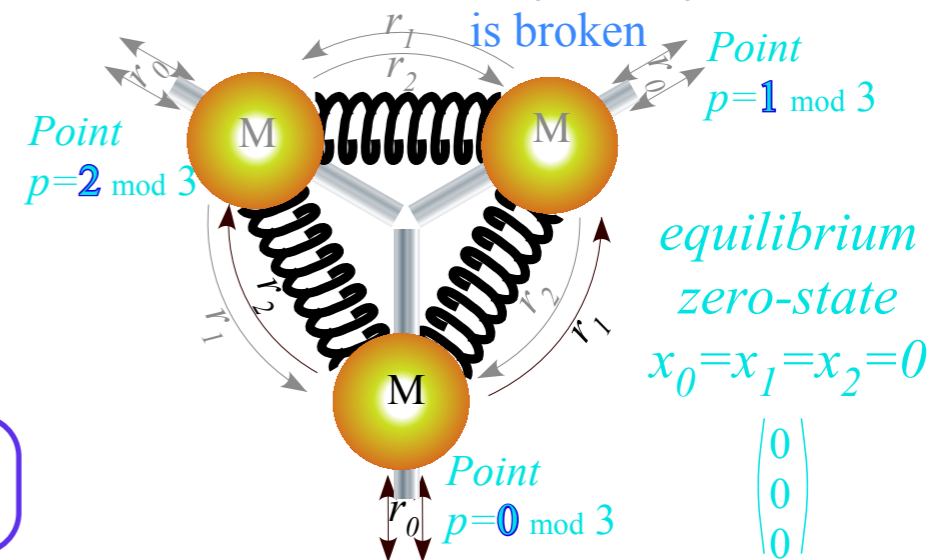
( $p=1$ ) unit base state  $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$   
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( $p=2$ ) unit base state  $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$   
 $|2\rangle = \mathbf{r}^2 |0\rangle = \mathbf{r}^{-1} |0\rangle$



Constants  $r_k$  that are grayed-out may change values if  $C_3$  symmetry is broken

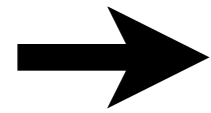


equilibrium zero-state  
 $x_0 = x_1 = x_2 = 0$

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

*C<sub>3</sub>  $\mathbf{g}^\dagger\mathbf{g}$ -product-table and basic group representation theory*

*C<sub>3</sub>  $\mathbf{H}$ -and- $\mathbf{r}^p$ -matrix representations and conjugation symmetry*



*C<sub>3</sub> Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations*

*C<sub>3</sub> character table and modular labeling*

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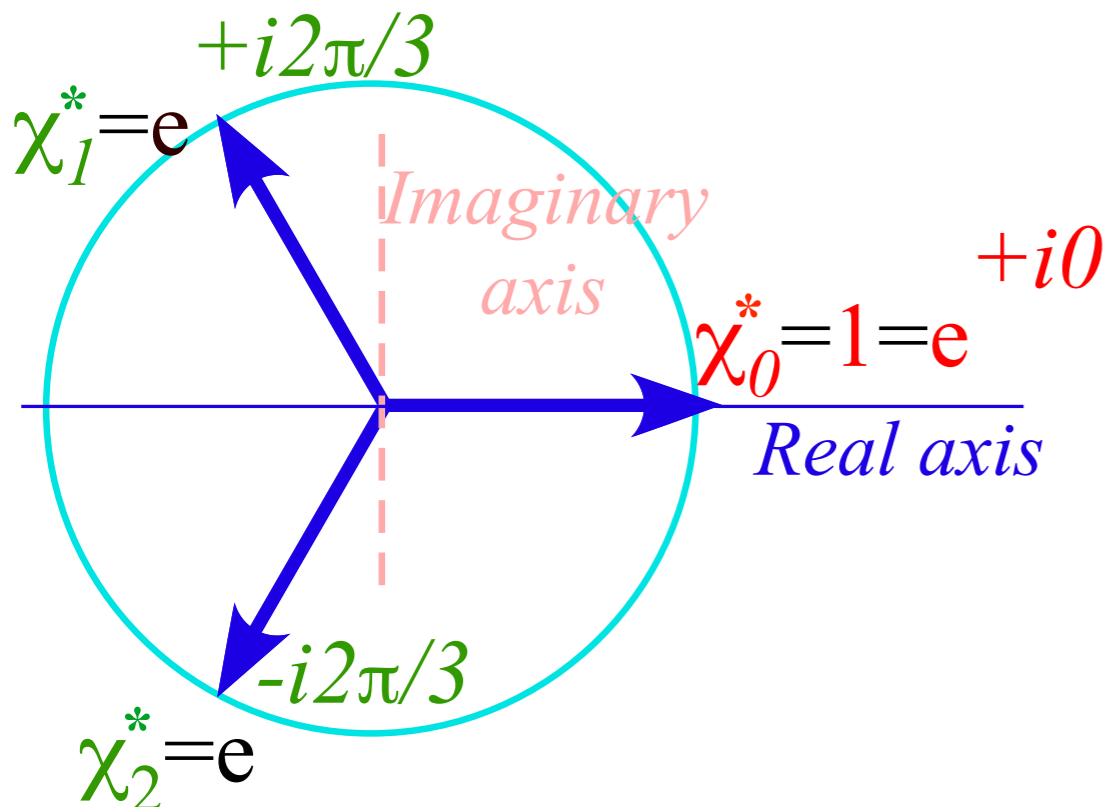
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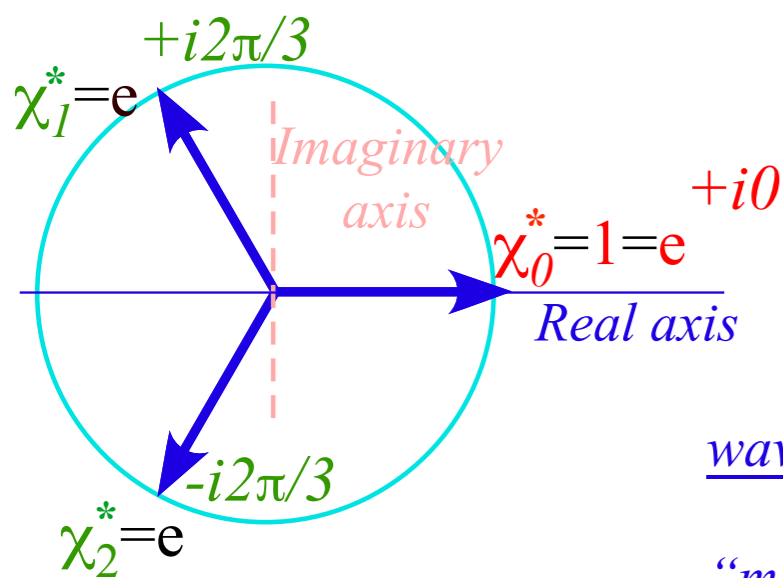
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$C_3$  mode phase character table

	$p=0$	$p=1$	$p=2$
$m=0$	$\chi_{00} = 1$	$\chi_{01} = 1$	$\chi_{02} = 1$
$m=1$	$\chi_{10} = 1$	$\chi_{11} = e^{-i2\pi/3}$	$\chi_{12} = e^{i2\pi/3}$
$m=2$	$\chi_{20} = 1$	$\chi_{21} = e^{i2\pi/3}$	$\chi_{22} = e^{-i2\pi/3}$

$\frac{\text{wave-number}}{m =}$   
 “momentum”

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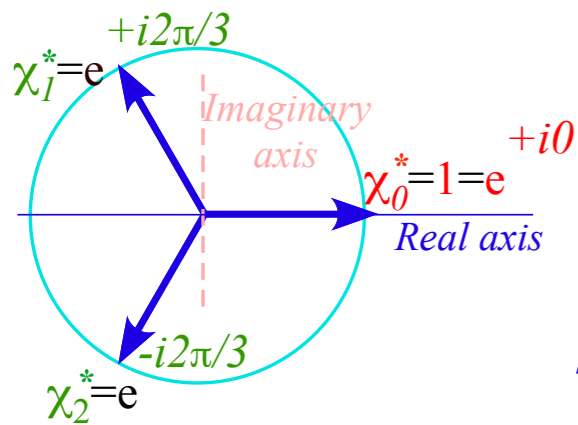
We know there is an idempotent projector **P<sup>(m)</sup>** such that  $\mathbf{r} \cdot \mathbf{P}^{(m)} = \chi_m \mathbf{P}^{(m)}$  for each eigenvalue  $\chi_m$  of **r**,

They must be *orthonormal* ( $\mathbf{P}^{(m)} \mathbf{P}^{(n)} = \delta_{mn} \mathbf{P}^{(m)}$ ) and sum to unit **1** by a *completeness* relation:

$$\mathbf{r} \cdot \mathbf{P}^{(m)} = \chi_m \mathbf{P}^{(m)} \quad \text{Ortho-Completeness} \quad \mathbf{1} = \mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)}$$

$$\chi_0 = e^{i0} = 1, \quad \chi_1 = e^{-i2\pi/3}, \quad \chi_2 = e^{-i4\pi/3}. \quad \mathbf{r}^1 \text{-Spectral-Decomp.} \quad \mathbf{r}^1 = \chi_0 \mathbf{P}^{(0)} + \chi_1 \mathbf{P}^{(1)} + \chi_2 \mathbf{P}^{(2)}$$

$$(\chi_0)^2 = 1, \quad (\chi_1)^2 = \chi_2, \quad (\chi_2)^2 = \chi_1. \quad \mathbf{r}^2 \text{-Spectral-Decomp.} \quad \mathbf{r}^2 = (\chi_0)^2 \mathbf{P}^{(0)} + (\chi_1)^2 \mathbf{P}^{(1)} + (\chi_2)^2 \mathbf{P}^{(2)}$$



$C_3$  mode phase character table

	$p=0$	$p=1$	$p=2$
$m=0$	$\chi_{00} = 1$	$\chi_{01} = 1$	$\chi_{02} = 1$
$m=1$	$\chi_{10} = 1$	$\chi_{11} = e^{-i2\pi/3}$	$\chi_{12} = e^{i2\pi/3}$
$m=2$	$\chi_{20} = 1$	$\chi_{21} = e^{i2\pi/3}$	$\chi_{22} = e^{-i2\pi/3}$

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$C_3$  character conjugate

$$\chi_{mp}^* = e^{imp2\pi/3}$$

is wave function

$$\psi_m(\mathbf{r}_p) = \frac{e^{ik_m \cdot \mathbf{r}_p}}{\sqrt{3}}$$

wave-number  
 $m =$   
“momentum”

# $C_3$ Spectral resolution: 3<sup>rd</sup> roots of unity

“Chi”(χ) refers to characters or characteristic roots

We can spectrally resolve **H** if we resolve **r** since **H** is a combination of powers **r<sup>p</sup>**.

**r**- symmetry implies cubic **r<sup>3</sup>=1**, or **r<sup>3</sup>-1=0** resolved by three 3<sup>rd</sup> roots of unity  $\chi_m^* = e^{im2\pi/3} = \psi_m$ .

Complex numbers *z* make it easy to find cube roots of  $z = 1 = e^{2\pi im}$ . (Answer:  $z^{1/3} = e^{2\pi im/3}$ )

$1 = \mathbf{r}^3$  implies :  $0 = \mathbf{r}^3 - 1 = (\mathbf{r} - \chi_0 \mathbf{1})(\mathbf{r} - \chi_1 \mathbf{1})(\mathbf{r} - \chi_2 \mathbf{1})$  where :  $\chi_m = e^{-im\frac{2\pi}{3}} = \psi_m^*$

$$\left\{ \begin{array}{l} \chi_0 = e^{-i0\frac{2\pi}{3}} = 1 \\ \chi_1 = e^{-i1\frac{2\pi}{3}} = \psi_1^* \\ \chi_2 = e^{-i2\frac{2\pi}{3}} = \psi_2^* \end{array} \right.$$

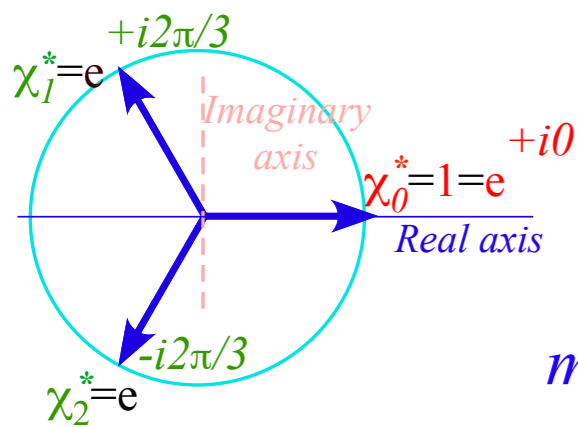
We know there is an idempotent projector **P<sup>(m)</sup>** such that  $\mathbf{r} \cdot \mathbf{P}^{(m)} = \chi_m \mathbf{P}^{(m)}$  for each eigenvalue  $\chi_m$  of **r**,

They must be *orthonormal* ( $\mathbf{P}^{(m)} \mathbf{P}^{(n)} = \delta_{mn} \mathbf{P}^{(m)}$ ) and sum to unit **1** by a *completeness* relation:

$$\mathbf{r} \cdot \mathbf{P}^{(m)} = \chi_m \mathbf{P}^{(m)} \quad \text{Ortho-Completeness} \quad \mathbf{1} = \mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)}$$

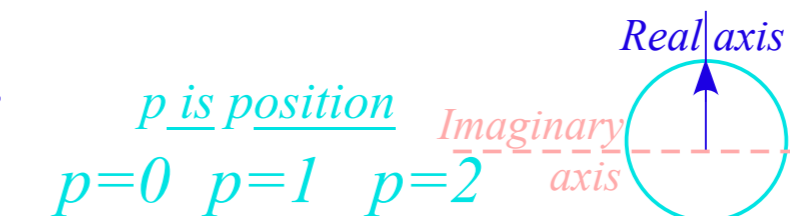
$$\chi_0 = e^{i0} = 1, \quad \chi_1 = e^{-i2\pi/3}, \quad \chi_2 = e^{-i4\pi/3}. \quad \mathbf{r}^1\text{-Spectral-Decomp.} \quad \mathbf{r}^1 = \chi_0 \mathbf{P}^{(0)} + \chi_1 \mathbf{P}^{(1)} + \chi_2 \mathbf{P}^{(2)}$$

$$(\chi_0)^2 = 1, \quad (\chi_1)^2 = \chi_2, \quad (\chi_2)^2 = \chi_1. \quad \mathbf{r}^2\text{-Spectral-Decomp.} \quad \mathbf{r}^2 = (\chi_0)^2 \mathbf{P}^{(0)} + (\chi_1)^2 \mathbf{P}^{(1)} + (\chi_2)^2 \mathbf{P}^{(2)}$$



$C_3$  mode phase character table

	$p=0$	$p=1$	$p=2$
$m=0_3$	$\chi_{00} = 1$	$\chi_{01} = 1$	$\chi_{02} = 1$
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$m=2_3$	$\chi_{20} = 1$	$\chi_{21} = e^{i2\pi/3}$	$\chi_{22} = e^{-i2\pi/3}$



$C_3$  character conjugate

$$\chi_{mp}^* = e^{imp2\pi/3}$$

is wave function

$$\psi_m(\mathbf{r}_p) = e^{ik_m \cdot \mathbf{r}_p}$$

norm:  $1/\sqrt{3}$

WaveIt App

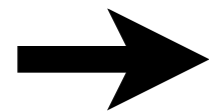
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*C<sub>3</sub> g†g-product-table and basic group representation theory*

*C<sub>3</sub> H-and-r<sup>p</sup>-matrix representations and conjugation symmetry*

*C<sub>3</sub> Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations*

*C<sub>3</sub> character table and modular labeling*



*Ortho-completeness inversion for operators and states*

*Comparing wave function operator algebra to bra-ket algebra*

*Modular quantum number arithmetic*

*C<sub>3</sub>-group jargon and structure of various tables*

*C<sub>3</sub> Eigenvalues and wave dispersion functions*

*Standing waves vs Moving waves*

*C<sub>6</sub> Spectral resolution: 6<sup>th</sup> roots of unity and higher*

*Complete sets of coupling parameters and Fourier dispersion*

*Gauge shifts due to complex coupling*

Given unitary *Ortho-Completeness operator* relations:

$$\mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} = \mathbf{1} = \mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)}$$

$$\chi_0 \mathbf{P}^{(0)} + \chi_1 \mathbf{P}^{(1)} + \chi_2 \mathbf{P}^{(2)} = \mathbf{r}^1 = \mathbf{1} \mathbf{P}^{(0)} + e^{-i2\pi/3} \mathbf{P}^{(1)} + e^{i2\pi/3} \mathbf{P}^{(2)}$$

$$(\chi_0)^2 \mathbf{P}^{(0)} + (\chi_1)^2 \mathbf{P}^{(1)} + (\chi_2)^2 \mathbf{P}^{(2)} = \mathbf{r}^2 = \mathbf{1} \mathbf{P}^{(0)} + e^{i2\pi/3} \mathbf{P}^{(1)} + e^{-i2\pi/3} \mathbf{P}^{(2)}$$



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or ket relations: (to  $|\mathbf{1}\rangle = |\mathbf{r}^0\rangle$ )

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Inverting *O-C* is easy: just  $\dagger$ -conjugate!

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$$\mathbf{P}^{(1)} = \frac{1}{3}(\mathbf{r}^0 + \chi_1^* \mathbf{r}^1 + \chi_2^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{+i2\pi/3} \mathbf{r}^1 + e^{-i2\pi/3} \mathbf{r}^2)$$

$$\mathbf{P}^{(2)} = \frac{1}{3}(\mathbf{r}^0 + \chi_2^* \mathbf{r}^1 + \chi_1^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{-i2\pi/3} \mathbf{r}^1 + e^{+i2\pi/3} \mathbf{r}^2)$$

or ket relations: (to  $|\mathbf{1}\rangle = |\mathbf{r}^0\rangle$ )

$$\sqrt{3}|\mathbf{1}\rangle = |\mathbf{0}_3\rangle + |\mathbf{1}_3\rangle + |\mathbf{2}_3\rangle$$

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$$\mathbf{P}^{(1)} = \frac{1}{3}(\mathbf{r}^0 + \chi_1^* \mathbf{r}^1 + \chi_2^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{+i2\pi/3} \mathbf{r}^1 + e^{-i2\pi/3} \mathbf{r}^2)$$

$$\mathbf{P}^{(2)} = \frac{1}{3}(\mathbf{r}^0 + \chi_2^* \mathbf{r}^1 + \chi_1^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{-i2\pi/3} \mathbf{r}^1 + e^{+i2\pi/3} \mathbf{r}^2)$$

or ket relations: (to  $|\mathbf{1}\rangle = |\mathbf{r}^0\rangle$ )

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$$|\mathbf{0}_3\rangle = \mathbf{P}^{(0)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + |\mathbf{r}^1\rangle + |\mathbf{r}^2\rangle}{\sqrt{3}}$$

$$|\mathbf{1}_3\rangle = \mathbf{P}^{(1)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + e^{+i2\pi/3} |\mathbf{r}^1\rangle + e^{-i2\pi/3} |\mathbf{r}^2\rangle}{\sqrt{3}}$$

$$|\mathbf{2}_3\rangle = \mathbf{P}^{(2)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + e^{-i2\pi/3} |\mathbf{r}^1\rangle + e^{+i2\pi/3} |\mathbf{r}^2\rangle}{\sqrt{3}}$$

Given unitary *Ortho-Completeness operator relations*:

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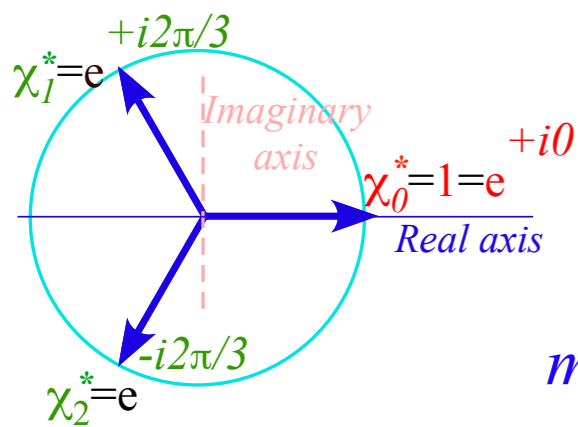
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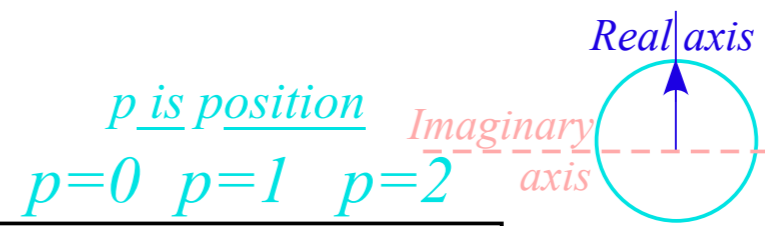
$$\mathbf{P}^{(2)} = \frac{1}{3}(\mathbf{r}^0 + \chi_2^* \mathbf{r}^1 + \chi_1^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{-i2\pi/3} \mathbf{r}^1 + e^{+i2\pi/3} \mathbf{r}^2)$$

$$\begin{aligned} |\mathbf{0}_3\rangle &= \mathbf{P}^{(0)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + |\mathbf{r}^1\rangle + |\mathbf{r}^2\rangle}{\sqrt{3}} \\ |\mathbf{1}_3\rangle &= \mathbf{P}^{(1)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + e^{+i2\pi/3} |\mathbf{r}^1\rangle + e^{-i2\pi/3} |\mathbf{r}^2\rangle}{\sqrt{3}} \\ |\mathbf{2}_3\rangle &= \mathbf{P}^{(2)}|\mathbf{1}\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + e^{-i2\pi/3} |\mathbf{r}^1\rangle + e^{+i2\pi/3} |\mathbf{r}^2\rangle}{\sqrt{3}} \end{aligned}$$



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$m=2_3$	$\chi_{20}=1$	$\chi_{21}=e^{i2\pi/3}$	$\chi_{22}=e^{-i2\pi/3}$



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$$\chi_{mp}^* = e^{imp2\pi/3}$$

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$$\psi_m(\mathbf{r}_p) = \frac{e^{ik_m \cdot \mathbf{r}_p}}{\sqrt{3}}$$

norm:  $1/\sqrt{3}$

WaveIt App  
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Given unitary *Ortho-Completeness* operator relations:

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$$\begin{aligned} \sqrt{3}|\mathbf{1}\rangle &= |\mathbf{0}_3\rangle + |\mathbf{1}_3\rangle + |\mathbf{2}_3\rangle \\ \sqrt{3}|\mathbf{r}^1\rangle &= |\mathbf{0}_3\rangle + e^{-i2\pi/3} |\mathbf{1}_3\rangle + e^{i2\pi/3} |\mathbf{2}_3\rangle \\ \sqrt{3}|\mathbf{r}^2\rangle &= |\mathbf{0}_3\rangle + e^{i2\pi/3} |\mathbf{1}_3\rangle + e^{-i2\pi/3} |\mathbf{2}_3\rangle \end{aligned}$$

Inverting *O-C* is easy: just  $\dagger$ -conjugate! (and norm by  $\frac{1}{3}$ )

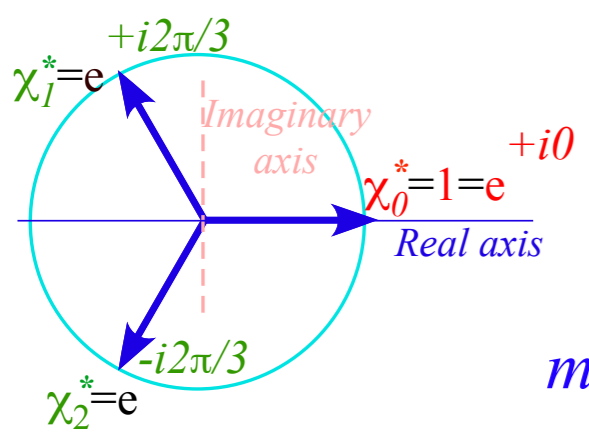
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$$\begin{aligned} \mathbf{P}^{(0)} &= \frac{1}{3}(\mathbf{r}^0 + \mathbf{r}^1 + \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2) \\ \mathbf{P}^{(1)} &= \frac{1}{3}(\mathbf{r}^0 + \chi_1^* \mathbf{r}^1 + \chi_2^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{+i2\pi/3} \mathbf{r}^1 + e^{-i2\pi/3} \mathbf{r}^2) \\ \mathbf{P}^{(2)} &= \frac{1}{3}(\mathbf{r}^0 + \chi_2^* \mathbf{r}^1 + \chi_1^* \mathbf{r}^2) = \frac{1}{3}(\mathbf{1} + e^{-i2\pi/3} \mathbf{r}^1 + e^{+i2\pi/3} \mathbf{r}^2) \end{aligned}$$

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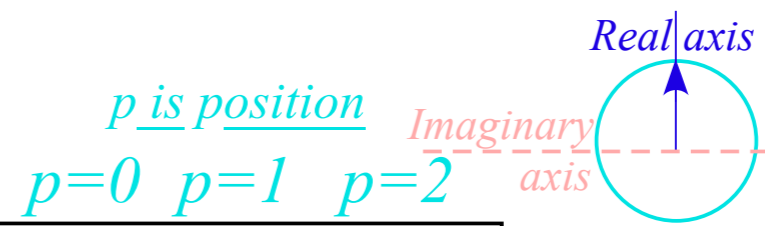
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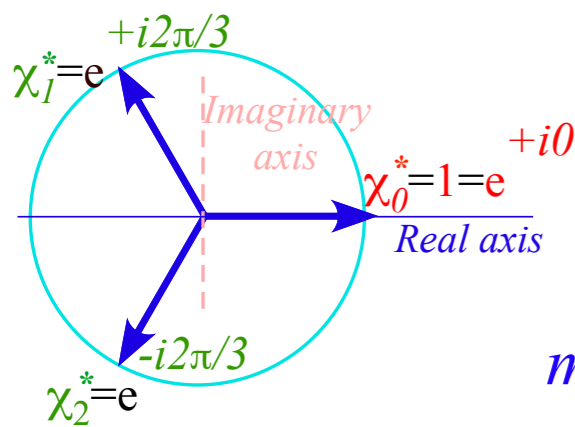
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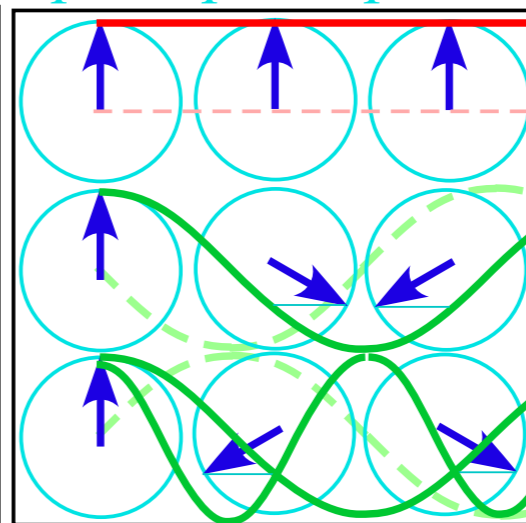
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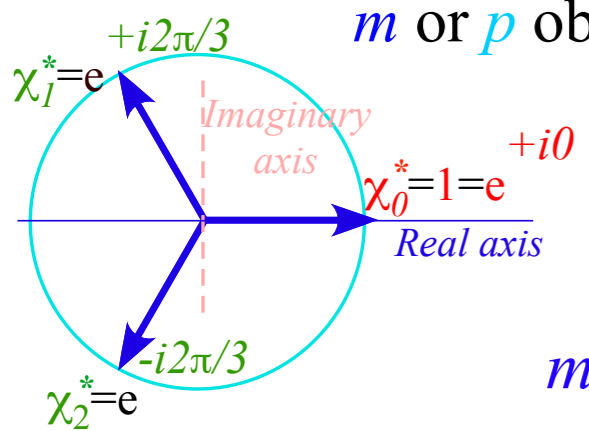
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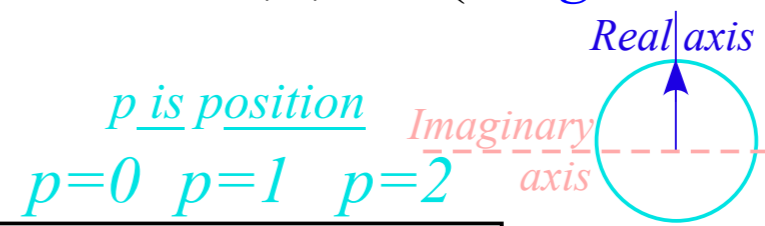
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# Comparing wave function operator algebra to bra-ket algebra

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$$\mathbf{x}_p = L \cdot \mathbf{p}$$

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$$k_m = 2\pi m / 3L = 2\pi / \lambda_m$$

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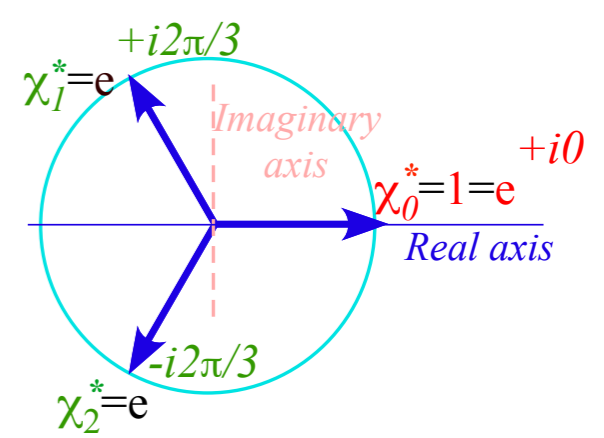
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# Modular quantum number arithmetic



Two distinct types of modular “quantum” numbers:

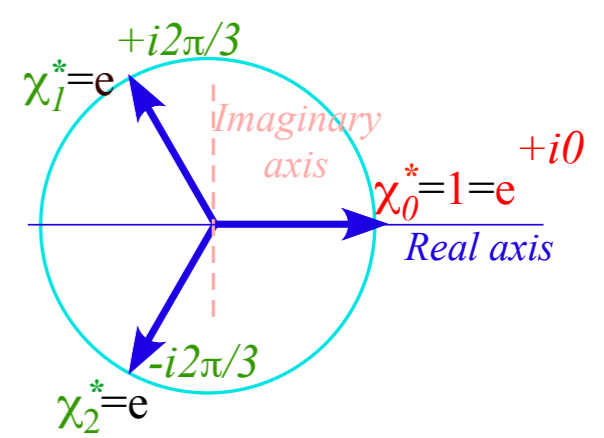
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$m$  or  $p$  obey *modular arithmetic* so sums or products  $=0,1,\text{ or }2$  (*integers-modulo-3*)

For example, for  $m=2$  and  $p=2$  the number  $(\rho_m)^p = (e^{im2\pi/3})^p$  is  $e^{imp \cdot 2\pi/3} = e^{i4 \cdot 2\pi/3} = e^{i1 \cdot 2\pi/3} = e^{i3 \cdot 2\pi/3} = e^{i2\pi/3} = \rho_1$ .

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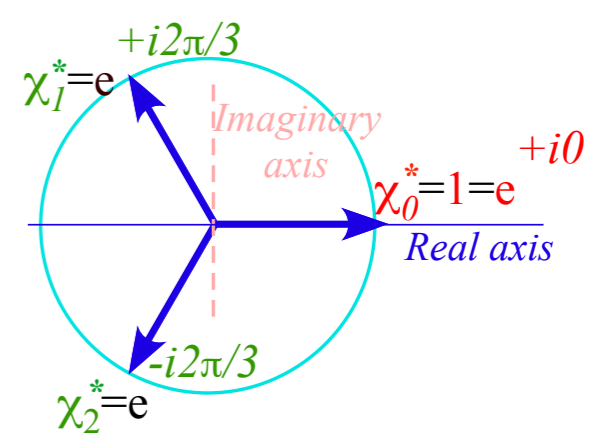
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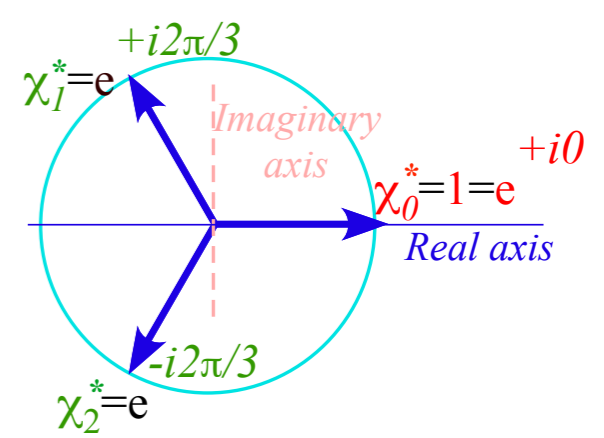
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Thus,  $(\rho_2)^2 = \rho_1$ . Also,  $5 \bmod 3 = 2$  so  $(\rho_1)^5 = \rho_2$ , and  $6 \bmod 3 = 0$  so  $(\rho_1)^6 = \rho_0$ .

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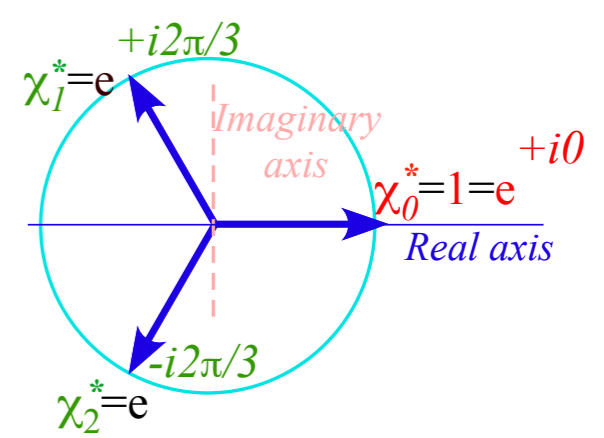
For example, for  $m=2$  and  $p=2$  the number  $(\rho_m)^p = (e^{im2\pi/3})^p$  is  $e^{imp \cdot 2\pi/3} = e^{i4 \cdot 2\pi/3} = e^{i1 \cdot 2\pi/3} e^{i3 \cdot 2\pi/3} = e^{i2\pi/3} = \rho_1$ .

That is,  $(2\text{-times-}2) \bmod 3$  is not  $4$  but  $1$  ( $4 \bmod 3 = 1$ ), the remainder of  $4$  divided by  $3$ .

Thus,  $(\rho_2)^2 = \rho_1$ . Also,  $5 \bmod 3 = 2$  so  $(\rho_1)^5 = \rho_2$ , and  $6 \bmod 3 = 0$  so  $(\rho_1)^6 = \rho_0$ .

Other examples:  $-1 \bmod 3 = 2$  [ $(\rho_1)^{-1} = (\rho_{-1})^1 = \rho_2$ ] and  $-2 \bmod 3 = 1$ .

# Modular quantum number arithmetic



Two distinct types of modular “quantum” numbers:

$p=0,1,\text{ or }2$  is *power*  $p$  of operator  $\mathbf{r}^p$  labeling oscillator *position point*  $p$

$m=0,1,\text{ or }2$  that is the *mode momentum*  $m$  of waves

$m$  or  $p$  obey *modular arithmetic* so sums or products  $=0,1,\text{ or }2$  (*integers-modulo-3*)

For example, for  $m=2$  and  $p=2$  the number  $(\rho_m)^p = (e^{im2\pi/3})^p$  is  $e^{imp \cdot 2\pi/3} = e^{i4 \cdot 2\pi/3} = e^{i1 \cdot 2\pi/3} e^{i3 \cdot 2\pi/3} = e^{i2\pi/3} = \rho_1$ .

That is,  $(2\text{-times-}2) \bmod 3$  is not 4 but 1 ( $4 \bmod 3 = 1$ ), the remainder of 4 divided by 3.

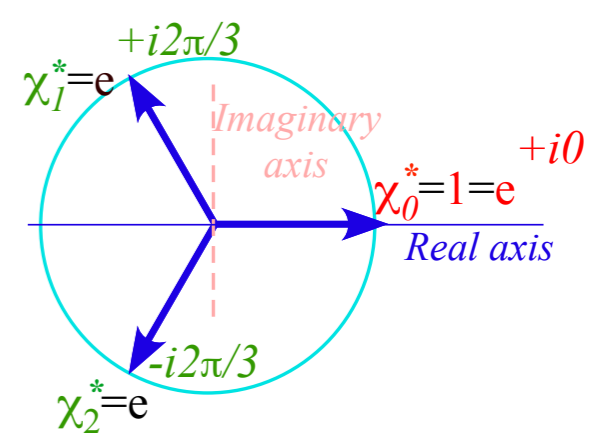
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Other examples:  $-1 \bmod 3 = 2$  [ $(\rho_1)^{-1} = (\rho_{-1})^1 = \rho_2$ ] and  $-2 \bmod 3 = 1$ .

Imagine going around ring reading off address points  $p = \dots 0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2, \dots$

..for regular integer points  $\dots -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, \dots$

# Modular quantum number arithmetic



Two distinct types of modular “quantum” numbers:

$p=0,1, or  $2$  is *power*  $p$  of operator  $\mathbf{r}^p$  labeling oscillator *position point*  $p$$

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For example, for  $m=2$  and  $p=2$  the number  $(\rho_m)^p=(e^{im2\pi/3})^p$  is  $e^{imp\cdot 2\pi/3}=e^{i4\cdot 2\pi/3}=e^{i1\cdot 2\pi/3}=e^{i2\pi/3}=\rho_1$ .

That is,  $(2\text{-times-}2) \bmod 3$  is not  $4$  but  $1$  ( $4 \bmod 3=1$ ), the remainder of  $4$  divided by  $3$ .

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Other examples:  $-1 \bmod 3=2$  [ $(\rho_1)^{-1}=(\rho_{-1})^1=\rho_2$ ] and  $-2 \bmod 3=1$ .

Imagine going around ring reading off address points  $p=\dots 0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2, \dots$

..for regular integer points  $\dots -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, \dots$

$e^{imp2\pi/3}$  must always equal  $e^{i(mp \bmod 3)2\pi/3}$ .

$$(\rho_m)^p=(e^{im2\pi/3})^p = e^{imp\cdot 2\pi/3}=\rho_{mp} = e^{i(mp \bmod 3)2\pi/3}=\rho_{mp \bmod 3}$$

$C_3$   $\mathbf{g}^\dagger \mathbf{g}$ -product-table and basic group representation theory

$C_3$   $\mathbf{H}$ -and- $\mathbf{r}^p$ -matrix representations and conjugation symmetry

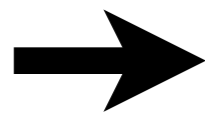
$C_3$  Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations

$C_3$  character table and modular labeling

Ortho-completeness inversion for operators and states

Comparing wave function operator algebra to bra-ket algebra

Modular quantum number arithmetic



$C_3$ -group jargon and structure of various tables

$C_3$  Eigenvalues and wave dispersion functions

Standing waves vs Moving waves

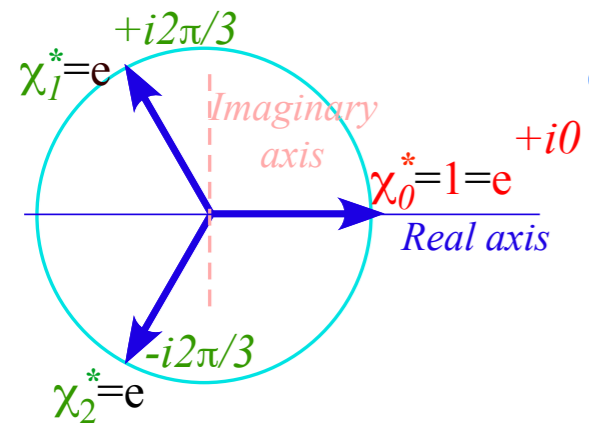
$C_6$  Spectral resolution: 6<sup>th</sup> roots of unity and higher

Complete sets of coupling parameters and Fourier dispersion

Gauge shifts due to complex coupling



# $C_3$ -group jargon and structure of various tables



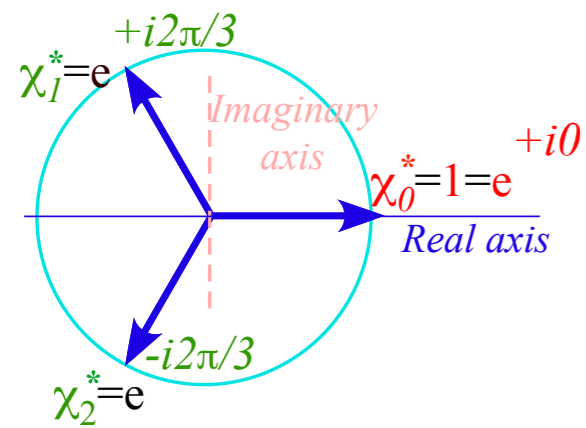
$C_3$ -group  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$ -table

obeyed by  $\{\chi_0=1, \chi_1=e^{-i2\pi/3}, \chi_2=e^{+i2\pi/3}\}$

$C_3$	$\mathbf{r}^0=1$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=1$	1	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	1	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	1

$C_3$	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	$\chi_0$	$\chi_1$	$\chi_2$
$\chi_2=\chi_1^{-1}$	$\chi_2$	$\chi_0$	$\chi_1$
$\chi_1=\chi_2^{-2}$	$\chi_1$	$\chi_2$	$\chi_0$

# $C_3$ -group jargon and structure of various tables



$C_3$ -group  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$ -table  
 obeyed by  $\{\chi_0=1, \chi_1=e^{-i2\pi/3}, \chi_2=e^{+i2\pi/3}\}$

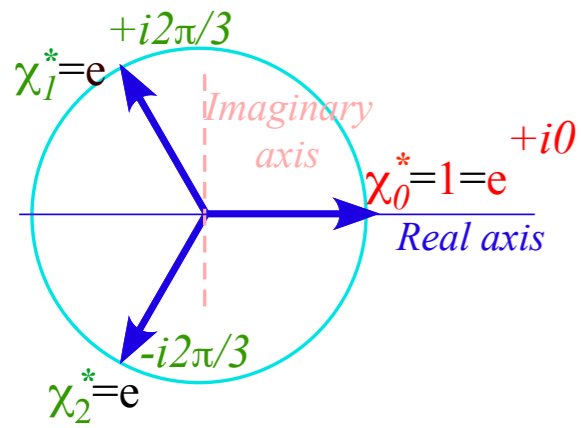
Set  $\{\chi_0, \chi_1, \chi_2\}$  is an  
 irreducible representation  
 (irrep) of  $C_3$

$$\{D(\mathbf{r}^0)=\chi_0, D(\mathbf{r}^1)=\chi_1, D(\mathbf{r}^2)=\chi_2\}$$

$C_3$	$\mathbf{r}^0=1$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=1$	1	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	1	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	1

$C_3$	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	$\chi_0$	$\chi_1$	$\chi_2$
$\chi_2=\chi_1^{-1}$	$\chi_2$	$\chi_0$	$\chi_1$
$\chi_1=\chi_2^{-2}$	$\chi_1$	$\chi_2$	$\chi_0$

# $C_3$ -group jargon and structure of various tables



$C_3$ -group  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$ -table  
 obeyed by  $\{\chi_0=1, \chi_1=e^{-i2\pi/3}, \chi_2=e^{+i2\pi/3}\}$

Set  $\{\chi_0, \chi_1, \chi_2\}$  is an  
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$$\{D(\mathbf{r}^0)=\chi_0, D(\mathbf{r}^1)=\chi_1, D(\mathbf{r}^2)=\chi_2\}$$

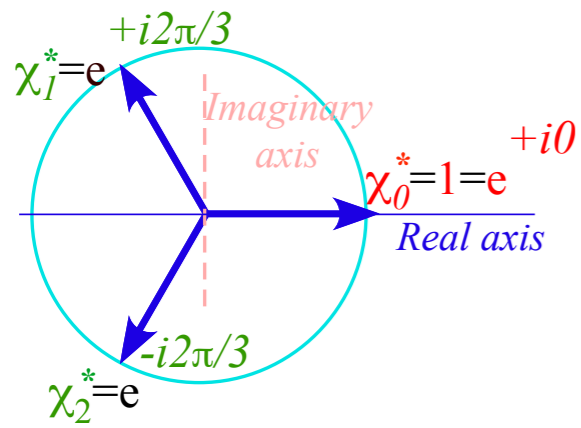
$C_3$	$\mathbf{r}^0=1$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=1$	1	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	1	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	1

$C_3$	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	$\chi_0$	$\chi_1$	$\chi_2$
$\chi_2=\chi_1^{-1}$	$\chi_2$	$\chi_0$	$\chi_1$
$\chi_1=\chi_2^{-2}$	$\chi_1$	$\chi_2$	$\chi_0$

In fact, all three irreps  $\{D^{(0)}, D^{(1)}, D^{(2)}\}$  listed in character table obey  $C_3$ -group table

$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$
$D^{(0)}(\mathbf{g})$	$\chi_0^{(0)}$	$\chi_1^{(0)}$	$\chi_2^{(0)}$	$D^{(0)}(\mathbf{g})$	1	1	1
$D^{(1)}(\mathbf{g})$	$\chi_0^{(1)}$	$\chi_1^{(1)}$	$\chi_2^{(1)}$	$D^{(1)}(\mathbf{g})$	1	$e^{-\frac{2\pi i}{3}}$	$e^{+\frac{2\pi i}{3}}$
$D^{(2)}(\mathbf{g})$	$\chi_0^{(2)}$	$\chi_1^{(2)}$	$\chi_2^{(2)}$	$D^{(2)}(\mathbf{g})$	1	$e^{+\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$

# $C_3$ -group jargon and structure of various tables



$C_3$ -group  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$ -table  
 obeyed by  $\{\chi_0=1, \chi_1=e^{-i2\pi/3}, \chi_2=e^{+i2\pi/3}\}$

Set  $\{\chi_0, \chi_1, \chi_2\}$  is an  
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$$\{D(\mathbf{r}^0)=\chi_0, D(\mathbf{r}^1)=\chi_1, D(\mathbf{r}^2)=\chi_2\}$$

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$\mathbf{r}^0=1$	1	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	1	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	1

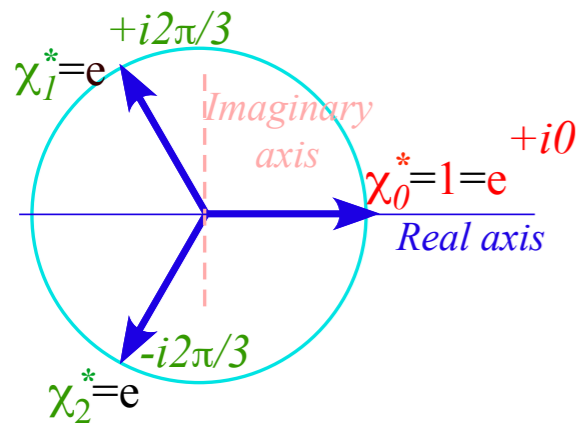
$C_3$	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	$\chi_0$	$\chi_1$	$\chi_2$
$\chi_2=\chi_1^{-1}$	$\chi_2$	$\chi_0$	$\chi_1$
$\chi_1=\chi_2^{-2}$	$\chi_1$	$\chi_2$	$\chi_0$

In fact, all **three** irreps  $\{D^{(0)}, D^{(1)}, D^{(2)}\}$  listed in character table obey  $C_3$ -group table

$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$
$D^{(0)}(\mathbf{g})$	$\chi_0^{(0)}$	$\chi_1^{(0)}$	$\chi_2^{(0)}$	$D^{(0)}(\mathbf{g})$	1	1	1
$D^{(1)}(\mathbf{g})$	$\chi_0^{(1)}$	$\chi_1^{(1)}$	$\chi_2^{(1)}$	$D^{(1)}(\mathbf{g})$	1	$e^{-\frac{2\pi i}{3}}$	$e^{+\frac{2\pi i}{3}}$
$D^{(2)}(\mathbf{g})$	$\chi_0^{(2)}$	$\chi_1^{(2)}$	$\chi_2^{(2)}$	$D^{(2)}(\mathbf{g})$	1	$e^{+\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$

The *identity irrep*  
 $D^{(0)}=\{1,1,1\}$   
 obeys any group table.

# $C_3$ -group jargon and structure of various tables



$C_3$ -group  $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$ -table  
 obeyed by  $\{\chi_0=1, \chi_1=e^{-i2\pi/3}, \chi_2=e^{+i2\pi/3}\}$

Set  $\{\chi_0, \chi_1, \chi_2\}$  is an  
 irreducible representation  
 (irrep) of  $C_3$

$$\{D(\mathbf{r}^0)=\chi_0, D(\mathbf{r}^1)=\chi_1, D(\mathbf{r}^2)=\chi_2\}$$

$C_3$	$\mathbf{r}^0=1$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=1$	1	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	1	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	1

$C_3$	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	$\chi_0$	$\chi_1$	$\chi_2$
$\chi_2=\chi_1^{-1}$	$\chi_2$	$\chi_0$	$\chi_1$
$\chi_1=\chi_2^{-2}$	$\chi_1$	$\chi_2$	$\chi_0$

In fact, all **three** irreps  $\{D^{(0)}, D^{(1)}, D^{(2)}\}$  listed in character table obey  $C_3$ -group table

$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{g} =$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$
$D^{(0)}(\mathbf{g})$	$\chi_0^{(0)}$	$\chi_1^{(0)}$	$\chi_2^{(0)}$	$D^{(0)}(\mathbf{g})$	1	1	1
$D^{(1)}(\mathbf{g})$	$\chi_0^{(1)}$	$\chi_1^{(1)}$	$\chi_2^{(1)}$	$D^{(1)}(\mathbf{g})$	1	$e^{-\frac{2\pi i}{3}}$	$e^{+\frac{2\pi i}{3}}$
$D^{(2)}(\mathbf{g})$	$\chi_0^{(2)}$	$\chi_1^{(2)}$	$\chi_2^{(2)}$	$D^{(2)}(\mathbf{g})$	1	$e^{+\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$

The *identity irrep*  
 $D^{(0)}=\{1,1,1\}$   
 obeys any group table.

Irrep  $D^{(2)}=\{1, e^{+i2\pi/3}, e^{-i2\pi/3}\}$  is a conjugate irrep to  $D^{(1)}=\{1, e^{-i2\pi/3}, e^{+i2\pi/3}\}$

$$D^{(2)}=D^{(1)*}$$

*C<sub>3</sub>  $\mathbf{g}^\dagger\mathbf{g}$ -product-table and basic group representation theory*

*C<sub>3</sub>  $\mathbf{H}$ -and- $\mathbf{r}^p$ -matrix representations and conjugation symmetry*

*C<sub>3</sub> Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations*

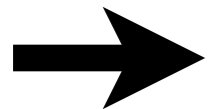
*C<sub>3</sub> character table and modular labeling*

*Ortho-completeness inversion for operators and states*

*Comparing wave function operator algebra to bra-ket algebra*

*Modular quantum number arithmetic*

*C<sub>3</sub>-group jargon and structure of various tables*



*C<sub>3</sub> Eigenvalues and wave dispersion functions*

*Standing waves vs Moving waves*

*C<sub>6</sub> Spectral resolution: 6<sup>th</sup> roots of unity and higher*

*Complete sets of coupling parameters and Fourier dispersion*

*Gauge shifts due to complex coupling*

# *Eigenvalues and wave dispersion functions*

$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

# *Eigenvalues and wave dispersion functions*

$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}})$$

*(Here we assume  $r_1 = r_2 = r$ )  
(all-real)*



# Eigenvalues and wave dispersion functions

$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

(Here we assume  $r_1 = r_2 = r$ )  
(all-real)

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

# Eigenvalues and wave dispersion functions

$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

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$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

Quantum  $\mathbf{H}$ -values:

$$\begin{pmatrix} r_0 & r & r \\ r & r_0 & r \\ r & r & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = (r_0 + 2r \cos(\frac{2m\pi}{3})) \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

# Eigenvalues and wave dispersion functions - Moving waves

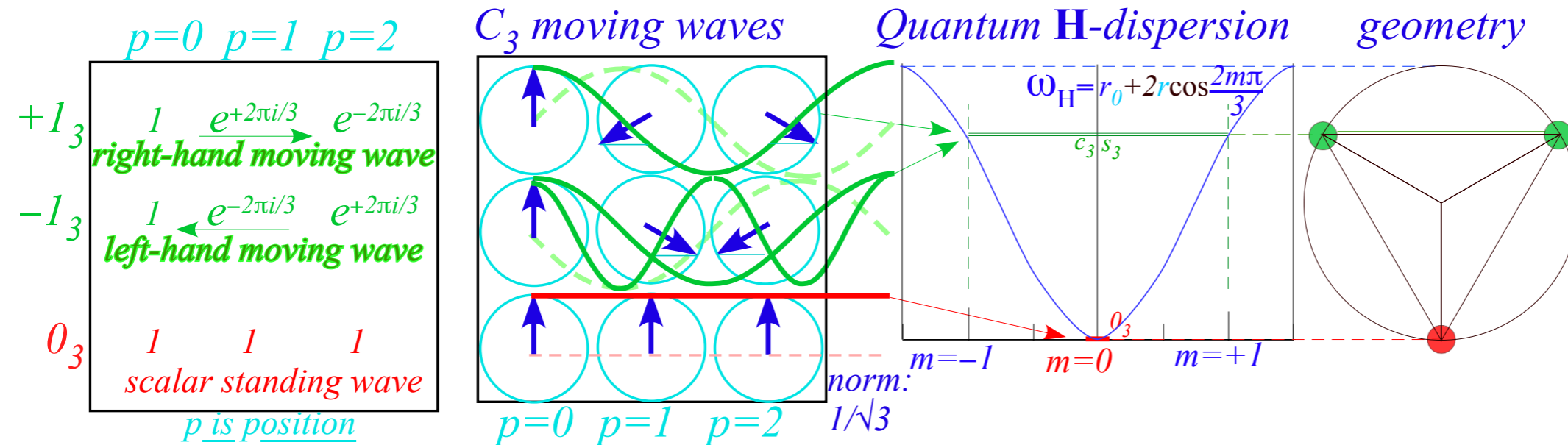
$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

(Here we assume  $r_1 = r_2 = r$ )  
(all-real)

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

Quantum  $\mathbf{H}$ -values:

$$\begin{pmatrix} r_0 & r & r \\ r & r_0 & r \\ r & r & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = (r_0 + 2r \cos(\frac{2m\pi}{3})) \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$



# Eigenvalues and wave dispersion functions - Moving waves

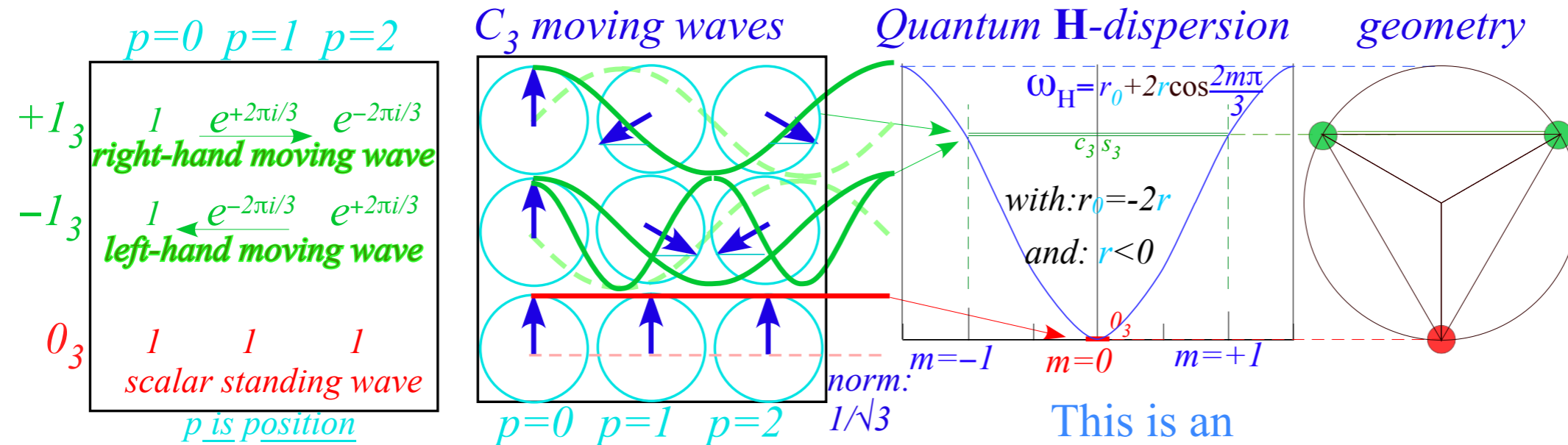
$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

(Here we assume  $r_1 = r_2 = r$ )  
(all-real)

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i2\frac{m\pi}{3}} + e^{-i2\frac{m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

Quantum  $\mathbf{H}$ -values:

$$\begin{pmatrix} r_0 & r & r \\ r & r_0 & r \\ r & r & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = (r_0 + 2r \cos(\frac{2m\pi}{3})) \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$



This is an  
exciton-like  
dispersion function  
 $\omega_H(m) = r_0(1 - \cos \frac{2m\pi}{3})$

$$\omega_H(m) \sim 2r_0 \left(\frac{m\pi}{3}\right)^2$$

# Eigenvalues and wave dispersion functions - Moving waves

$$\langle m | \mathbf{H} | m \rangle = \langle m | r_0 \mathbf{r}^0 + r_1 \mathbf{r}^1 + r_2 \mathbf{r}^2 | m \rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

(Here we assume  $r_1 = r_2 = r$ )  
(all-real)

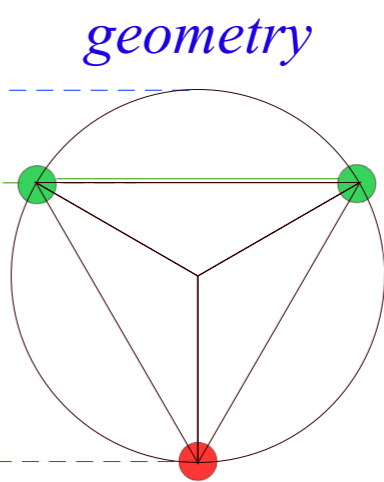
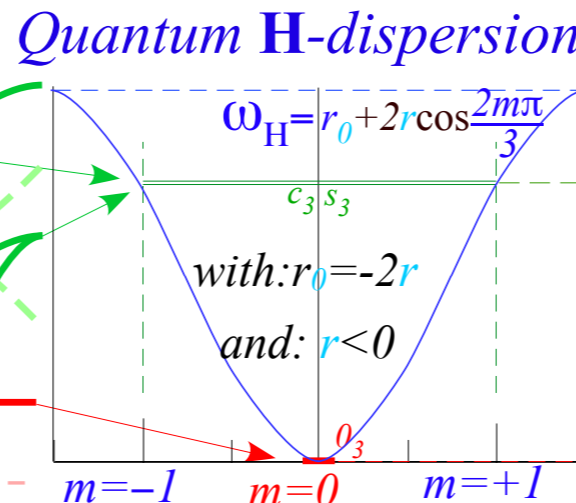
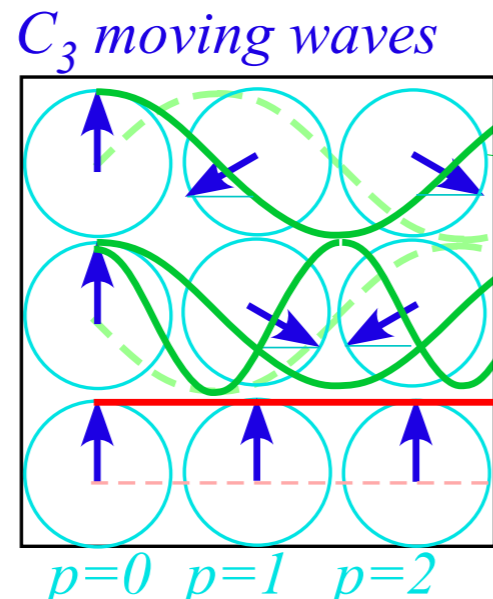
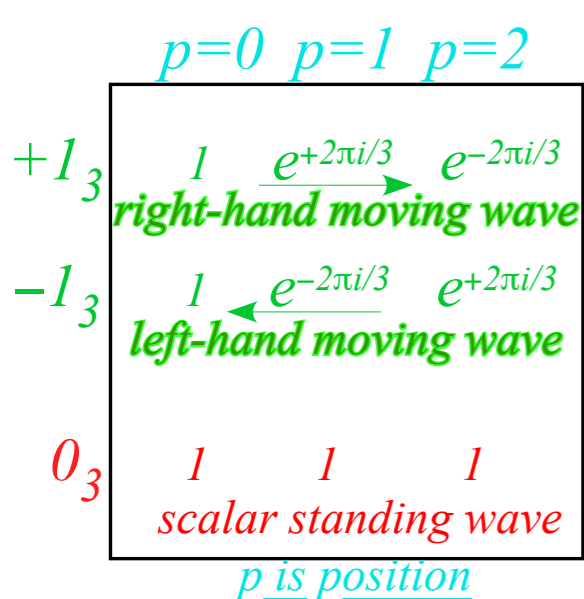
$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

Quantum  $\mathbf{H}$ -values:

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This is an  
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 $\omega_H(m) = r_0(1 - \cos \frac{2m\pi}{3})$

$$\omega_H(m) \sim 2r_0 \left(\frac{m\pi}{3}\right)^2$$

# Eigenvalues and wave dispersion functions - Moving waves

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$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}) = r_0 + 2r \cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0 + 2r & (\text{for } m = 0) \\ r_0 - r & (\text{for } m = \pm 1) \end{cases}$$

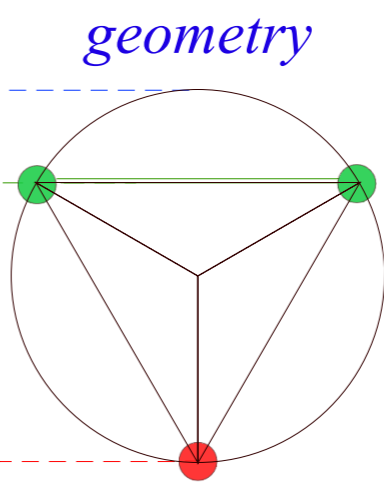
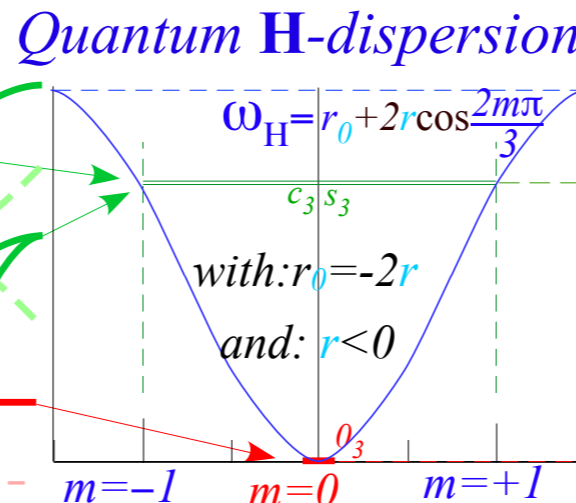
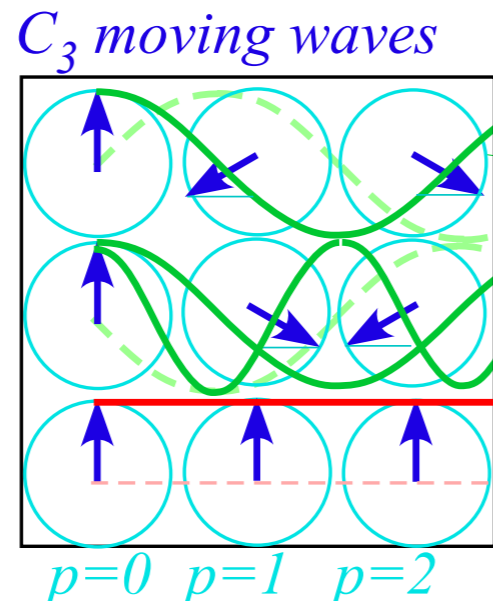
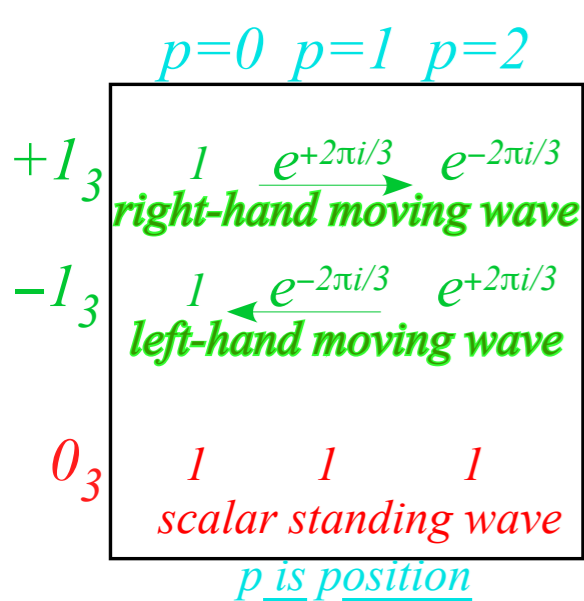
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$$\begin{pmatrix} r_0 & r & r \\ r & r_0 & r \\ r & r & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = (r_0 + 2r \cos(\frac{2m\pi}{3})) \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

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K-eigenvalue...  
needs Square-Root  
to be a frequency



This is an  
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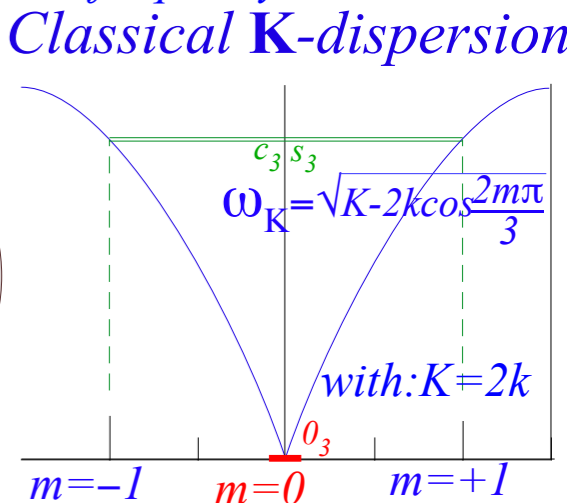
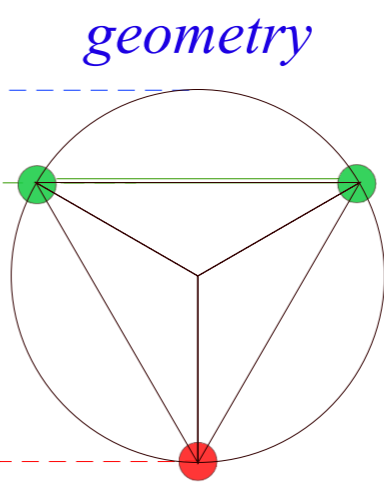
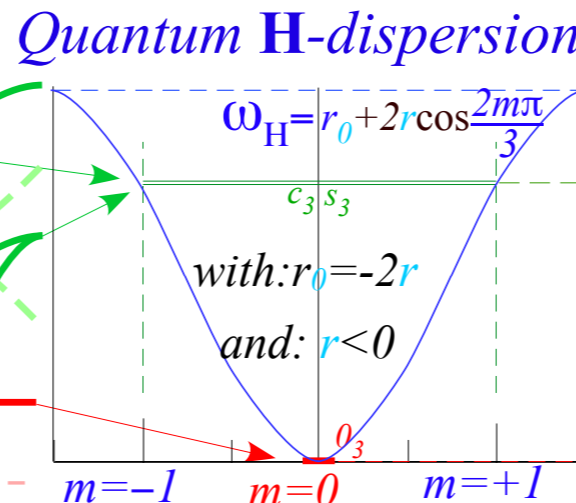
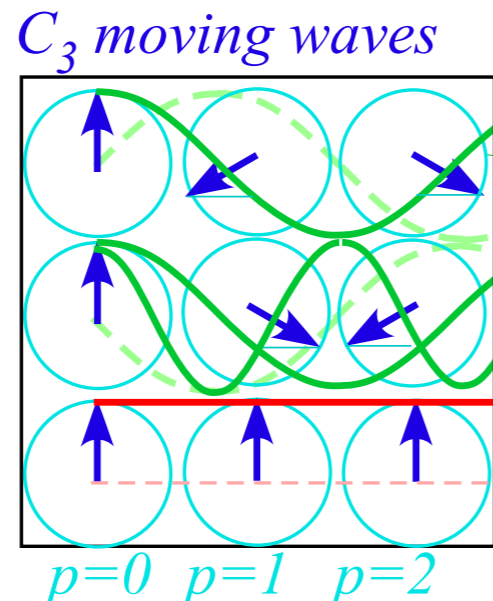
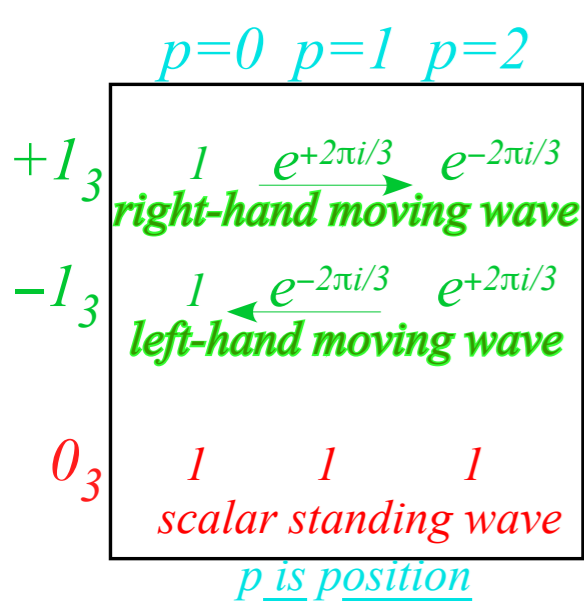
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exciton-like  
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$$\omega_H(m) = r_0(1 - \cos \frac{2m\pi}{3})$$

$\omega_H(m) \sim 2r_0 \left(\frac{m\pi}{3}\right)^2$   
 $\omega_H(m)$  is quadratic for low  $m$   
(long wavelength  $\lambda$ )

This is a  
phonon-like  
dispersion function

$$\omega_K(m) = \sqrt{2k - 2k \cos \frac{2m\pi}{3}}$$

$$= 2\sqrt{k} \sin \frac{m\pi}{3}$$

$\omega_K(m) \sim 2\sqrt{k} \left(\frac{m\pi}{3}\right)^1$   
 $\omega_K(m)$  is linear for low  $m$   
(long wavelength  $\lambda$ )

*C<sub>3</sub>  $\mathbf{g}^\dagger\mathbf{g}$ -product-table and basic group representation theory*

*C<sub>3</sub>  $\mathbf{H}$ -and- $\mathbf{r}^p$ -matrix representations and conjugation symmetry*

*C<sub>3</sub> Spectral resolution: 3<sup>rd</sup> roots of unity and ortho-completeness relations*

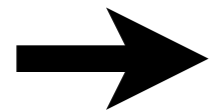
*C<sub>3</sub> character table and modular labeling*

*Ortho-completeness inversion for operators and states*

*Modular quantum number arithmetic*

*C<sub>3</sub>-group jargon and structure of various tables*

*C<sub>3</sub> Eigenvalues and wave dispersion functions*



*Standing waves vs Moving waves*

*C<sub>6</sub> Spectral resolution: 6<sup>th</sup> roots of unity and higher*

*Complete sets of coupling parameters and Fourier dispersion*

*Gauge shifts due to complex coupling*



# Eigenvalues and wave dispersion functions - Standing waves

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Standing waves possible if  $\mathbf{H}$  is all-real (No curly C-stuff allowed!)

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Standing waves possible if  $\mathbf{H}$  is all-real (No curly C-stuff allowed!)

Moving eigenwave	Standing eigenwaves	$\mathbf{H}$ - eigenfrequencies	$\mathbf{K}$ - eigenfrequencies
$ (+1)_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{+i2\pi/3} \\ e^{-i2\pi/3} \end{pmatrix}$ States $ (+)\rangle$ and $ (-)\rangle$ in any mixtures are still stationary due to $(\pm)$ -degeneracy ( $\cos(+x) = \cos(-x)$ )	$ c_3\rangle = \frac{ (+1)_3\rangle +  (-1)_3\rangle}{\sqrt{2}} = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$	$\omega^{(+1)_3} = r_0 + 2r \cos(\frac{+2m\pi}{3}) = r_0 - r$	$\sqrt{k_0 - 2k \cos(\frac{+2m\pi}{3})} = \sqrt{k_0 + k}$
$ (-1)_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-i2\pi/3} \\ e^{+i2\pi/3} \end{pmatrix}$	$ s_3\rangle = \frac{ (+1)_3\rangle -  (-1)_3\rangle}{i\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ +1 \\ -1 \end{pmatrix}$	$\omega^{(-1)_3} = r_0 + 2r \cos(\frac{-2m\pi}{3}) = r_0 - r$	$\sqrt{k_0 - 2k \cos(\frac{-2m\pi}{3})} = \sqrt{k_0 + k}$
	$ 0_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$	$\omega^{(0)_3} = r_0 + 2r$	$\sqrt{k_0 - 2k}$

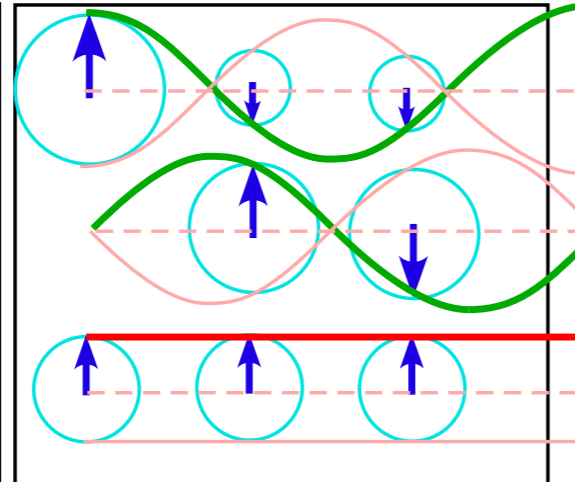
# Eigenvalues and wave dispersion functions - Standing waves

(Possible if  $\mathbf{H}$  is all-real)

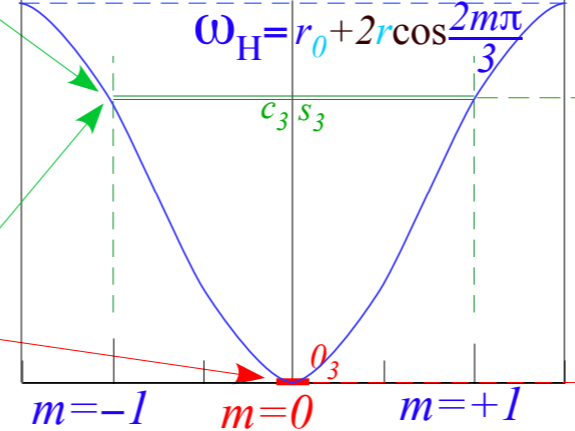
$p=0$   $p=1$   $p=2$

$c_3$	$2/\sqrt{6}$	$-1/\sqrt{6}$	$-1/\sqrt{6}$
	cosine standing wave		
$s_3$	0	$1/\sqrt{2}$	$-1/\sqrt{2}$
	sine standing wave		
$o_3$	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$
	scalar standing wave		

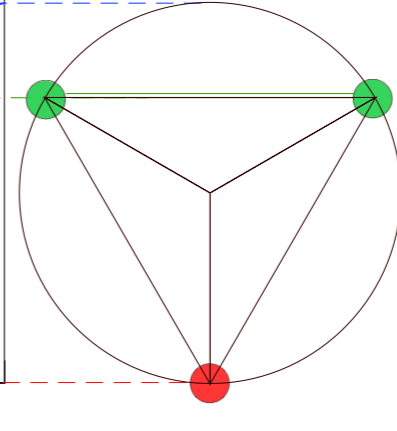
$C_3$  standing waves



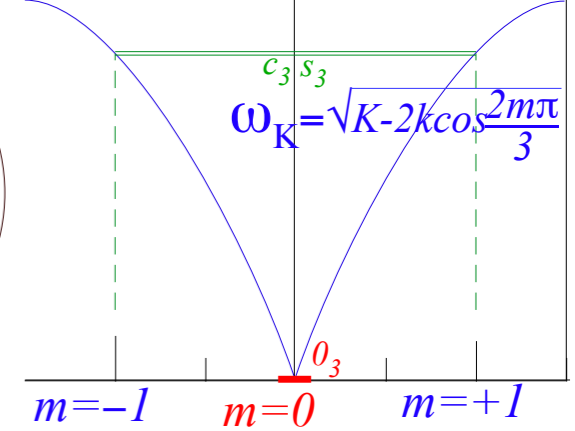
Quantum  $\mathbf{H}$ -dispersion



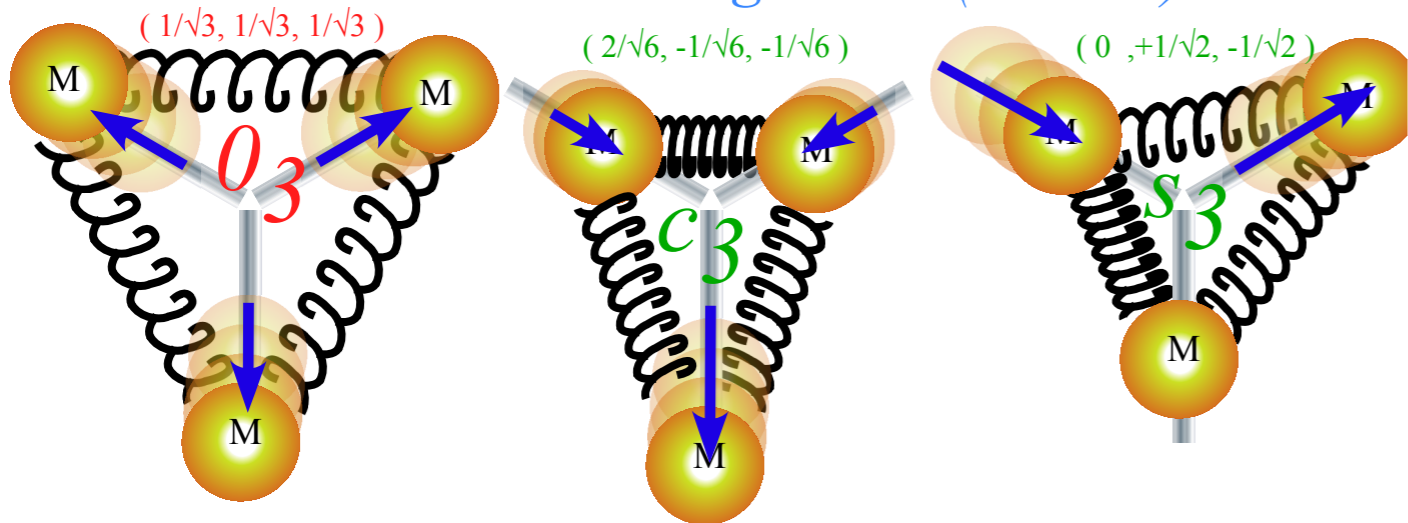
geometry



Classical  $\mathbf{K}$ -dispersion



Radial standing waves (all-real)



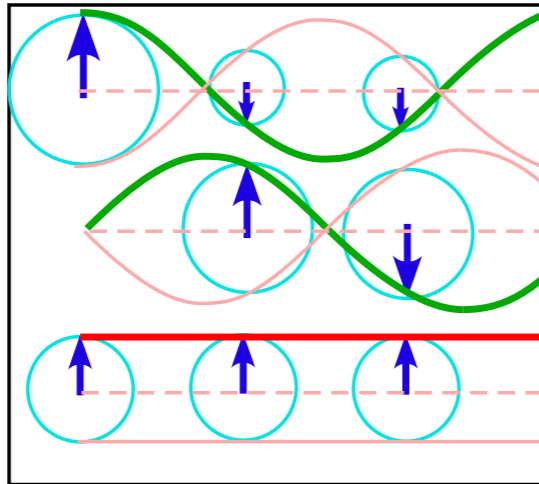
# Eigenvalues and wave dispersion functions - Standing waves

(Possible if  $\mathbf{H}$  is all-real)

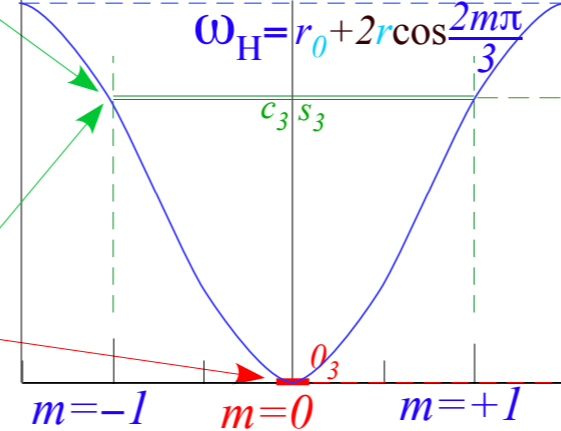
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	scalar standing wave		

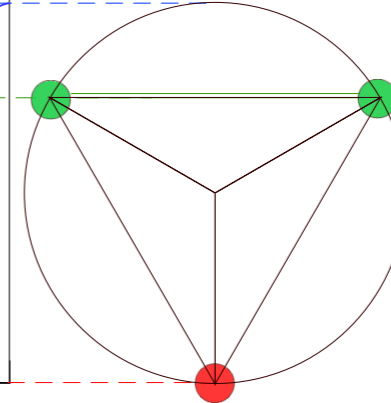
$C_3$  standing waves



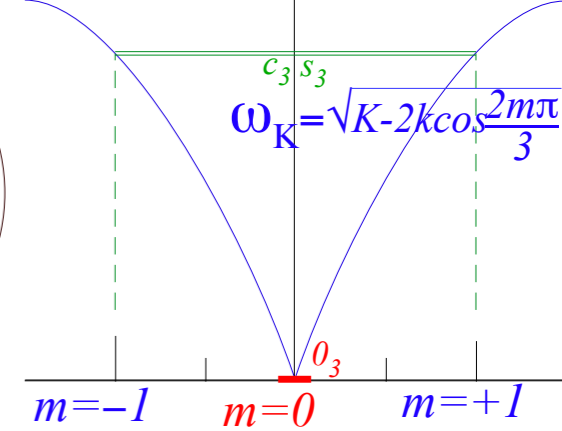
Quantum  $\mathbf{H}$ -dispersion



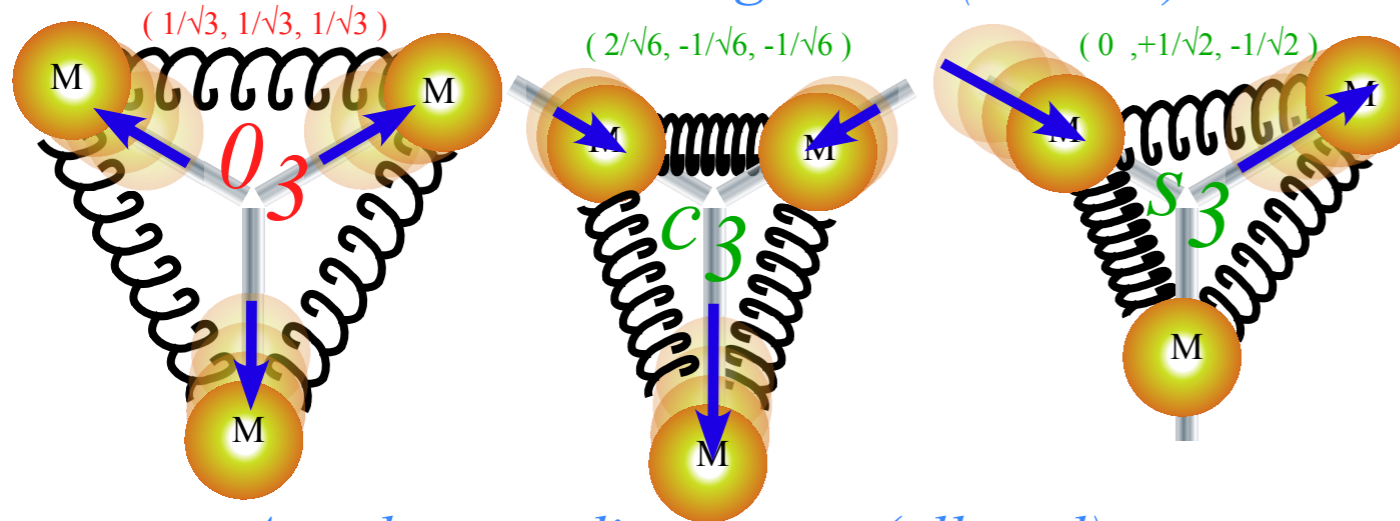
geometry



Classical  $\mathbf{K}$ -dispersion



Radial standing waves (all-real)



Angular standing waves (all-real)

