Group Theory in Quantum Mechanics

Lecture 11 *(2.19.15)*

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: 3rd 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: 6th roots of unity and higher*

- *Complete sets of coupling parameters and Fourier dispersion*
- *Gauge shifts due to complex coupling*

Introduction to C_N *beat dynamics and "Revivals" in Lecture 12*

WebApps used

[WaveIt App](#)

[MolVibes](#)

Review of C_2 spectral resolution for 2D oscillator Lecture 6

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: 3rd roots of unity and ortho-completeness relations
- *C_3 character table and modular labeling*

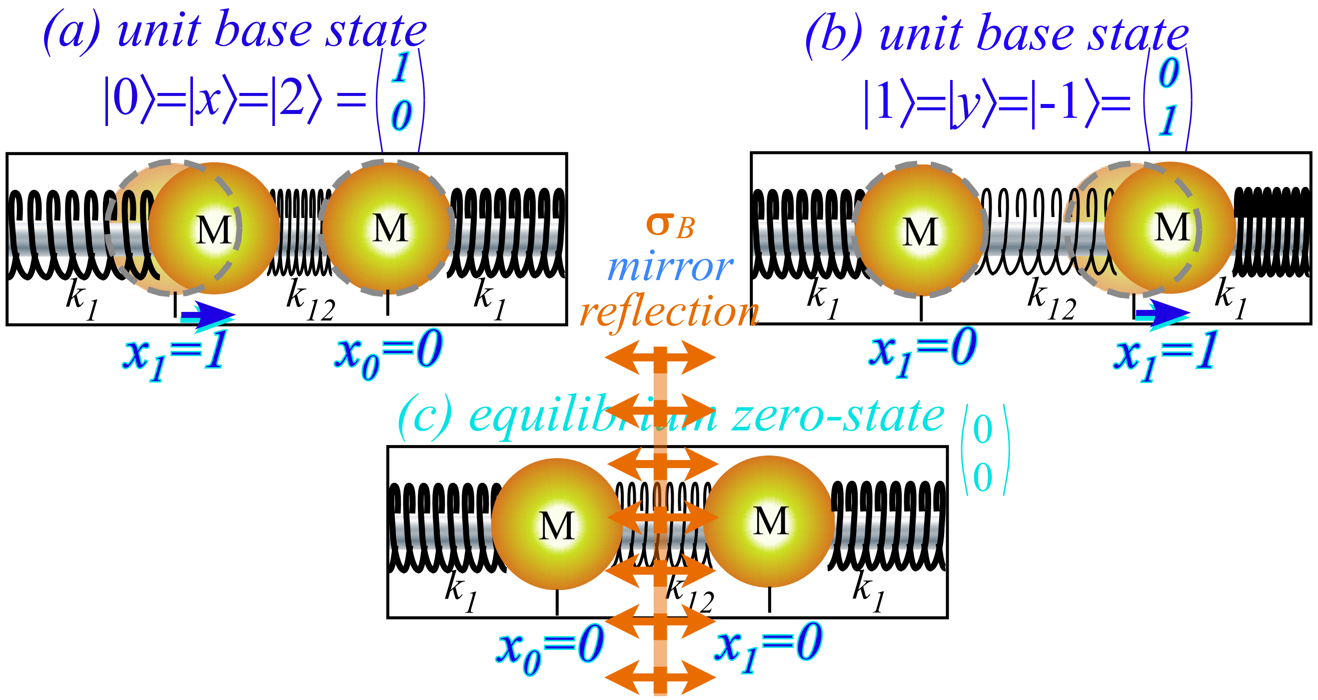
Ortho-completeness inversion for operators and states
- *Modular quantum number arithmetic*
- *C_3-group jargon and structure of various tables*

C_3 Eigenvalues and wave dispersion functions
- *Standing waves vs Moving waves*

C_6 Spectral resolution: 6th 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. $\{x_0,x_1\}$



2D HO Matrix operator equations

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

$$= -\begin{pmatrix}K_{11} & K_{12}\\ K_{21} & K_{22}\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$

$$|\ddot{\mathbf{x}}\rangle \;=\; -\;\mathbf{K}\;|\mathbf{x}\rangle$$

More conventional coordinate notation $\{x_0,x_1\} \longrightarrow \{x_1,x_2\}$

C_2 (Bilateral σ_B reflection) symmetry conditions:

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

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

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

K-matrix is made of its symmetry operators in *group* $C_2=\{\mathbf{1},\sigma_B\}$ with *product table*:

C_2	$\mathbf{1}$	σ_B
$\mathbf{1}$	$\mathbf{1}$	σ_B
σ_B	σ_B	$\mathbf{1}$

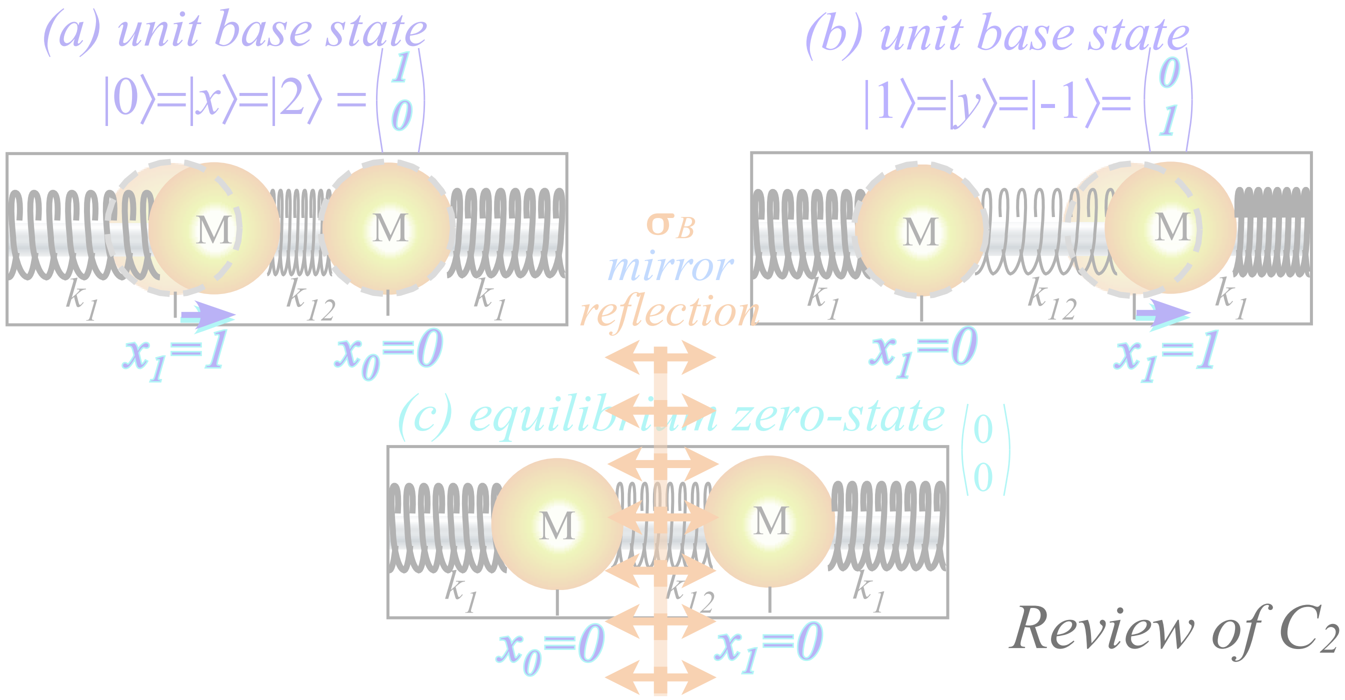
Symmetry *product table* gives C_2 group representations in *group basis* $\{|0\rangle=\mathbf{1}|0\rangle\equiv|\mathbf{1}\rangle \;,\; |1\rangle=\boldsymbol{\sigma}_B|0\rangle\equiv|\sigma_B\rangle\}$

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

Review of C_2 spectral resolution for 2D oscillator Lecture 6 p.11

C_2 Symmetric two-dimensional harmonic oscillators (2DHO)

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



2D HO Matrix operator equations

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

$$=-\begin{pmatrix}K_{11} & K_{12}\\ K_{21} & K_{22}\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$

$$|\ddot{\mathbf{x}}\rangle \quad = \quad -\ \mathbf{K} \quad |\mathbf{x}\rangle$$

More conventional coordinate notation $\{x_0,x_1\}\longrightarrow\{x_1,x_2\}$

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

C_2 (Bilateral σ_B reflection) symmetry conditions:

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

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

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

K-matrix is made of its symmetry operators in group $C_2=\{\mathbf{1},\sigma_B\}$ with product table:

C_2	$\mathbf{1}$	σ_B
$\mathbf{1}$	$\mathbf{1}$	σ_B
σ_B	σ_B	$\mathbf{1}$

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

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

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

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 $\{\mathbf{P}^+,\mathbf{P}^-\}$

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

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

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

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

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

C_2 Symmetric 2DHO eigensolutions

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

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

K-matrix is made of its symmetry operators

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

$C_2(\sigma_B)$ spectrally decomposed into $\{\mathbf{P}^+,\mathbf{P}^-\}$ projectors:

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

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

$$\mathbf{P}^+ = \frac{\mathbf{1}+\sigma_B}{2} = \begin{pmatrix}\frac{1}{2}&\frac{1}{2}\\ \frac{1}{2}&\frac{1}{2}\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\otimes\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\end{pmatrix} = |+\rangle\langle+|$$

factored projectors

$$\mathbf{P}^- = \frac{\mathbf{1}-\sigma_B}{2} = \begin{pmatrix}\frac{1}{2}&-\frac{1}{2}\\ -\frac{1}{2}&\frac{1}{2}\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{pmatrix}\otimes\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}\end{pmatrix} = |-\rangle\langle-|$$

Eigenvalues of σ_B :

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

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

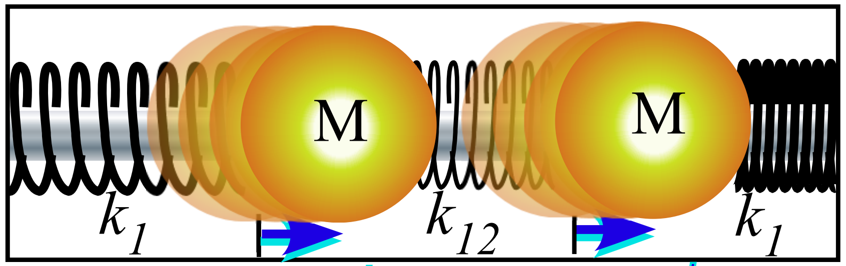
$$\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}k_1+k_{12}&-k_{12}\\-k_{12}&k_1+k_{12}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}\end{pmatrix}=\begin{pmatrix}k_1&0\\0&k_1+2k_{12}\end{pmatrix}$$

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

$$\varepsilon^+(\mathbf{K}) = K-k_{12}, \qquad \varepsilon^-(\mathbf{K}) = K+k_{12}$$

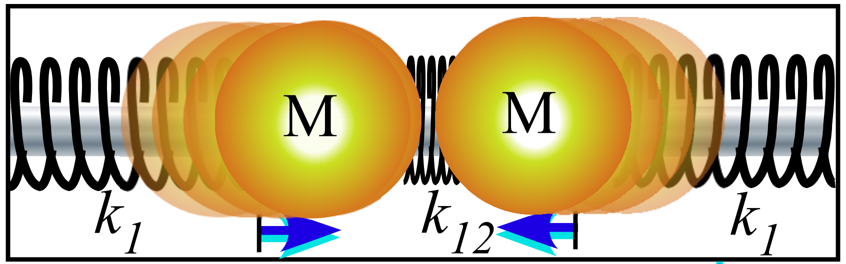
$$= k_1 \qquad\qquad = k_1+2k_{12}$$

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



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

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

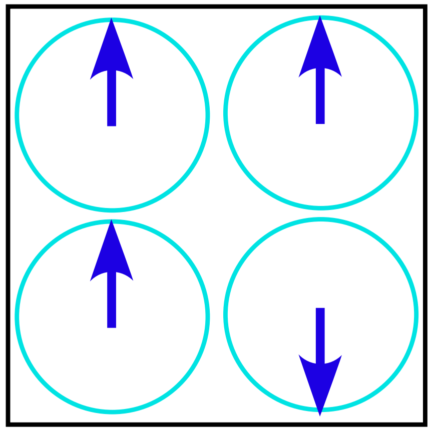


$x_0=1/\sqrt{2}$ $\quad x_1=-1/\sqrt{2}$

C_2 *mode phase character tables*

p is position

	$p=0$	$p=1$
$m=0_2$	1	1
$m=1_2$	1	-1



norm:
$1/\sqrt{2}$

m is wave-number
or "momentum"

(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!)

Review of C_2 spectral resolution for 2D oscillator Lecture 6 p.33

→ 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: 3rd roots of unity and ortho-completeness relations

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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 **g** in the 1st row
with its inverse $\mathbf{g}^\dagger=\mathbf{g}^{-1}$ in the 1st 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	$\mathbf{r}^0=\mathbf{1}$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=\ \mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{1}$

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

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so all *unit* $\mathbf{1}=\mathbf{g}^{-1}\mathbf{g}$ *elements* lie on diagonal.

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

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

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

C₃ **g†g**-*product-table and basic group representation theory*

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

C₃ **g†g**-*product-table*

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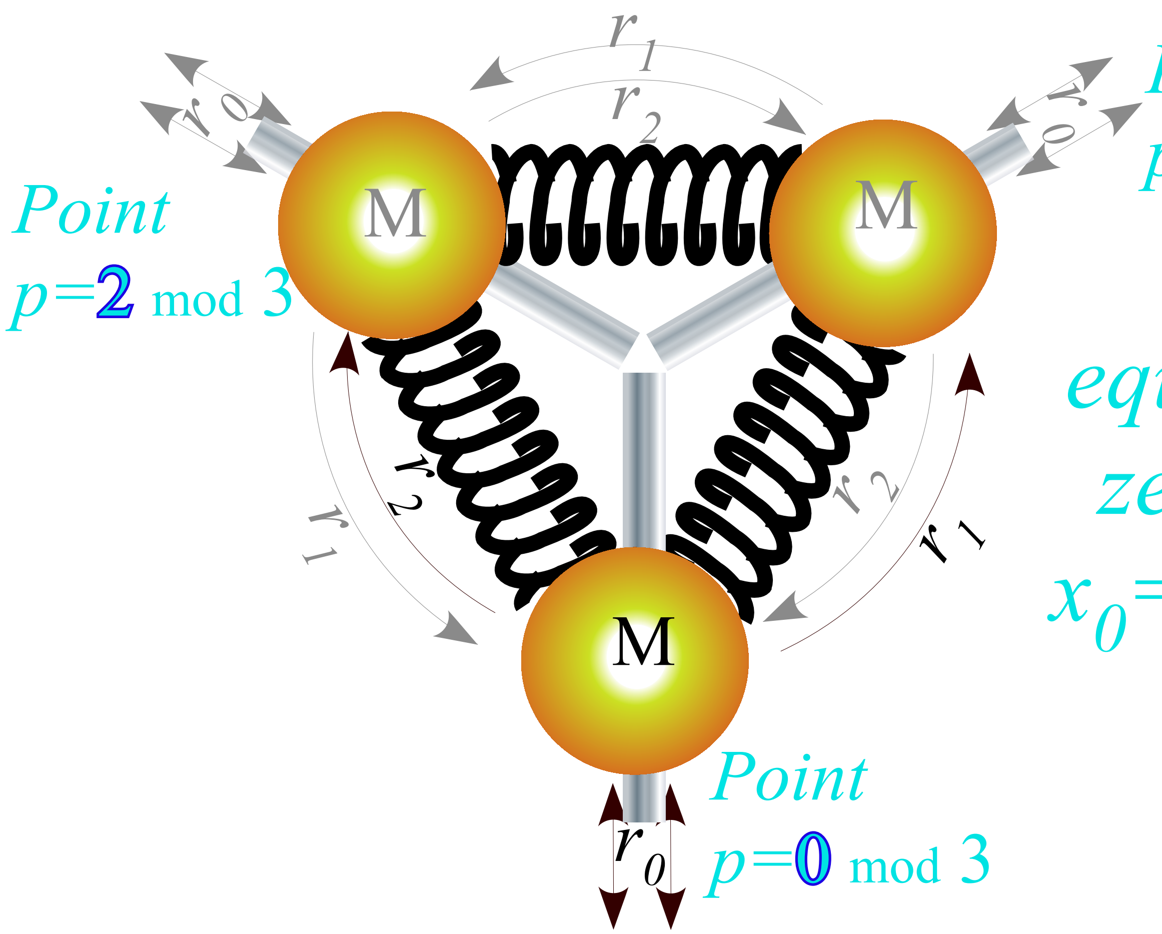
$$\mathbf{H}=\begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + r_1\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} + r_2\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

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

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.



equilibrium zero-state

$$x_0=x_1=x_2=0$$

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

C_3 **g†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 **g†g**-*product-table*
Pairs each operator **g** in the 1st row
with its inverse $\mathbf{g}^\dagger=\mathbf{g}^{-1}$ in the 1st column
so all *unit* $\mathbf{1}=\mathbf{g}^{-1}\mathbf{g}$ *elements* lie on diagonal.

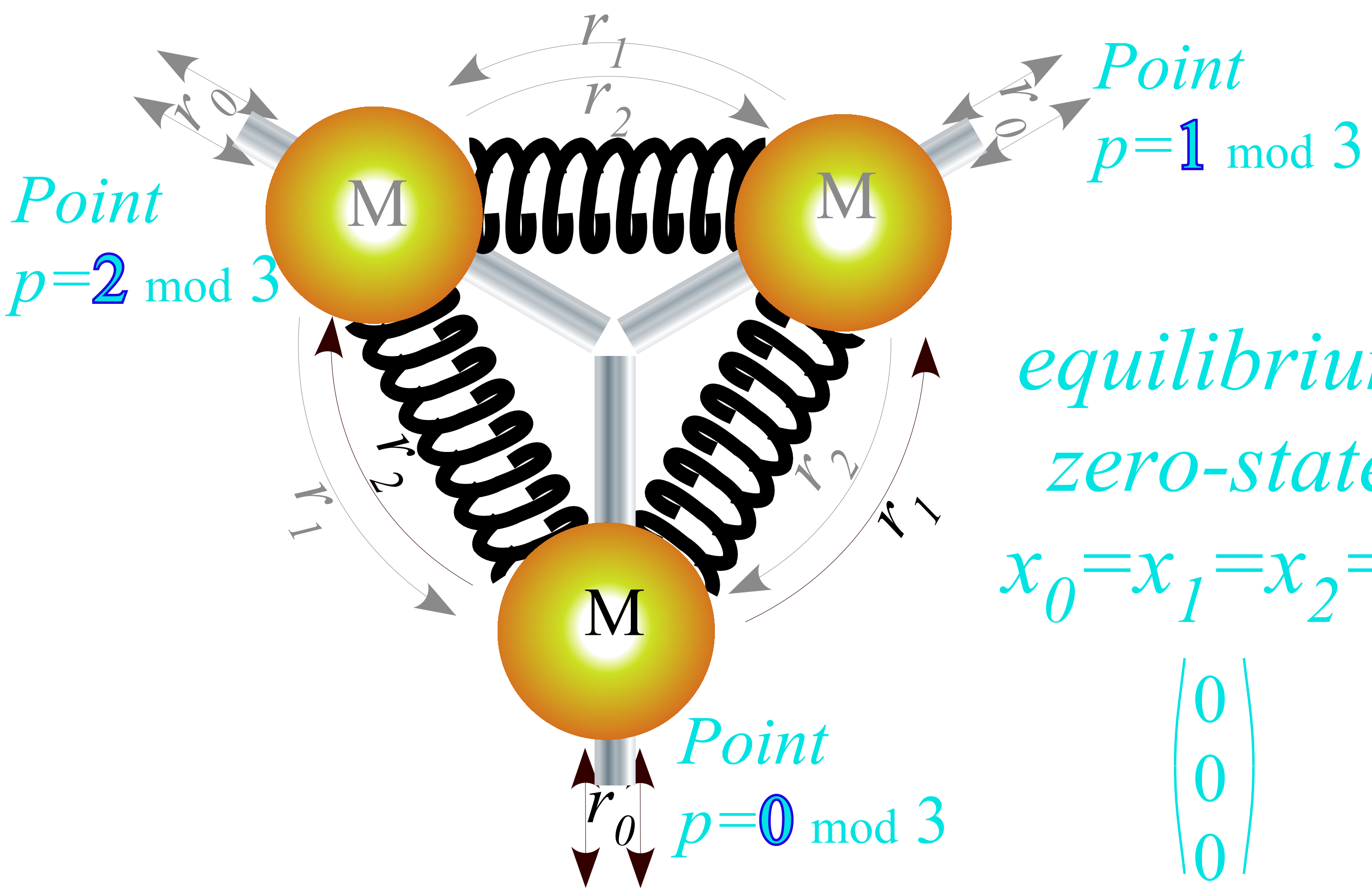
A C_3 **H**-*matrix* is then constructed directly from the **g†g**-*table* and so is each $\mathbf{r}^p$-*matrix representation*.

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

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

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

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.



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

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

C₃ **g†g**-*product-table and basic group representation theory*

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

C₃ **g†g**-*product-table*
Pairs each operator **g** in the 1st row
with its inverse $\mathbf{g}^\dagger=\mathbf{g}^{-1}$ in the 1st column
so all *unit* $\mathbf{1}=\mathbf{g}^{-1}\mathbf{g}$ *elements* lie on diagonal.

A C₃ **H**-*matrix* is then constructed directly from the **g†g**-*table* and so is each $\mathbf{r}^p$-*matrix representation*.

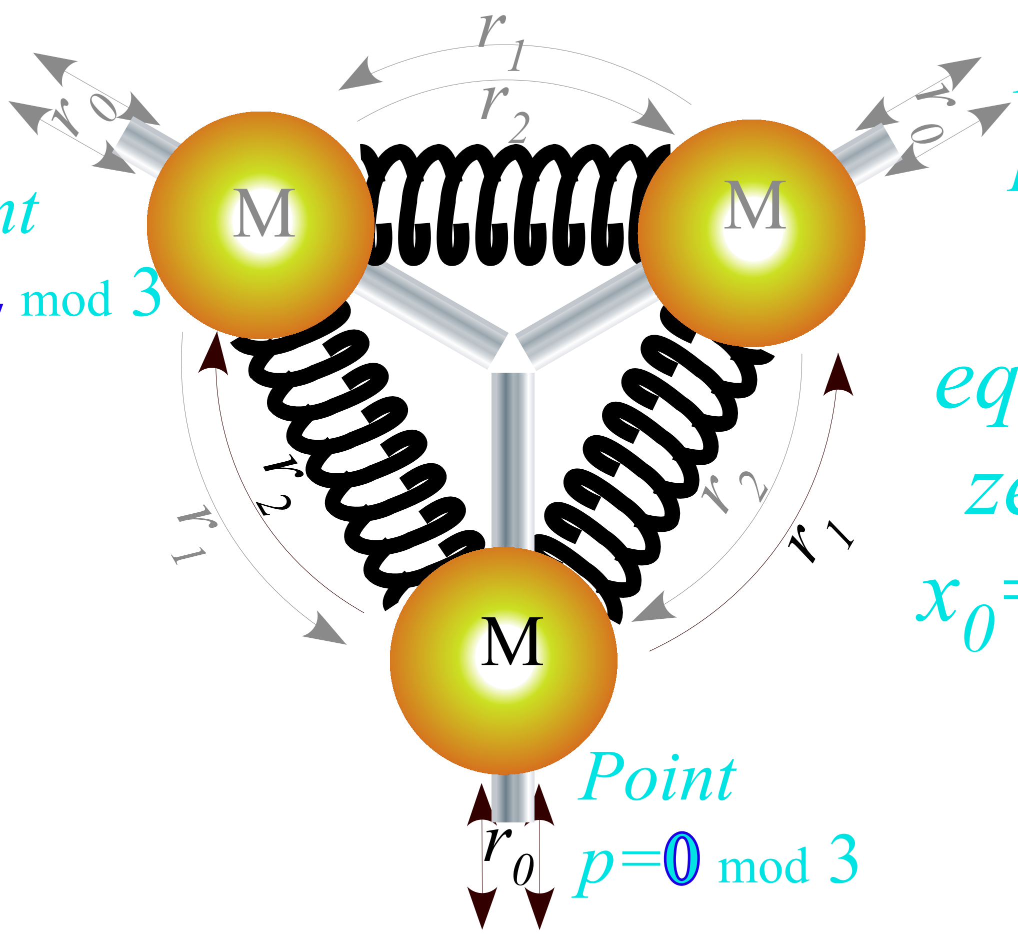
$$\mathbf{H}=\begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1&0&0\\0&1&0\\0&0&1\end{pmatrix} + r_1\begin{pmatrix} 0&1&0\\0&0&1\\1&0&0\end{pmatrix} + r_2\begin{pmatrix} 0&0&1\\1&0&0\\0&1&0\end{pmatrix}$$

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

Constants r_k that are *grayed-out*
may change values
if C₃ symmetry
is broken

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
However, no matter how C₃ is broken,
a Hermitian-symmetric Hamiltonian
$(H^*_{jk}=H_{kj})$ requires that $r_0^*=r_0$ and $r_1^*=r_2$.



equilibrium
zero-state
$$x_0=x_1=x_2=0$$
$$\begin{pmatrix}0\\0\\0\end{pmatrix}$$

C3 $\mathbf{g}^\dagger\mathbf{g}$-*product-table* *and basic group representation theory*

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

C3 $\mathbf{g}^\dagger\mathbf{g}$-*product-table*

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

A C3 **H**-*matrix* is then constructed directly from the $\mathbf{g}^\dagger\mathbf{g}$-*table* and so is each $\mathbf{r}^p$-*matrix representation*.

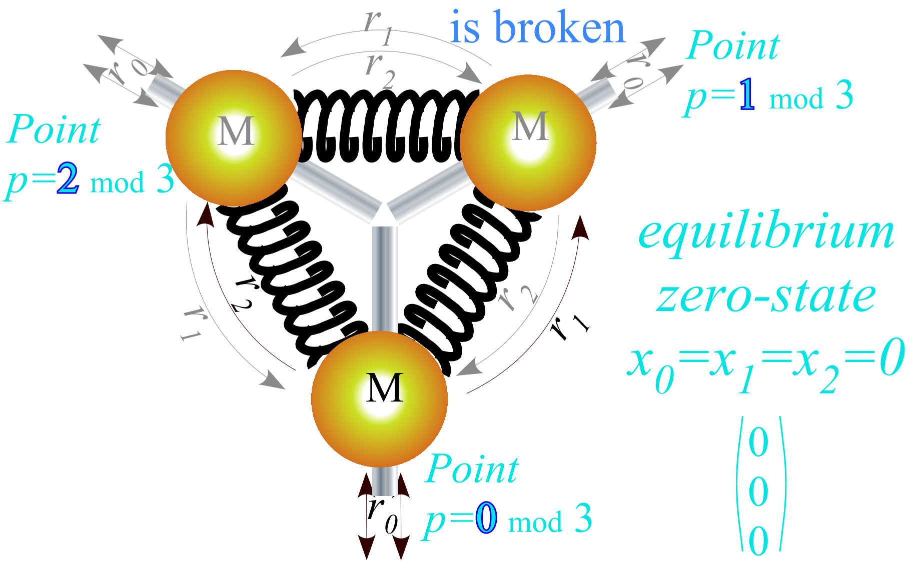
$$\mathbf{H}=\begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + r_1\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} + r_2\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

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

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 $r^*_1=r_2$.

Constants r_k that are *grayed-out*
may change values
if C3 symmetry
is broken

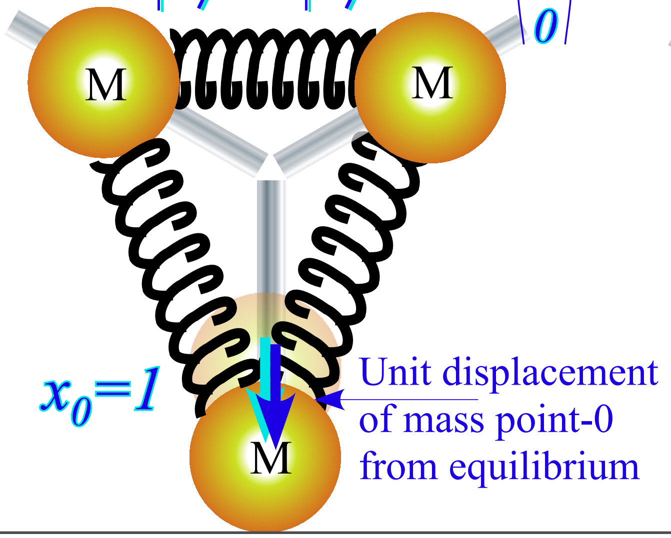


equilibrium
zero-state
$x_0=x_1=x_2=0$

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

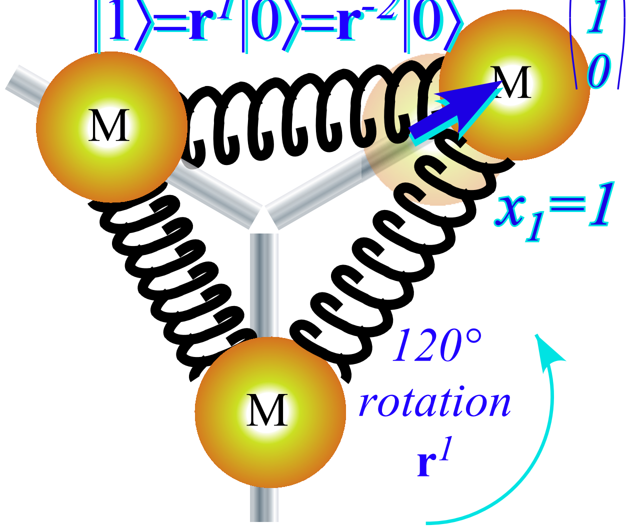
C3 operators $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$
also label unit
base states:
$|0\rangle = \mathbf{r}^0\,|0\rangle$
$|1\rangle = \mathbf{r}^1\,|0\rangle$
$|2\rangle = \mathbf{r}^2\,|0\rangle$
modulo-3

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

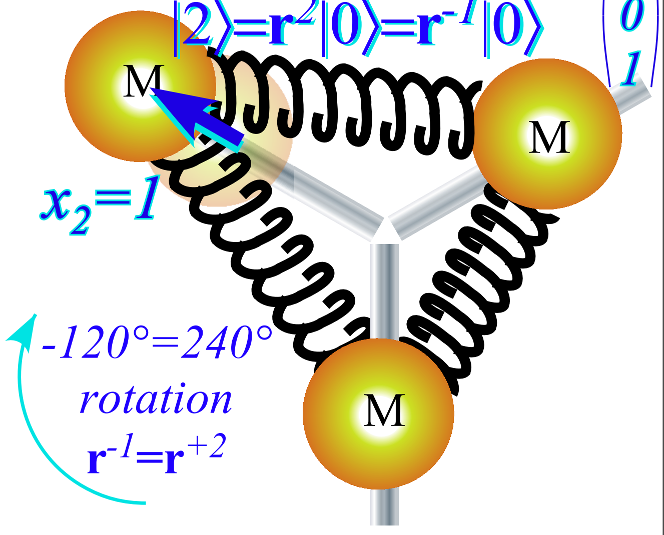


Unit displacement
of mass point-0
from equilibrium

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



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



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

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

C_3 Spectral resolution: 3rd roots of unity and ortho-completeness relations

C_3 character table and modular labeling

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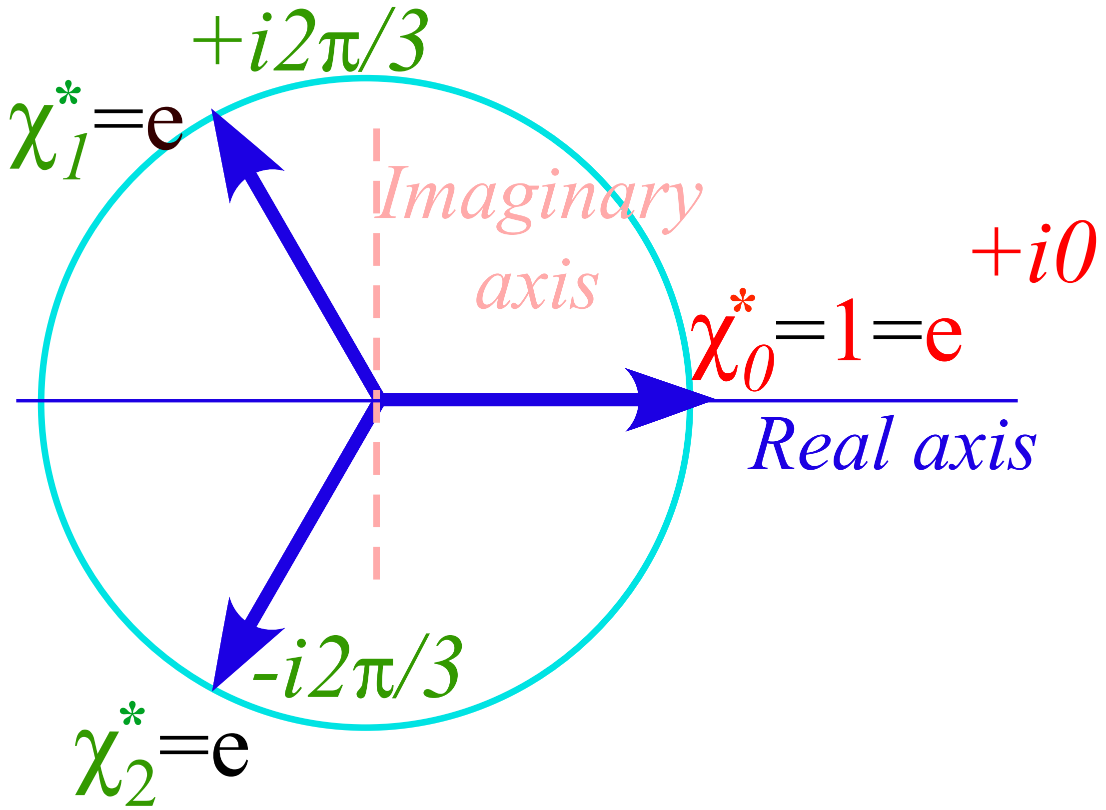

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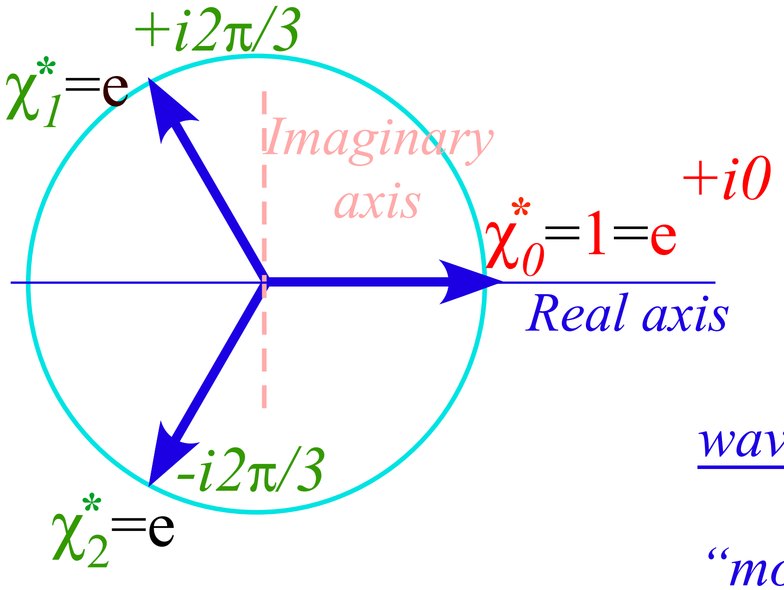

C_3 mode phase character table

wave-number $m=$ "momentum"

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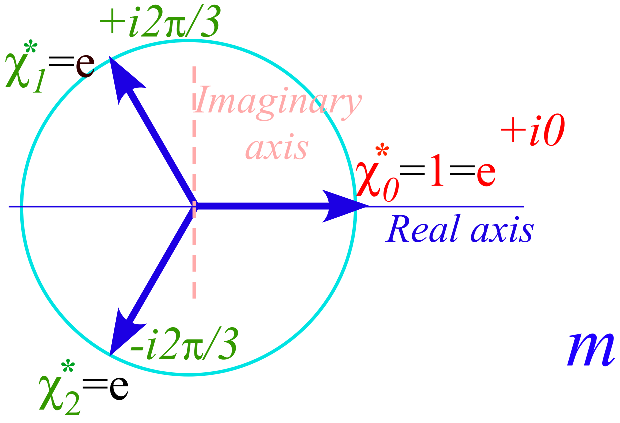

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wave-number
m=
"momentum"

WaveIt App

MolVibes

C_3 *character conjugate*

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

is wave function

$$\psi_m(r_p)=\frac{e^{ik_m\cdot r_p}}{\sqrt{3}}$$

C_3 Spectral resolution: 3rd roots of unity

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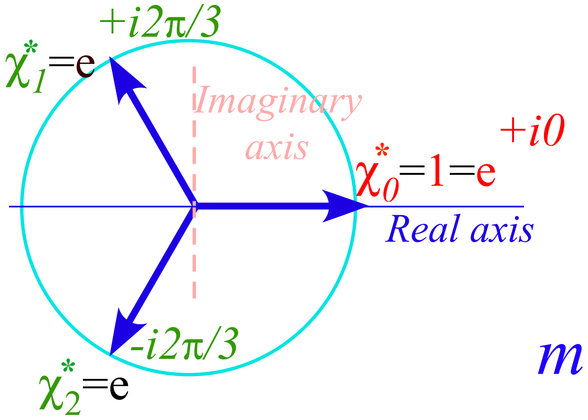

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C_3 mode phase character table

	p=0	*p*=1	*p*=2
$m=0_3$	$\chi_{00}=1$	$\chi_{01}=1$	$\chi_{02}=1$
$m=1_3$	$\chi_{10}=1$	$\chi_{11}=e^{-i2\pi/3}$	$\chi_{12}=e^{i2\pi/3}$
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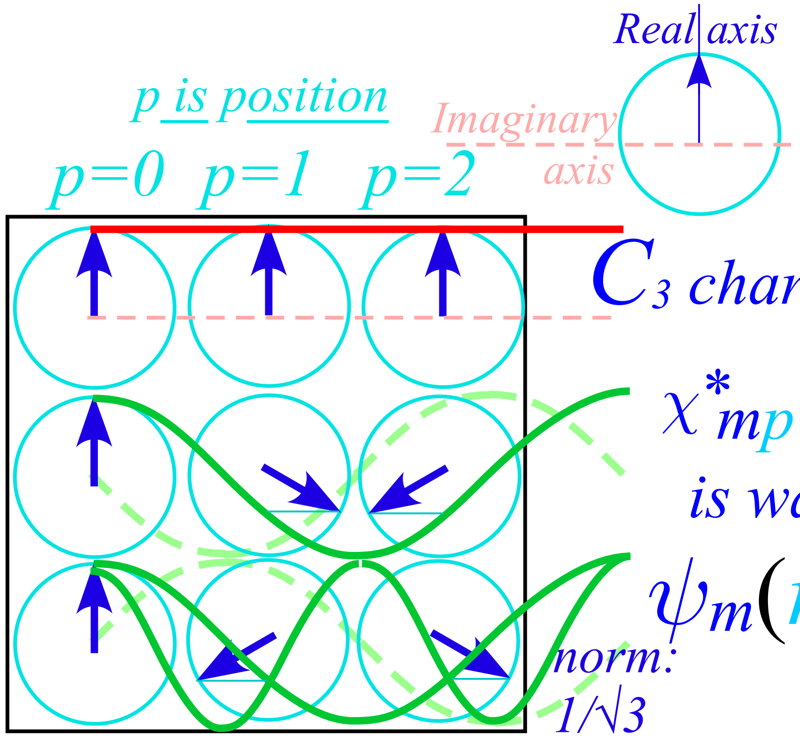
p is position



WaveIt App

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C_3 *character conjugate*

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

is wave function

$$\psi_m(r_p)=\frac{e^{ik_m\cdot r_p}}{\sqrt{3}}$$

C3 $\mathbf{g}^\dagger\mathbf{g}$-*product-table and basic group representation theory*
- C3 **H**-and-$\mathbf{r}^p$-*matrix representations and conjugation symmetry*

C3 Spectral resolution: 3rd roots of unity and ortho-completeness relations
- C3 *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*
- *C3-group jargon and structure of various tables*

C3 Eigenvalues and wave dispersion functions
- *Standing waves vs Moving waves*

C6 Spectral resolution: 6th 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:

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

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

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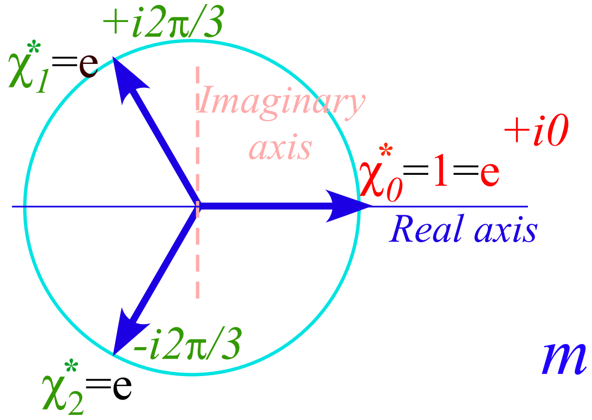

wave-number

m= “momentum”

C_3 mode phase character table

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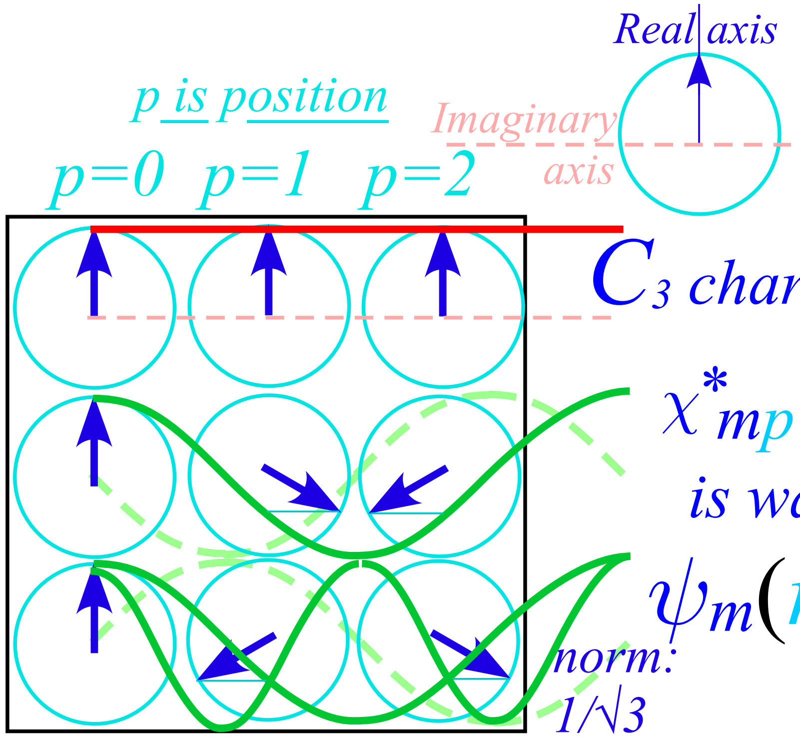

C_3 character conjugate

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WaveIt App

MolVibes

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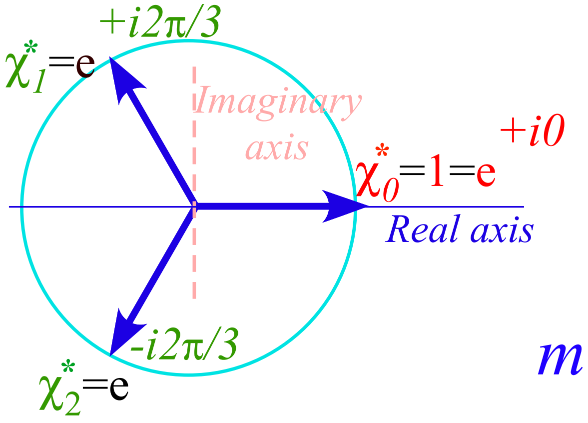

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wave-number m= "momentum"

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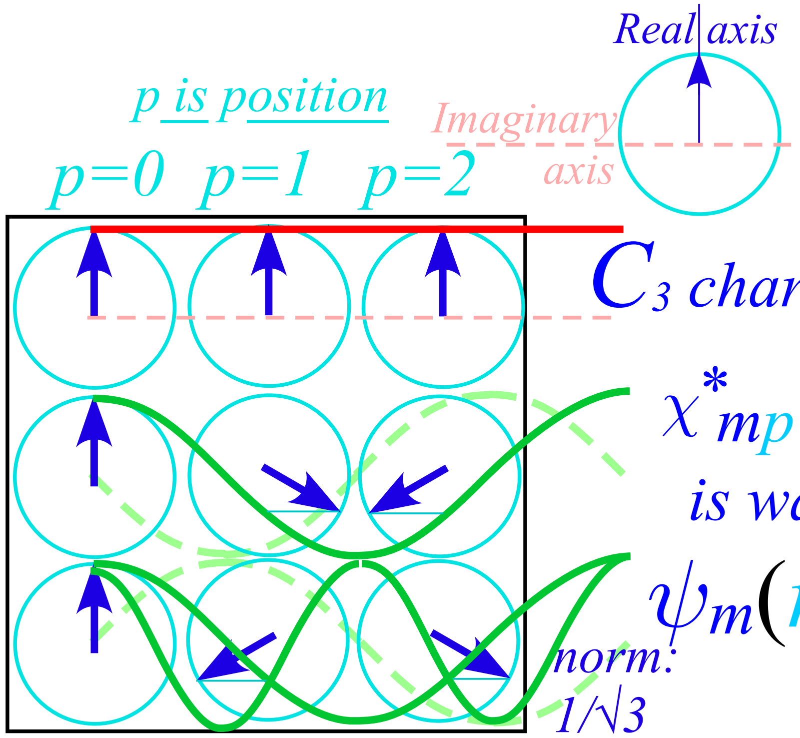

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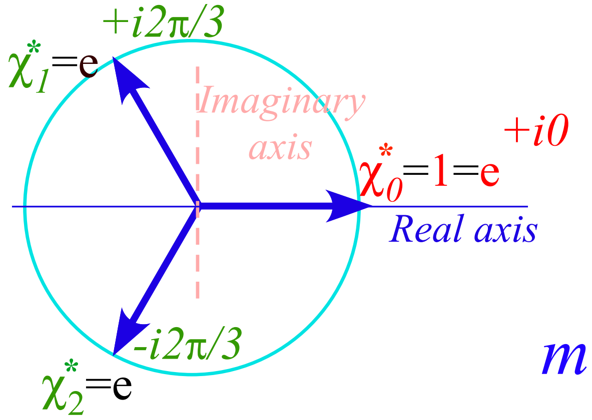

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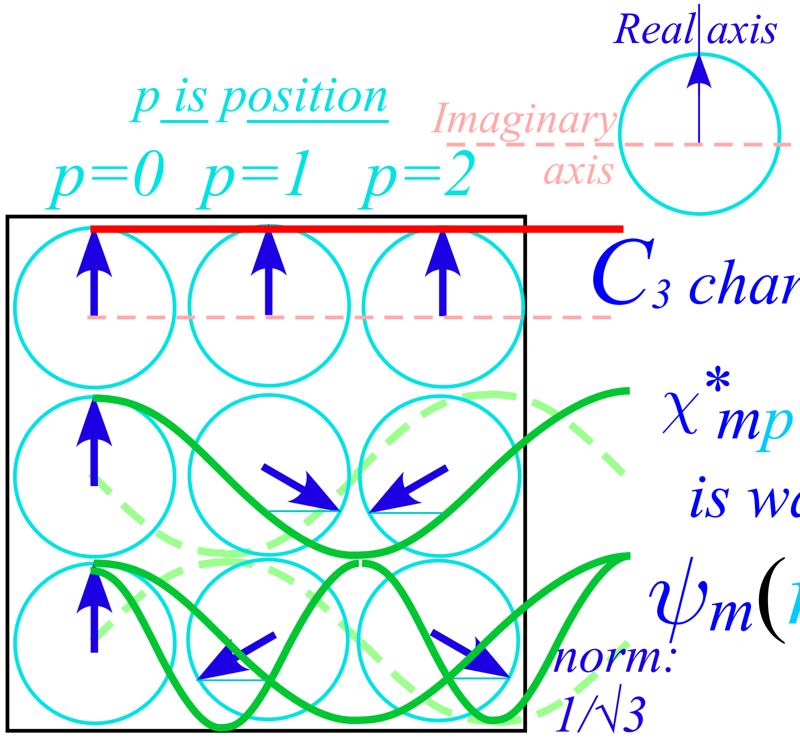

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$$\sqrt{3}|1\rangle = |0_3\rangle + |1_3\rangle + |2_3\rangle$$

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

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

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

$$\mathbf{P}^{(0)} = \tfrac{1}{3}(\mathbf{r}^0 + \mathbf{r}^1 + \mathbf{r}^2) = \tfrac{1}{3}(\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2)$$

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

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

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

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

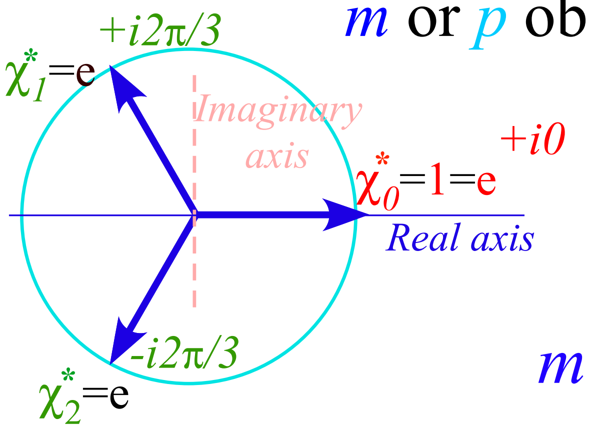
$$|2_3\rangle = \mathbf{P}^{(2)}|0\rangle\sqrt{3} = \frac{|\mathbf{r}^0\rangle + e^{-i2\pi/3}|\mathbf{r}^1\rangle + e^{+i2\pi/3}|\mathbf{r}^2\rangle}{\sqrt{3}}$$

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*

m=0,1,or *2* that is the *mode momentum m* of waves

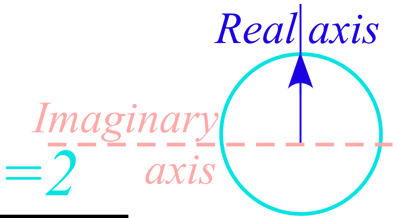
m or *p* obey *modular arithmetic* so sums or products =*0,1*,or *2* (*integers-modulo-3*)

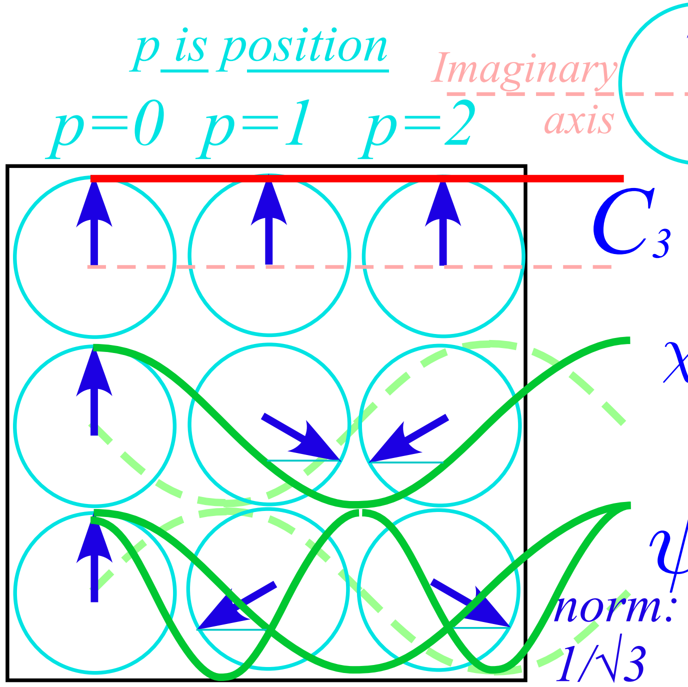


C_3 mode phase character table

	p=0	*p=1*	*p=2*
$m=0_3$	$\chi_{00}=1$	$\chi_{01}=1$	$\chi_{02}=1$
$m=1_3$	$\chi_{10}=1$	$\chi_{11}=e^{-i2\pi/3}$	$\chi_{12}=e^{i2\pi/3}$
$m=2_3$	$\chi_{20}=1$	$\chi_{21}=e^{i2\pi/3}$	$\chi_{22}=e^{-i2\pi/3}$

wave-number
m=
"momentum"





C_3 character conjugate

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

is wave function

$$\psi_m(r_p) = \frac{e^{ik_m \cdot r_p}}{\sqrt{3}}$$

WaveIt App

MolVibes

C_3 **g**†**g**-*product-table and basic group representation theory*

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

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$$\psi_m(x_p) = \frac{e^{ik_m \cdot x_p}}{\sqrt{3}}$$

$$= \frac{e^{imp2\pi/3}}{\sqrt{3}}$$

C_3 Lattice position vector

$x_p = L \cdot p$

Wavevector

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

Wavelength

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

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$$\mathbf{r}^p\,|q\rangle=|q+p\rangle \quad \text{implies:} \quad \langle q|\left(\mathbf{r}^p\right)^\dagger=\langle q|\mathbf{r}^{-p}=\langle q+p| \quad \text{implies:} \quad \langle q|\mathbf{r}^p=\langle q-p|$$

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Action of $\mathbf{r}^p$ on m-ket $|(m)\rangle=|k_m\rangle$ is inverse to action on coordinate bra $\langle x_q|=\langle q|$.

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(Norm factors left out) $\psi_{k_m}(x_q-p\cdot L)\quad=\langle x_q|\mathbf{r}^p|k_m\rangle=e^{ik_m(x_q-p\cdot L)}=e^{ik_m(x_q-x_p)}$

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$$\psi_{k_m}(x_q - p \cdot L) = \langle x_q|\mathbf{r}^p|k_m\rangle = e^{ik_m(x_q - p \cdot L)} = e^{ik_m(x_q - x_p)}$$

$$\langle q-p|(m)\rangle = \langle q|\mathbf{r}^p|(m)\rangle = e^{-ik_m x_p}\langle q|(m)\rangle$$

Comparing wave function operator algebra to bra-ket algebra

C₃ Plane wave function

$$\psi_m(x_p)=\frac{e^{ik_m\cdot x_p}}{\sqrt{3}}$$

$$=\frac{e^{imp2\pi/3}}{\sqrt{3}}$$

C₃ Lattice position vector

$x_p=L\cdot p$

Wavevector

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

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This implies: $\mathbf{r}^p|(m)\rangle=e^{-ik_m x_p}|(m)\rangle$

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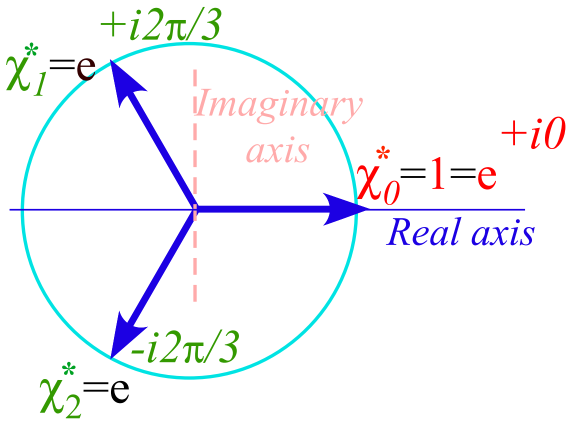


Two distinct types of modular "quantum" numbers:

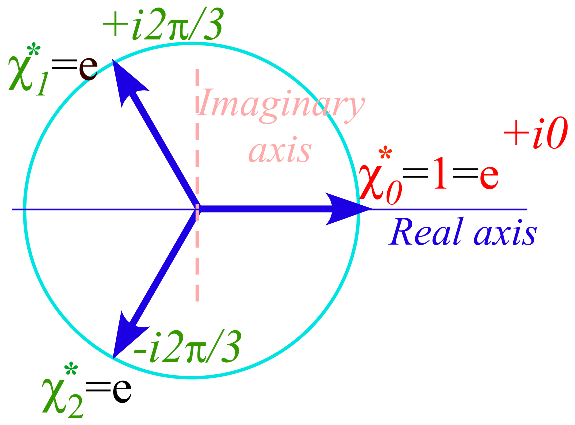
$p=0,1$,or 2 is *power p* of operator $\mathbf{r}^p$ labeling oscillator *position point p*

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

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

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

Modular quantum number arithmetic



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That is, (2-*times*-2)mod 3 is not 4 but 1 (4 mod $3=1$), the remainder of 4 divided by 3.

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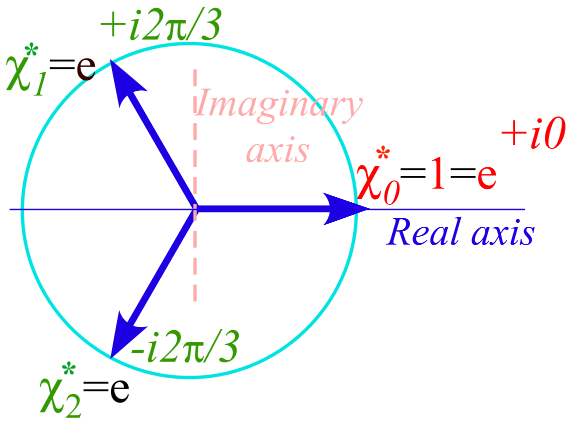

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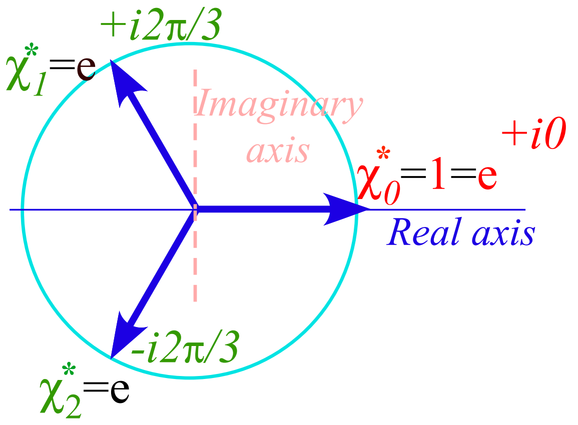
Thus, $(\rho_2)^2=\rho_1$. Also, *5* mod *3=2* so $(\rho_1)^5=\rho_2$, and *6* mod *3=0* so $(\rho_1)^6=\rho_0$.

Modular quantum number arithmetic



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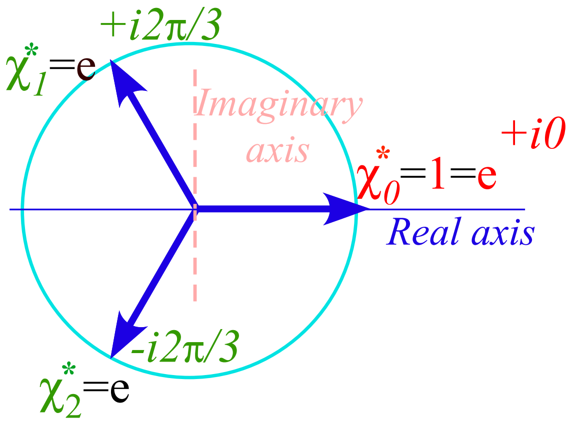

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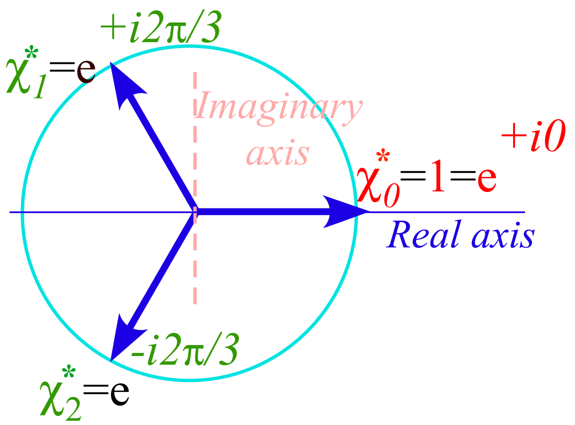
Other examples: -1 mod $3=2$ $[(\rho_1)^{-1}=(\rho_{-1})^1=\rho_2]$ and -2 mod $3=1$.

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

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

Modular quantum number arithmetic



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

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

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

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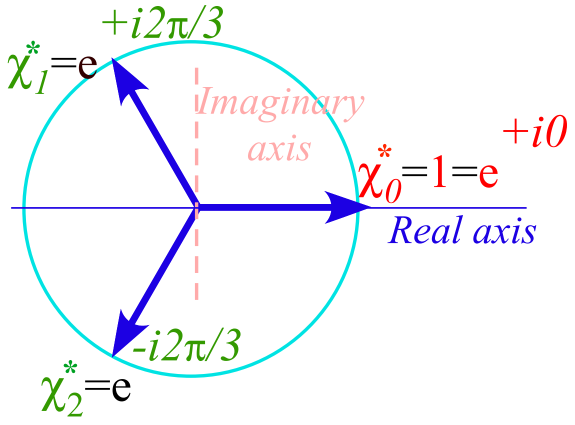


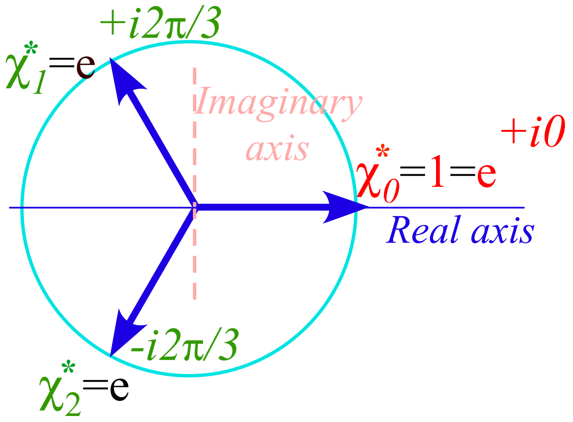
C_3-group $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$-table

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	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	χ_0	χ_1	χ_2
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

C_3-group jargon and structure of various tables



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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	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	χ_0	χ_1	χ_2
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

Set $\{\chi_0, \chi_1, \chi_2\}$ *is an*

irreducible representation

(irrep) of C_3

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

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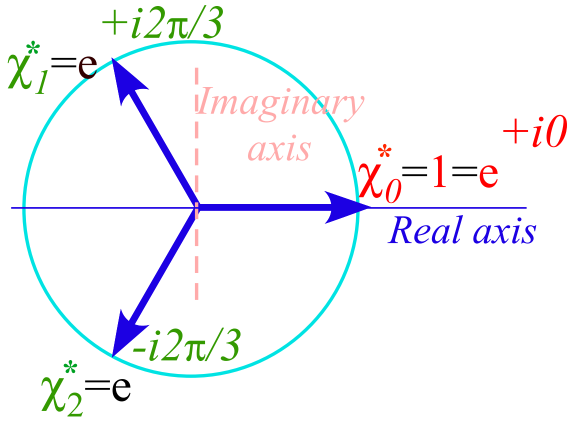

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C_3	$\mathbf{r}^0=\mathbf{1}$	$\mathbf{r}^1=\mathbf{r}^{-2}$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$\mathbf{r}^0=\ \mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
$\mathbf{r}^1=\mathbf{r}^{-2}$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

C_3	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	χ_0	χ_1	χ_2
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

Set $\{\chi_0, \chi_1, \chi_2\}$ *is an*
irreducible representation
(irrep) of C_3
$\{D(\mathbf{r}^0)=\chi_0,\ D(\mathbf{r}^1)=\chi_1,\ D(\mathbf{r}^2)=\chi_2\}$

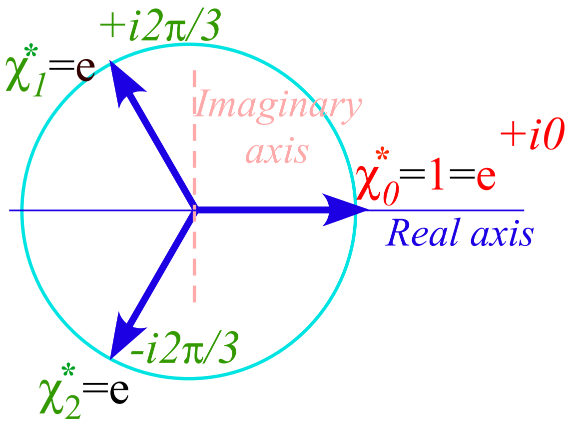
In fact, all ***three*** *irreps* $\{D^{(0)}, D^{(1)}, D^{(2)}\}$ listed in character table obey C_3-group table

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

=

$\mathbf{g}=$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$
$D^{(0)}(\mathbf{g})$	1	1	1
$D^{(1)}(\mathbf{g})$	1	$e^{-\frac{2\pi i}{3}}$	$e^{+\frac{2\pi i}{3}}$
$D^{(2)}(\mathbf{g})$	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 $\{\chi_0=1, \chi_1= e^{-i2\pi/3}, \chi_2= e^{+i2\pi/3}\}$

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	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	χ_0	χ_1	χ_2
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

Set $\{\chi_0, \chi_1, \chi_2\}$ is an
irreducible representation
(irrep) of C_3
$\{D(\mathbf{r}^0)=\chi_0, D(\mathbf{r}^1)=\chi_1, D(\mathbf{r}^2)=\chi_2\}$

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

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

=

$\mathbf{g}=$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$
$D^{(0)}(\mathbf{g})$	1	1	1
$D^{(1)}(\mathbf{g})$	1	$e^{-\frac{2\pi i}{3}}$	$e^{+\frac{2\pi i}{3}}$
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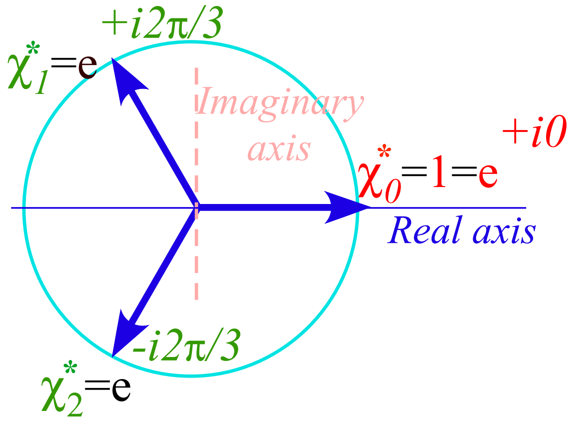
The *identity irrep*
$D^{(0)}=\{1,1,1\}$
obeys *any* group table.

C_3-group jargon and structure of various tables



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

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

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

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

C_3	$\chi_0=1$	$\chi_1=\chi_2^{-2}$	$\chi_2=\chi_1^{-1}$
$\chi_0=1=\chi_3$	χ_0	χ_1	χ_2
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

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

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

=

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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$_3$ **g**†**g**-*product-table and basic group representation theory*

C$_3$ **H**-and-**r**^{p}-*matrix representations and conjugation symmetry*

C$_3$ Spectral resolution: 3rd 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: 6th roots of unity and higher

Complete sets of coupling parameters and Fourier dispersion

Gauge shifts due to complex coupling

Eigenvalues and wave dispersion functions

$$\left\langle m\middle|\mathbf{H}\middle|m\right\rangle=\left\langle m\middle|r_0\mathbf{r}^0+r_1\mathbf{r}^1+r_2\mathbf{r}^2\middle|m\right\rangle=r_0e^{i0(m)\frac{2\pi}{3}}+r_1e^{i1(m)\frac{2\pi}{3}}+r_2e^{i2(m)\frac{2\pi}{3}}$$

Eigenvalues and wave dispersion functions

$$\langle m|\mathbf{H}|m\rangle=\langle m|r_0\mathbf{r}^0+r_1\mathbf{r}^1+r_2\mathbf{r}^2|m\rangle=r_0e^{i0(m)\frac{2\pi}{3}}+r_1e^{i1(m)\frac{2\pi}{3}}+r_2e^{i2(m)\frac{2\pi}{3}}$$

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

$$=r_0e^{i0(m)\frac{2\pi}{3}}+r(e^{i\frac{2m\pi}{3}}+e^{-i\frac{2m\pi}{3}})$$

Eigenvalues and wave dispersion functions

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

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

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

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

Quantum **H**-values:

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

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)

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r\left(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}\right) = r_0 + 2r\cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0+2r & (\text{for } m=0)\\ r_0-r & (\text{for } m=\pm1)\end{cases}$$

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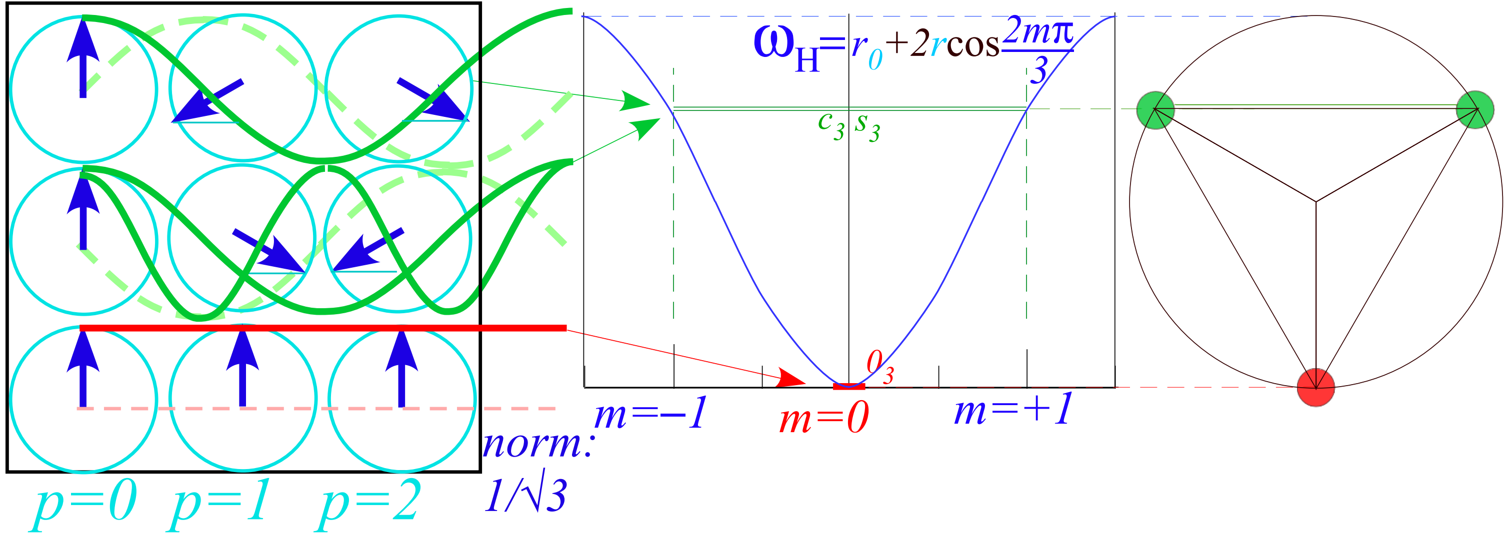
	p=0	*p=1*	*p=2*
$+1_3$	*1*	$e^{+2\pi i/3}$	$e^{-2\pi i/3}$
	right-hand moving wave		
-1_3	*1*	$e^{-2\pi i/3}$	$e^{+2\pi i/3}$
	left-hand moving wave		
0_3	*1*	*1*	*1*
	scalar standing wave		

p is position

C_3 moving waves *Quantum **H**-dispersion* *geometry*



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Eigenvalues and wave dispersion functions - Moving waves

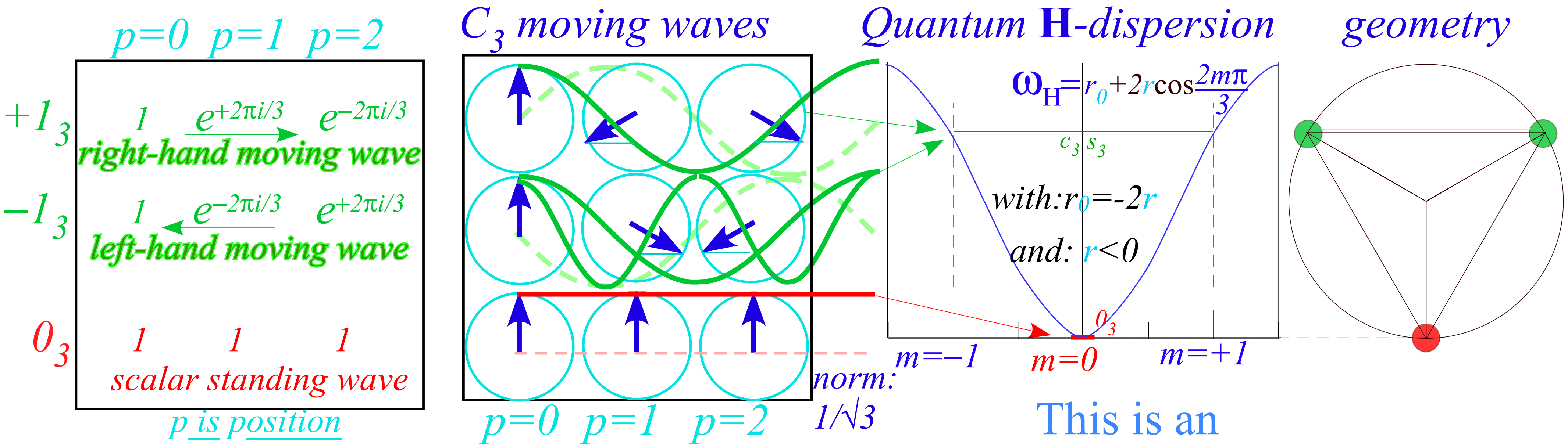
$$\langle m|\mathbf{H}|m\rangle = \langle m| r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 |m\rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

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

$$= r_0 e^{i0(m)\frac{2\pi}{3}} + r\left(e^{i\frac{2m\pi}{3}} + e^{-i\frac{2m\pi}{3}}\right) = r_0 + 2r\cos\left(\frac{2m\pi}{3}\right) = \begin{cases} r_0+2r & (\text{for } m=0)\\ r_0 - r & (\text{for } m=\pm1)\end{cases}$$

Quantum **H**-values:

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



This is an

exciton-like

dispersion function

$$\omega_H(m) = r_0\left(1-\cos\frac{2m\pi}{3}\right)$$

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

WaveIt App

MolVibes

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)

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

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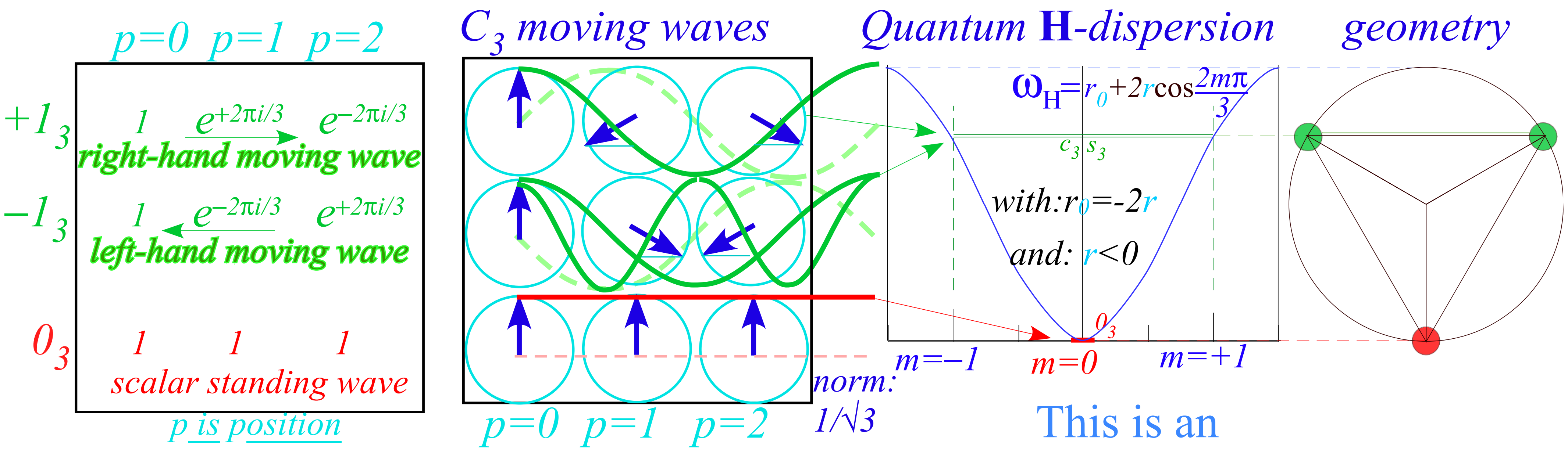
Classical **K**-values:

$$\begin{pmatrix} K & \text{-}k & \text{-}k \\ \text{-}k & K & \text{-}k \\ \text{-}k & \text{-}k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = \left(K - 2k\cos(\tfrac{2m\pi}{3})\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$



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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)

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

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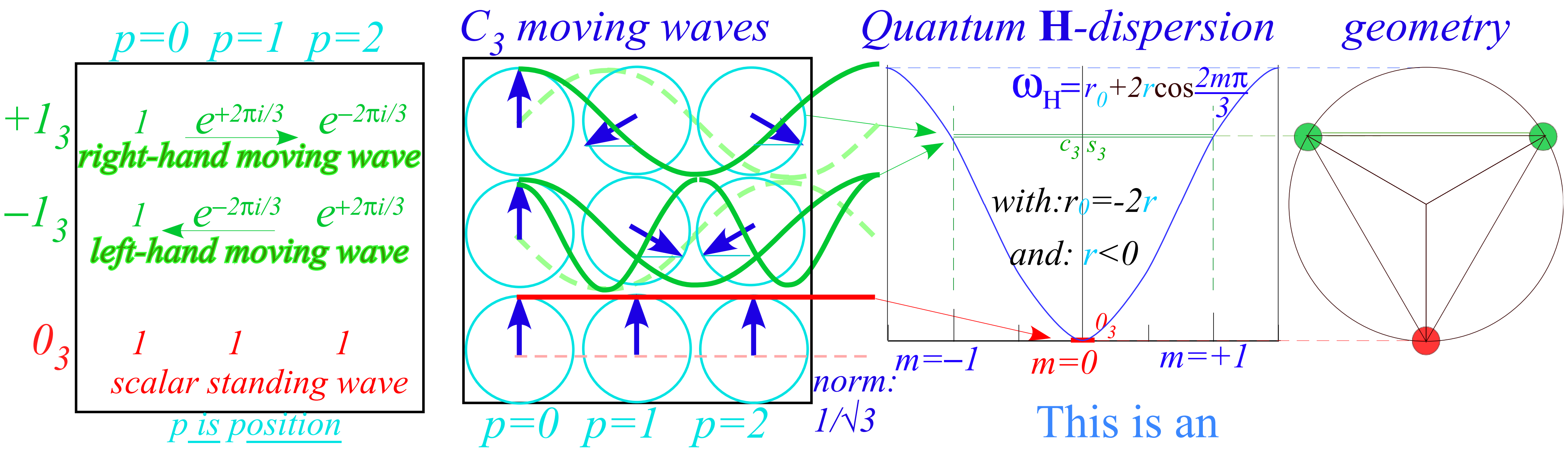
Classical **K**-values:

$$\begin{pmatrix} K & -k & -k \\ -k & K & -k \\ -k & -k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} \quad \text{K-eigenvalue...} \quad = \left(K - 2k\cos\left(\frac{2m\pi}{3}\right)\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

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



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Eigenvalues and wave dispersion functions - Moving waves

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$$\begin{pmatrix} K & \text{-}k & \text{-}k \\ \text{-}k & K & \text{-}k \\ \text{-}k & \text{-}k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} \begin{matrix}\text{K-eigenvalue...} \\ = \left(K - 2k\cos(\tfrac{2m\pi}{3})\right) \\ \text{needs } \textit{Square-Root} \\ \text{to be a } \textit{frequency}\end{matrix} \begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

	$p=0$	$p=1$	$p=2$
$+1_3$	1	$e^{+2\pi i/3}$	$e^{-2\pi i/3}$
	right-hand moving wave		
-1_3	1	$e^{-2\pi i/3}$	$e^{+2\pi i/3}$
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0_3	1	1	1
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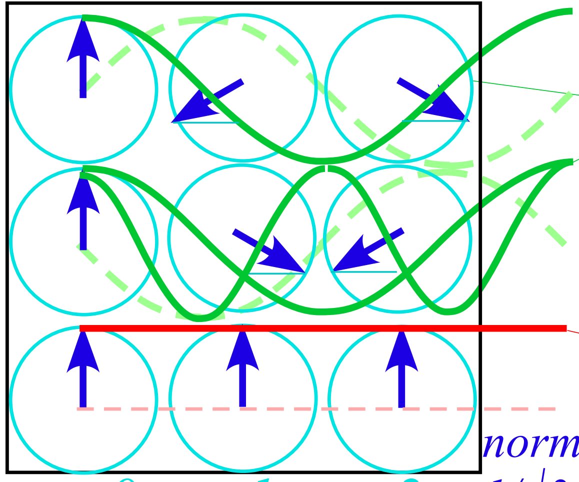
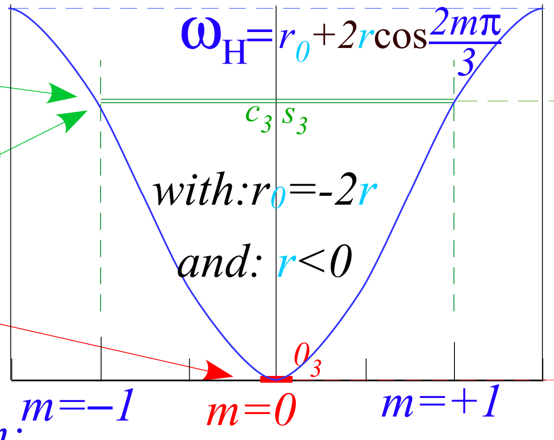
p is position

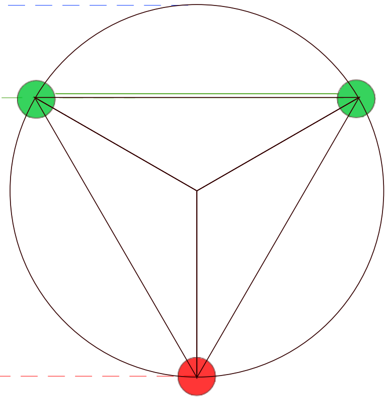
C_3 moving waves



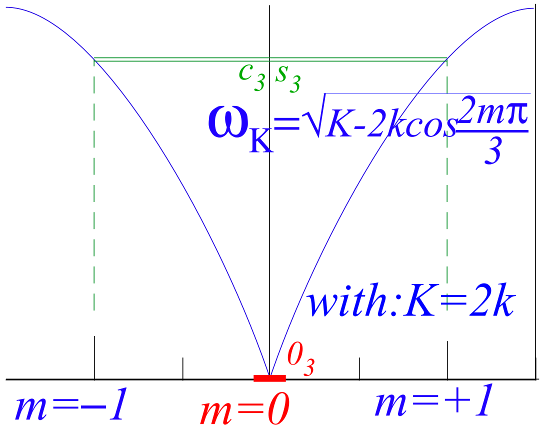
*Quantum **H**-dispersion*



geometry



*Classical **K**-dispersion*



This is an

exciton-like

dispersion function

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

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

$\omega_H(m)$ is *quadratic* for low m

(long wavelength λ)

This is a

phonon-like

dispersion function

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

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

$$\omega_K(m) \sim 2\sqrt{k}(\frac{m\pi}{3})^1$$

$\omega_K(m)$ is *linear* for low m

(long wavelength λ)

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C$_3$ **g†g**-*product-table and basic group representation theory*

C$_3$ **H**-and-**r**^{p}-*matrix representations and conjugation symmetry*

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

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

Quantum **H**-values:

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

Classical **K**-values:

$$\begin{pmatrix} K & -k & -k \\ -k & K & -k \\ -k & -k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = \left(K - 2k\cos\left(\tfrac{2m\pi}{3}\right)\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

Standing waves possible if **H** *is all-real (No curly C-stuff allowed!)*

Eigenvalues and wave dispersion functions - Standing 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)*

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

Quantum **H**-values:

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

Classical **K**-values:

$$\begin{pmatrix} K & -k & -k \\ -k & K & -k \\ -k & -k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = \left(K - 2k\cos(\tfrac{2m\pi}{3})\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$

Standing waves possible if **H** *is all-real (No curly C-stuff allowed!)*

Moving eigenwave	*Standing eigenwaves*	$\mathbf{H}-$*eigenfrequencies*	$\mathbf{K}-$*eigenfrequencies*
$\lvert(+1)_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^{+i2\pi/3} \\ e^{-i2\pi/3} \end{pmatrix}$	$\lvert c_3\rangle = \frac{\lvert(+1)_3\rangle + \lvert(-1)_3\rangle}{\sqrt{2}} = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$	$\omega^{(+1)_3} = r_0 + 2r\cos(\frac{+2m\pi}{3})$ $= r_0 - r$	$\sqrt{k_0 - 2k\cos(\frac{+2m\pi}{3})}$ $= \sqrt{k_0 + k}$
$\lvert(-1)_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^{-i2\pi/3} \\ e^{+i2\pi/3} \end{pmatrix}$	$\lvert s_3\rangle = \frac{\lvert(+1)_3\rangle - \lvert(-1)_3\rangle}{i\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ +1 \\ -1 \end{pmatrix}$	$\omega^{(-1)_3} = r_0 + 2r\cos(\frac{-2m\pi}{3})$ $= r_0 - r$	$\sqrt{k_0 - 2k\cos(\frac{-2m\pi}{3})}$ $= \sqrt{k_0 + k}$
	$\lvert(0)_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$	$\omega^{(0)_3} = r_0 + 2r$	$\sqrt{k_0 - 2k}$

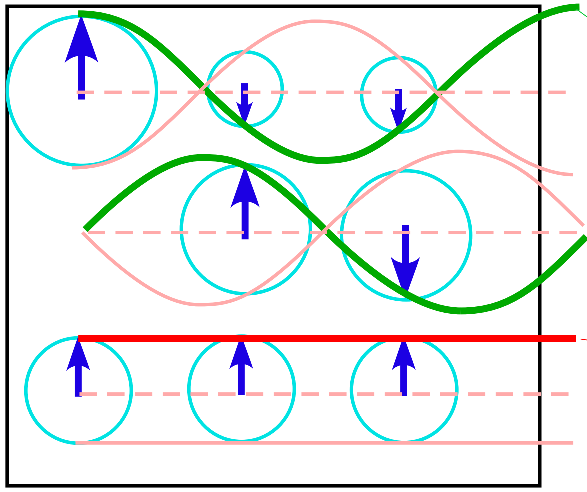
States $|(+)\rangle$ and $|(-)\rangle$ in *any mixtures* are still *stationary* due to $(\pm)$-*degeneracy* (cos(+*x*)=cos(-*x*))

Eigenvalues and wave dispersion functions - Standing waves

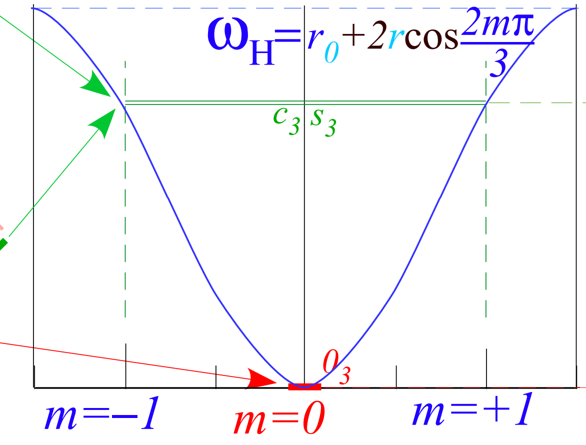
(Possible if **H** *is all-real)*

	$p=0$	$p=1$	$p=2$
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		
0_3	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$
	scalar standing wave		

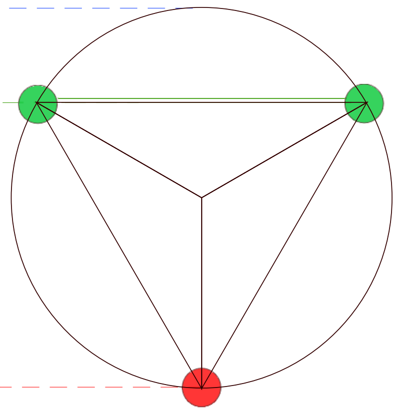
C_3 standing waves



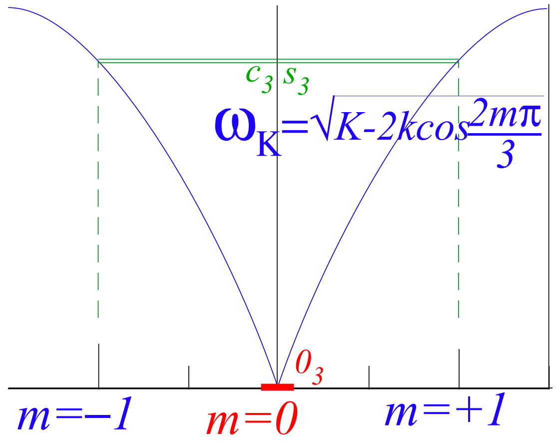
Quantum **H***-dispersion*



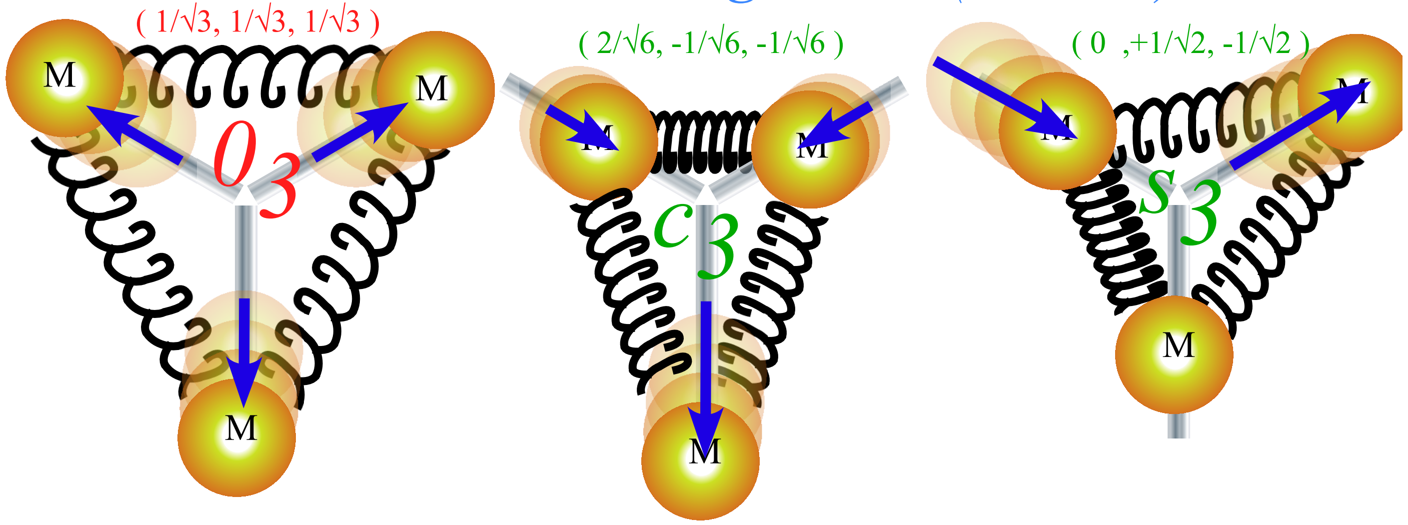
geometry



Classical **K***-dispersion*



Radial standing waves (all-real)



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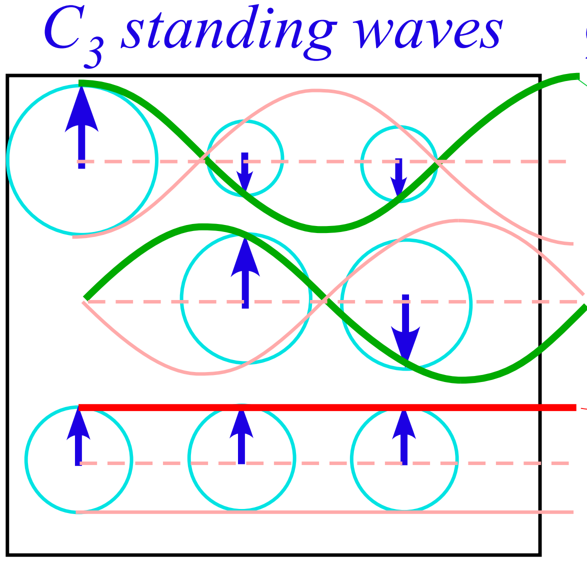
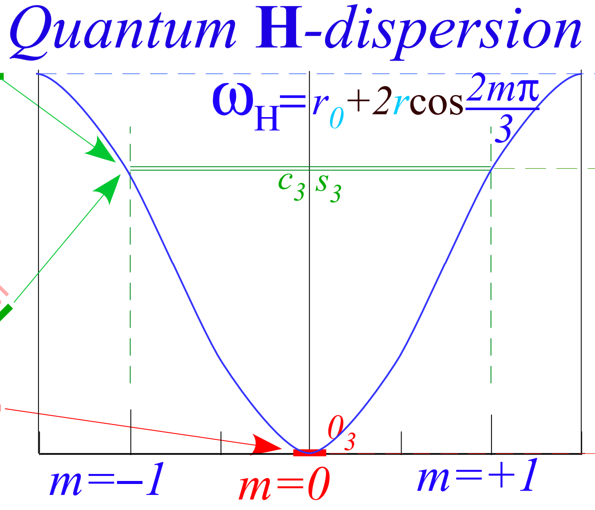
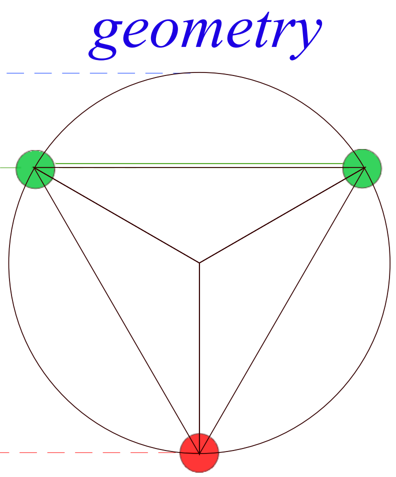
Eigenvalues and wave dispersion functions - Standing waves

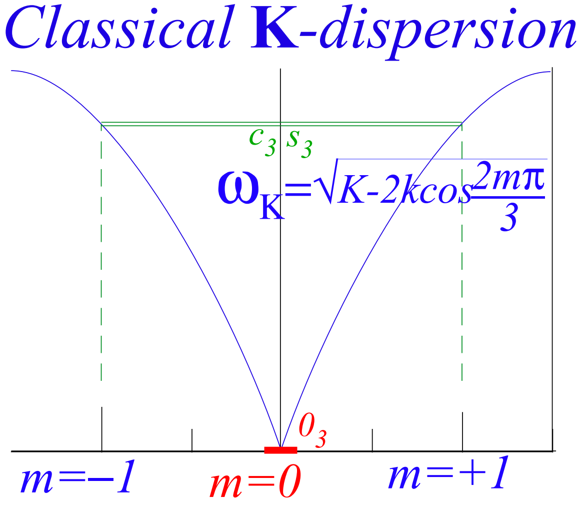
(Possible if **H** *is all-real)*

	$p=0$	$p=1$	$p=2$
c_3	2/√6	-1/√6	-1/√6
	cosine standing wave		
s_3	0	1/√2	-1/√2
	sine standing wave		
0_3	1/√3	1/√3	1/√3
	scalar standing wave		

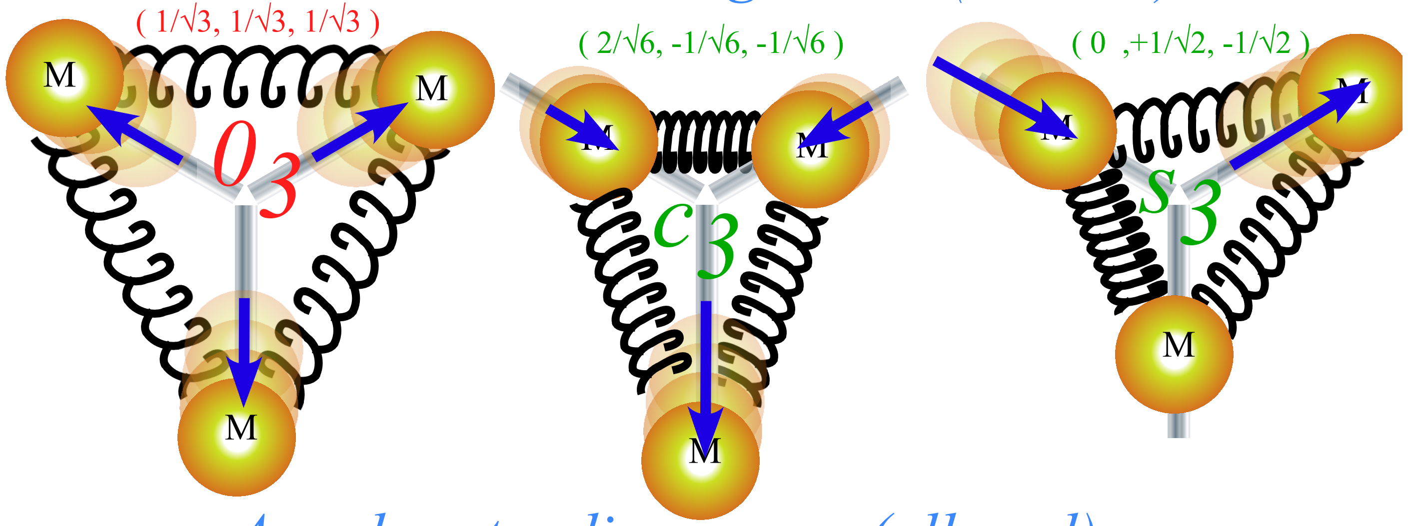




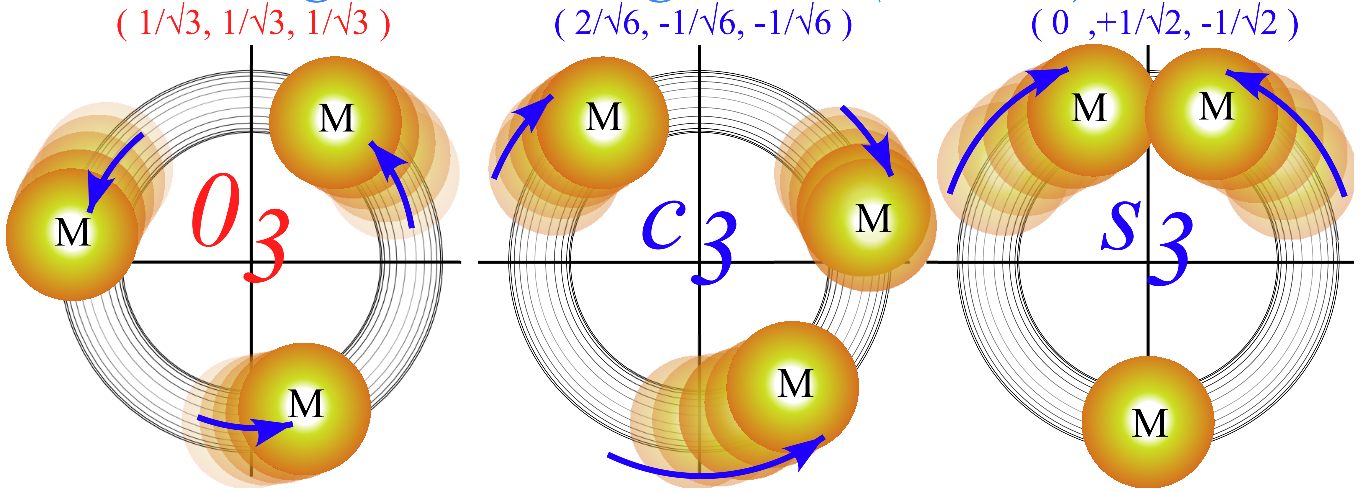




Radial standing waves (all-real)



Angular standing waves (all-real)



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C_3 **g**†**g**-*product-table and basic group representation theory*

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

C_3 Spectral resolution: 3rd roots of unity and ortho-completeness relations

C_3 character table and modular labeling

Ortho-completeness ***inversion*** *for operators and states*

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: 6th roots of unity and higher*

Complete sets of coupling parameters and Fourier dispersion

Gauge shifts due to complex coupling

1st Step in Abelian symmetry analysis

Expand C_6 symmetric $\mathbf{H}$ *matrix using C_6 group table($\overset{gg^\dagger}{form}$)*

$$\mathbf{H}= r_0\mathbf{r}^0+r_1\mathbf{r}^1+r_2\mathbf{r}^2+\ldots+r_{n-1}\mathbf{r}^{n-1}=\Sigma r_q\mathbf{r}^k$$

		$g^\dagger$					
	C_6	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
	1	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
	$\mathbf{r}$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
	$\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$
g	$\mathbf{r}^3$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$
	$\mathbf{r}^4$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$
	$\mathbf{r}^5$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**

$$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$$

$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} + r_1\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + r_2\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + r_3\begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} + r_4\begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + r_5\begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

C_6 group table gives $\mathbf{r}$*-matrices,...*

(known as a *regular* representation of the group)

1^{st} Step in Abelian symmetry analysis

Expand C_6 symmetric **H** *matrix using C_6 group table($\overset{gg^\dagger}{form}$)*

$$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + \ldots + r_{n-1}\mathbf{r}^{n-1} = \Sigma\, r_q\mathbf{r}^k$$

$g \backslash g^\dagger$ C_6	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
1	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{r}$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
$\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$
$\mathbf{r}^3$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$	$\mathbf{r}^4$
$\mathbf{r}^4$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**	$\mathbf{r}^5$
$\mathbf{r}^5$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	**1**

$$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$$

$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} + r_1 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + r_2 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + r_3 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} + r_4 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + r_5 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

C_6 group table gives ***r****-matrices,...*

Put "1" wherever $\mathbf{r}^3$ appears in product-table

(known as a *regular* representation of the group)

1^{st} Step in Abelian symmetry analysis

Expand C_6 symmetric $\mathbf{H}$ matrix using C_6 group table($\underset{form}{gg^\dagger}$)

$$\mathbf{H}= r_0\mathbf{r}^0+r_1\mathbf{r}^1+r_2\mathbf{r}^2+\ldots+r_{n-1}\mathbf{r}^{n-1}=\Sigma\, r_q\mathbf{r}^k$$

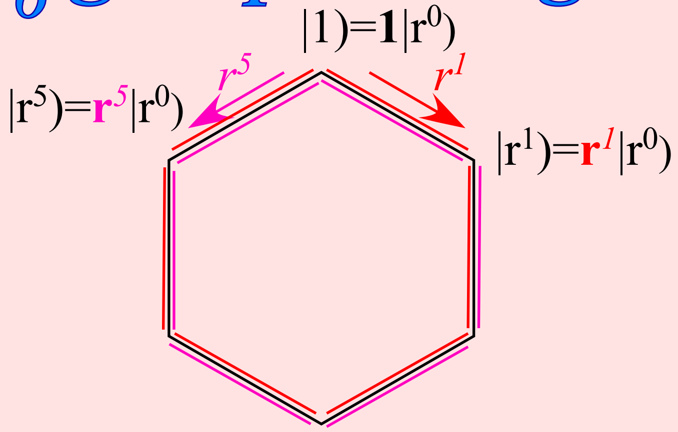
$g^\dagger$

C_6	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{r}$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
$\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$
g $\mathbf{r}^3$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$
$\mathbf{r}^4$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$
$\mathbf{r}^5$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$

$$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$$

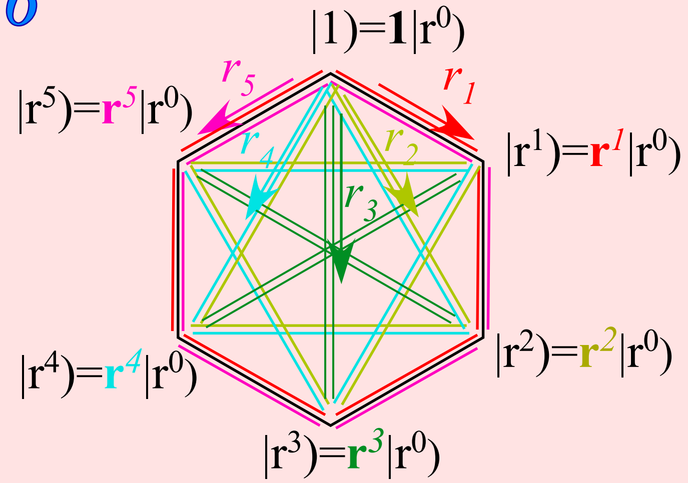
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} + r_1\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + r_2\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + r_3\begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} + r_4\begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + r_5\begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

C_6 group table gives $\mathbf{r}$-matrices,...C_6-allowed $\mathbf{H}$-matrices...



Nearest neighbor coupling

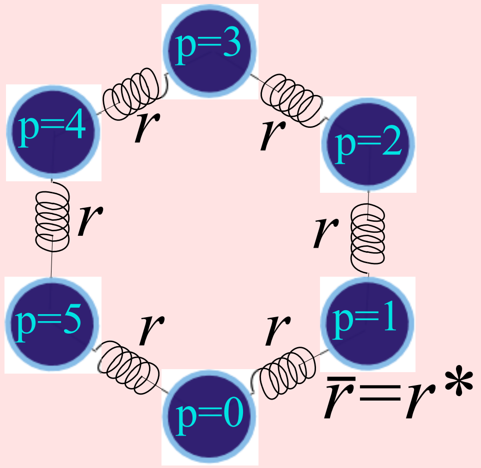
$$\begin{pmatrix} r_0 & r_5 & & & & r_1 \\ r_1 & r_0 & r_5 & & & \\ & r_1 & r_0 & r_5 & & \\ & & r_1 & r_0 & r_5 & \\ & & & r_1 & r_0 & r_5 \\ r_5 & & & & r_1 & r_0 \end{pmatrix}$$



<u>ALL</u> neighbor coupling

$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix}$$

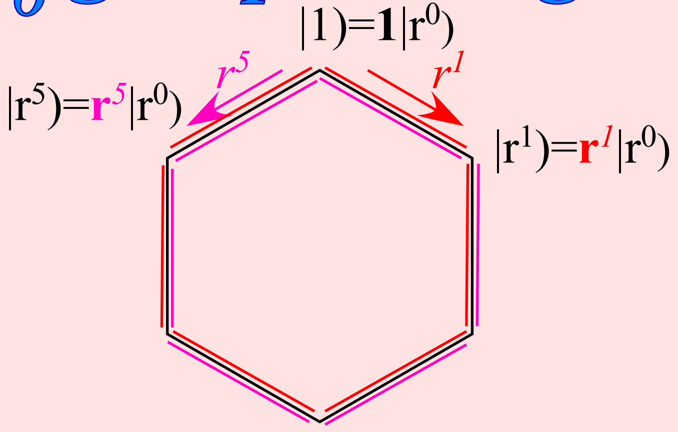
(a) 1^{st} Neighbor C_6



$$\mathbf{H}^{B1(6)}=\begin{array}{c|c} \begin{matrix} p=0 & 1 & 2 & 3 & 4 & 5 \end{matrix} & \\ \begin{pmatrix} H_1 & -r & \cdot & \cdot & \cdot & -\bar{r} \\ -\bar{r} & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -\bar{r} & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -\bar{r} & H_1 & -r & \cdot \\ \cdot & \cdot & \cdot & -\bar{r} & H_1 & -r \\ -r & \cdot & \cdot & \cdot & -\bar{r} & H_1 \end{pmatrix} & \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} \end{array}$$

$$= H_1\mathbf{1} - r\mathbf{r} - \bar{r}\mathbf{r}^{-1}$$

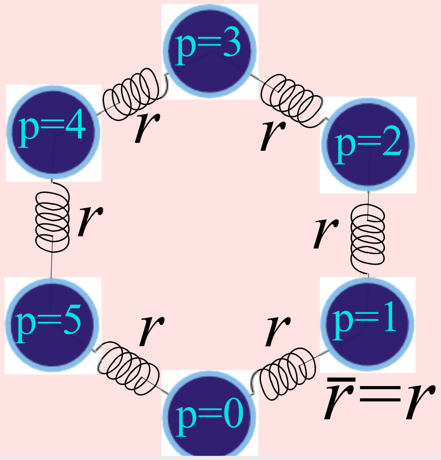
C_6 group table gives r-matrices,..



Nearest neighbor coupling

$$\begin{pmatrix} r_0 & r_5 & & & & r_1 \\ r_1 & r_0 & r_5 & & & \\ & r_1 & r_0 & r_5 & & \\ & & r_1 & r_0 & r_5 & \\ & & & r_1 & r_0 & r_5 \\ r_5 & & & & r_1 & r_0 \end{pmatrix}$$

(a) 1^{st} Neighbor C_6



$\bar{r}=r^*=r$

$$\mathbf{H}^{B1(6)}=2r\mathbf{1}-r\mathbf{r}^{1}-r\mathbf{r}^{-1}$$

$$\left|\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p\\
\hline
2r & -r & \cdot & \cdot & \cdot & -r & 0\\
-r & 2r & -r & \cdot & \cdot & \cdot & 1\\
\cdot & -r & 2r & -r & \cdot & \cdot & 2\\
\cdot & \cdot & -r & 2r & -r & \cdot & 3\\
\cdot & \cdot & \cdot & -r & 2r & -r & 4\\
-r & \cdot & \cdot & \cdot & -r & 2r & 5
\end{array}\right.$$

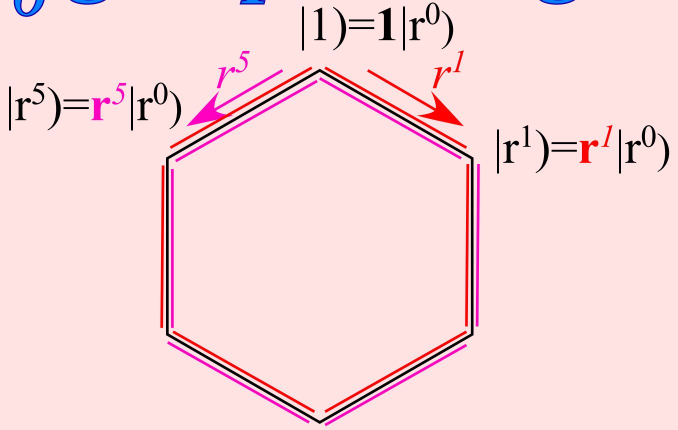
Conjugation symmetry

Hermitian Hamiltonian $(\mathbf{H}^*_{jk}=\mathbf{H}_{kj})$ requires $r_0^*=r_0$ and $r_1=r_5^*$.

Elementary Bloch model
assumes both are real
(r_1=-r=r_5^*)

r_1 equals conjugate of r_5: ($r_1=r_5^*$)

C_6 group table gives $\mathbf{r}$-matrices,..

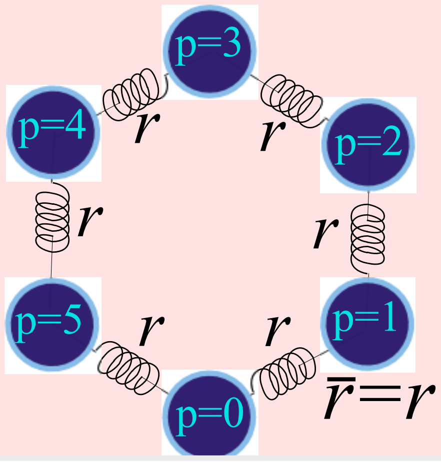


Elementary - Bloch - Model : Nearest neighbor coupling:

$$\mathbf{H}^{B1(6)}=r_0\mathbf{1}+r_1\mathbf{r}^1+r_5\mathbf{r}^5 \qquad =2r\mathbf{1}-r\mathbf{r}^1+-r\mathbf{r}^{-1}$$

$$\begin{pmatrix}
r_0 & r_5 & \cdot & \cdot & \cdot & r_1\\
r_1 & r_0 & r_5 & \cdot & \cdot & \cdot\\
\cdot & r_1 & r_0 & r_5 & \cdot & \cdot\\
\cdot & \cdot & r_1 & r_0 & r_5 & \cdot\\
\cdot & \cdot & \cdot & r_1 & r_0 & r_5\\
r_5 & \cdot & \cdot & \cdot & r_1 & r_0
\end{pmatrix}
=
\left|\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p\\
\hline
2r & -r & \cdot & \cdot & \cdot & -r & 0\\
-r & 2r & -r & \cdot & \cdot & \cdot & 1\\
\cdot & -r & 2r & -r & \cdot & \cdot & 2\\
\cdot & \cdot & -r & 2r & -r & \cdot & 3\\
\cdot & \cdot & \cdot & -r & 2r & -r & 4\\
-r & \cdot & \cdot & \cdot & -r & 2r & 5
\end{array}\right.$$

(a) 1st Neighbor C_6

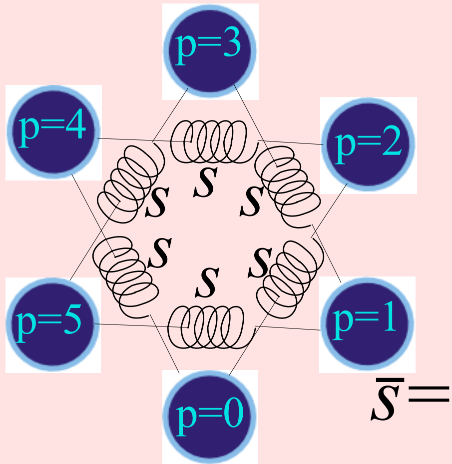


$\bar{r}=r^*=r$

$$\mathbf{H}^{B1(6)}=2r\mathbf{1}-r\mathbf{r}^{1}-r\mathbf{r}^{-1}$$

$$\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p \\
\hline
2r & -r & \cdot & \cdot & \cdot & -r & 0 \\
-r & 2r & -r & \cdot & \cdot & \cdot & 1 \\
\cdot & -r & 2r & -r & \cdot & \cdot & 2 \\
\cdot & \cdot & -r & 2r & -r & \cdot & 3 \\
\cdot & \cdot & \cdot & -r & 2r & -r & 4 \\
-r & \cdot & \cdot & \cdot & -r & 2r & 5
\end{array}$$

(b) 2nd Neighbor C_6



$\bar{s}=s^*=s$

$$\mathbf{H}^{B2(6)}=H_2\mathbf{1}-s\mathbf{r}^{2}-s\mathbf{r}^{-2}$$

$$\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p \\
\hline
H_2 & \cdot & -s & \cdot & -s & \cdot & 0 \\
\cdot & H_2 & \cdot & -s & \cdot & -s & 1 \\
-s & \cdot & H_2 & \cdot & -s & \cdot & 2 \\
\cdot & -s & \cdot & H_2 & \cdot & -s & 3 \\
-s & \cdot & -s & \cdot & H_2 & \cdot & 4 \\
\cdot & -s & \cdot & -s & \cdot & H_2 & 5
\end{array}$$

Conjugation symmetry

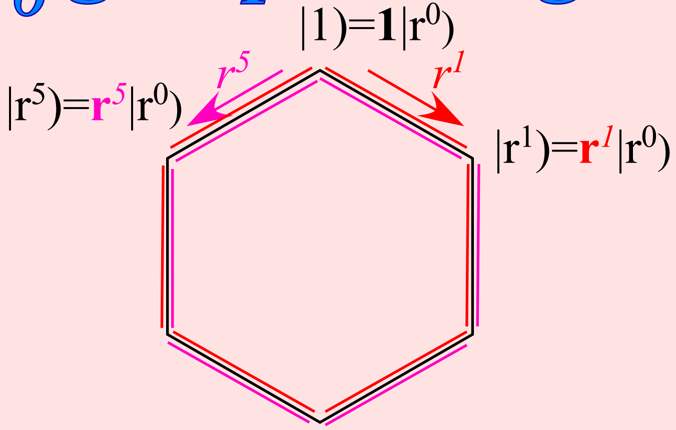
$(\mathbf{H}^*_{jk}=\mathbf{H}_{kj})$

requires $r_0^*=r_0$ and $r_2=r_4^*$.

r_1 equals conjugate of r_5: ($r_1=r_5^* = -r$)

$(r_2=r_4^* = -s)$ *We assume both are real*

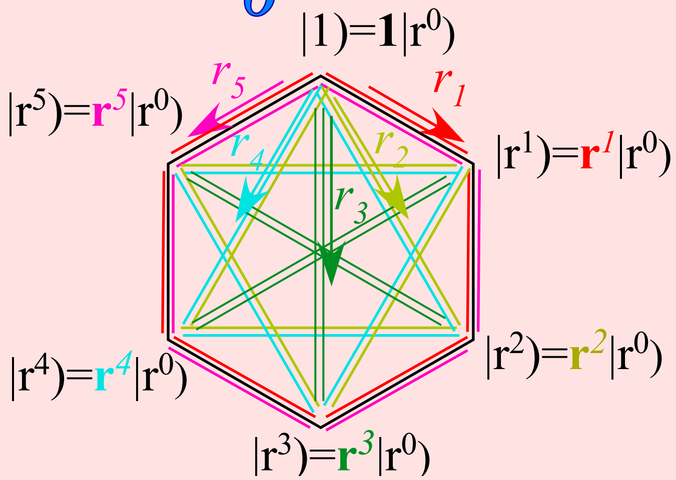
C_6 group table gives $\mathbf{r}$-matrices,..., and all C_6-allowed $\mathbb{H}$-matrices...



2^{nd} Nearest neighbor coupling:

$$\mathbf{H}^{B1(6)}=r_0\mathbf{1}+r_2\mathbf{r}^2+r_4\mathbf{r}^4$$

$$\begin{pmatrix}
r_0 & \cdot & r_4 & \cdot & r_2 & \cdot \\
\cdot & r_0 & \cdot & r_4 & \cdot & r_2 \\
r_2 & \cdot & r_0 & \cdot & r_4 & \cdot \\
\cdot & r_2 & \cdot & r_0 & \cdot & r_4 \\
r_4 & \cdot & r_2 & \cdot & r_0 & \cdot \\
\cdot & r_4 & \cdot & r_2 & \cdot & r_0
\end{pmatrix}$$

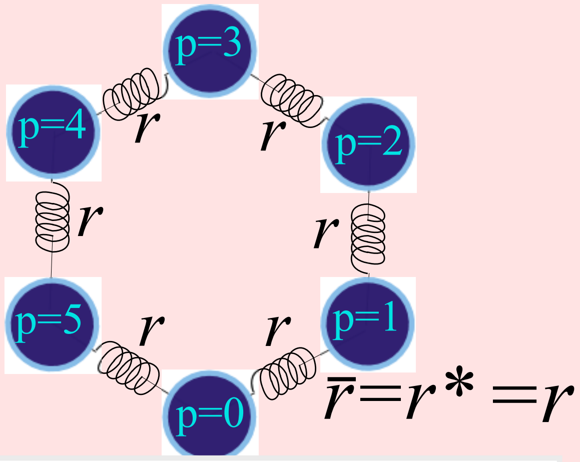


All – neighbor coupling:

$$\mathbf{H}^{A(6)}=r_0\mathbf{1}+r_1\mathbf{r}^1+r_2\mathbf{r}^2+r_3\mathbf{r}^3+r_4\mathbf{r}^4+r_5\mathbf{r}^5$$

$$\begin{pmatrix}
r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\
r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\
r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\
r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\
r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\
r_5 & r_4 & r_3 & r_2 & r_1 & r_0
\end{pmatrix}$$

(a) 1st Neighbor C_6

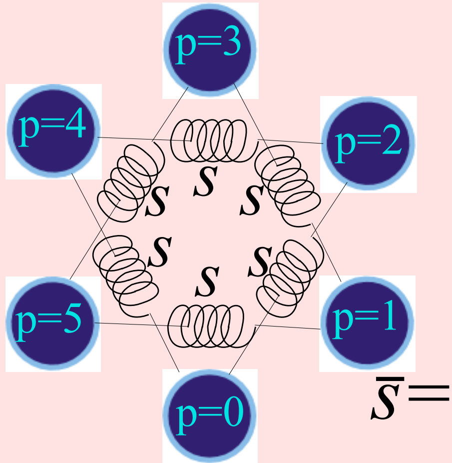


$\bar{r}=r^*=r$

$$\mathbf{H}^{B1(6)}=2r\mathbf{1}-r\mathbf{r}^{1}-r\mathbf{r}^{-1}$$

$$\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p \\
\hline
2r & -r & \cdot & \cdot & \cdot & -r & 0 \\
-r & 2r & -r & \cdot & \cdot & \cdot & 1 \\
\cdot & -r & 2r & -r & \cdot & \cdot & 2 \\
\cdot & \cdot & -r & 2r & -r & \cdot & 3 \\
\cdot & \cdot & \cdot & -r & 2r & -r & 4 \\
-r & \cdot & \cdot & \cdot & -r & 2r & 5
\end{array}$$

Neighbor C_6

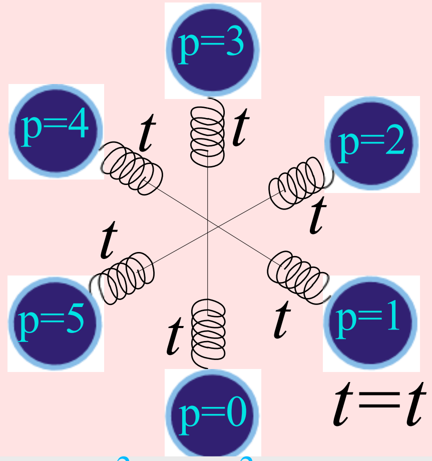


$\bar{s}=s^*=s$

$$\mathbf{H}^{B2(6)}=H_2\mathbf{1}-s\mathbf{r}^{2}-s\mathbf{r}^{-2}$$

$$\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p \\
\hline
H_2 & \cdot & -s & \cdot & -s & \cdot & 0 \\
\cdot & H_2 & \cdot & -s & \cdot & -s & 1 \\
-s & \cdot & H_2 & \cdot & -s & \cdot & 2 \\
\cdot & -s & \cdot & H_2 & \cdot & -s & 3 \\
-s & \cdot & -s & \cdot & H_2 & \cdot & 4 \\
\cdot & -s & \cdot & -s & \cdot & H_2 & 5
\end{array}$$

(c) 3rd Neighbor C_6



$t=t^*$

$$\mathbf{H}^{B3(6)}=H_3\mathbf{1}-t\mathbf{r}^{3}-t\mathbf{r}^{-3}$$

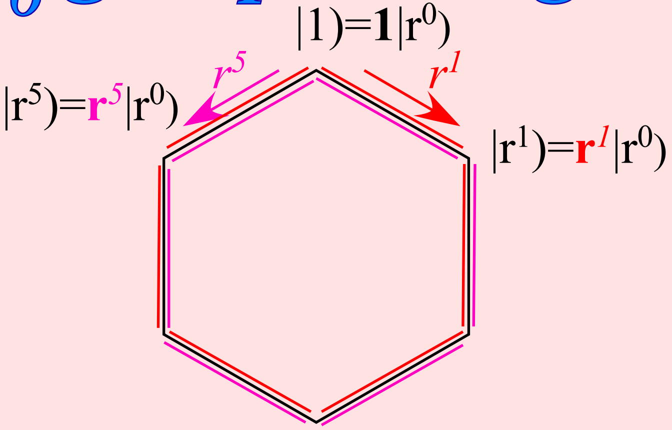
$$\begin{array}{cccccc|c}
0 & 1 & 2 & 3 & 4 & 5 & p \\
\hline
H_3 & \cdot & \cdot & -t & \cdot & \cdot & 0 \\
\cdot & H_3 & \cdot & \cdot & -t & \cdot & 1 \\
\cdot & \cdot & H_3 & \cdot & \cdot & -t & 2 \\
-t & \cdot & \cdot & H_3 & \cdot & \cdot & 3 \\
\cdot & -t & \cdot & \cdot & H_3 & \cdot & 4 \\
\cdot & \cdot & -t & \cdot & \cdot & H_3 & 5
\end{array}$$

r_1 equals conjugate of r_5: ($r_1=r_5^*=-r$)

$(r_2=r_4^*=-s)$

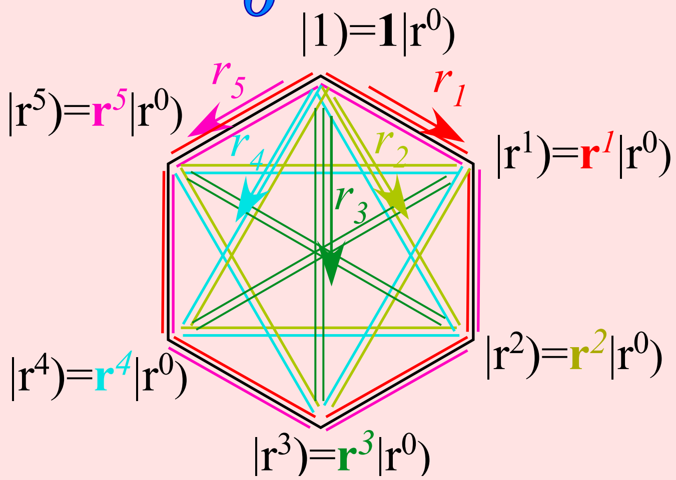
$(r_3=r_3^*=t)$ *must* be real

C_6 group table gives $\mathbf{r}$-matrices,..., and all C_6-allowed $\mathbb{H}$-matrices...



Nearest neighbor coupling

$$\begin{pmatrix}
r_0 & r_5 & & & & r_1 \\
r_1 & r_0 & r_5 & & & \\
 & r_1 & r_0 & r_5 & & \\
 & & r_1 & r_0 & r_5 & \\
 & & & r_1 & r_0 & r_5 \\
r_5 & & & & r_1 & r_0
\end{pmatrix}$$



ALL neighbor coupling

$$\begin{pmatrix}
r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\
r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\
r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\
r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\
r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\
r_5 & r_4 & r_3 & r_2 & r_1 & r_0
\end{pmatrix}$$

2^{nd} Step

H diagonalized by spectral resolution of $r, r^2,\ldots,r^6 = 1$

All $x=r^p$ satisfy $x^6=1$ and use **6^{th}-roots-of-1** *for eigenvalues*

$$D^m(\mathbf{r})=e^{-2\pi i m/6}=\chi_1{}^m=\psi_1{}^{m*}$$

$$D^m(\mathbf{r}^p)=e^{-2\pi i m\cdot p/6}=\chi_p{}^m=\psi_p{}^{m*}$$

$\psi_1{}^0=1$

$\psi_1{}^1=e^{2\pi i/6}$

$\psi_1{}^2=\psi_2{}^1=e^{4\pi i/6}$

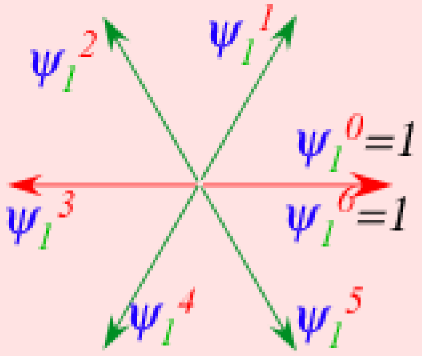
$\psi_1{}^3=\psi_3{}^1=-1$

$\psi_1{}^4=\psi_4{}^1=\psi_1{}^{-2}=e^{-4\pi i/6}$

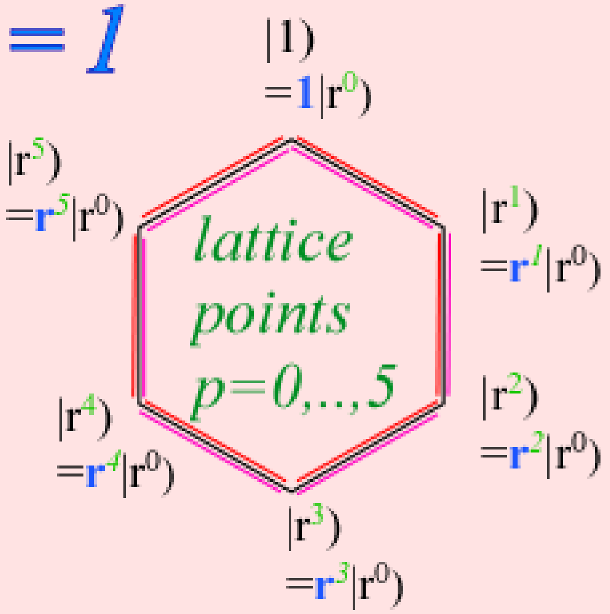
$\psi_1{}^5=\psi_5{}^1=\psi_1{}^{-1}=e^{-2\pi i/6}$

p=power (exponent) or position point

m = momentum or wave-number



6^{th}-roots of 1
m=0,...,5



Groups "know" their roots and will tell you them if you ask nicely!

You efficiently get:

- *invariant projectors*
- *irreducible projectors*
- *irreducible representations (irreps)*
- *H eigenvalues*
- *H eigenvectors*
- *T matrices*
- *dispersion functions*

2^{nd} Step (contd.)

H diagonalized by spectral resolution of $r, r^2, \ldots, r^6 = 1$

top-row flip
not needed...

$$\mathbf{P}^{(m)} = \mathbf{P}^{(m)\dagger}$$

All $x = r^p$ satisfy $x^6 = 1$ and use *6th-roots-of-1* *for eigenvalues*

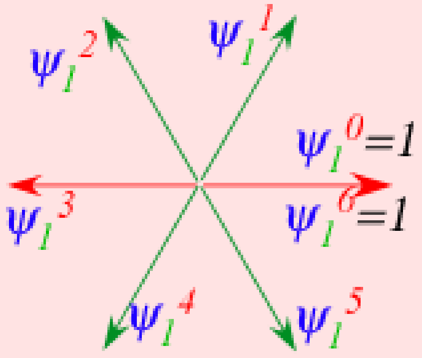
$$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1{}^m = \psi_1{}^{m*}$$

$$D^m(\mathbf{r}^p) = e^{-2\pi i m \cdot p/6} = \chi_p{}^m = \psi_p{}^{m*}$$

$\psi_1{}^0 = 1$
$\psi_1{}^1 = e^{2\pi i/6}$
$\psi_1{}^2 = \psi_2{}^1 = e^{4\pi i/6}$
$\psi_1{}^3 = \psi_3{}^1 = -1$
$\psi_1{}^4 = \psi_4{}^1 = \psi_1{}^{-2} = e^{-4\pi i/6}$
$\psi_1{}^5 = \psi_5{}^1 = \psi_1{}^{-1} = e^{-2\pi i/6}$

p=power (exponent)
or position point

m = momentum
or wave-number



$$\begin{array}{c|cccccc}
6 \text{ ring} & \mathbf{P}^{(0)} & \mathbf{P}^{(1)} & \mathbf{P}^{(2)} & \mathbf{P}^{(3)} & \mathbf{P}^{(4)} & \mathbf{P}^{(5)} \\ \hline
\mathbf{P}^{(0)} & \mathbf{P}^{(0)} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\mathbf{P}^{(1)} & \cdot & \mathbf{P}^{(1)} & \cdot & \cdot & \cdot & \cdot \\
\mathbf{P}^{(2)} & \cdot & \cdot & \mathbf{P}^{(2)} & \cdot & \cdot & \cdot \\
\mathbf{P}^{(3)} & \cdot & \cdot & \cdot & \mathbf{P}^{(3)} & \cdot & \cdot \\
\mathbf{P}^{(4)} & \cdot & \cdot & \cdot & \cdot & \mathbf{P}^{(4)} & \cdot \\
\mathbf{P}^{(5)} & \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{P}^{(5)}
\end{array}$$

$$\mathbf{r}^p = \chi_p{}^0\,\mathbf{P}^{(0)} + \chi_p{}^1\,\mathbf{P}^{(1)} + \chi_p{}^2\,\mathbf{P}^{(2)} + \chi_p{}^3\,\mathbf{P}^{(3)} + \chi_p{}^4\,\mathbf{P}^{(4)} + \chi_p{}^5\,\mathbf{P}^{(5)}$$

$$\begin{pmatrix}
\chi_p{}^0 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \chi_p{}^1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \chi_p{}^2 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \chi_p{}^3 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \chi_p{}^4 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \chi_p{}^5
\end{pmatrix}
= \chi_p{}^0 \begin{pmatrix}
1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
+ \chi_p{}^1 \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
+ \chi_p{}^2 \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
+ \chi_p{}^3 \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
+ \chi_p{}^4 \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
+ \chi_p{}^5 \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{pmatrix}$$

Projectors $\mathbf{P}^{(m)}$ ***are eigenvalue "placeholders" having orthogonal-idempotent products, eigen-equations,***

$$\mathbf{P}^{(m)}\mathbf{P}^{(n)} = \delta^{mn}\mathbf{P}^{(m)} \qquad \mathbf{r}^p\,\mathbf{P}^{(n)} = \chi_p{}^n\mathbf{P}^{(n)}$$

and one completeness rule: $\mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \ldots + \mathbf{P}^{(5)} = \mathbf{1}$

2^{nd} Step (contd.)

H diagonalized by spectral resolution of $r, r^2, \ldots, r^6 = 1$

top-row flip
not needed...

$\mathbf{P}^{(m)} = \mathbf{P}^{(m)\dagger}$

All $x = r^p$ satisfy $x^6 = 1$ and use **6th-roots-of-1** *for eigenvalues*

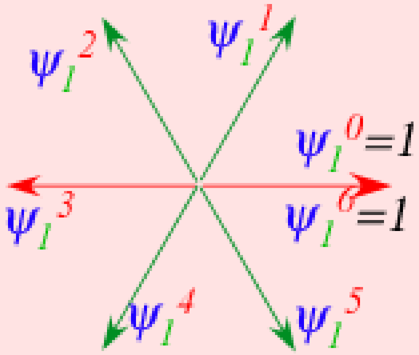
$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1^m = \psi_1^{m*}$

$D^m(\mathbf{r}^p) = e^{-2\pi i m\cdot p/6} = \chi_p^m = \psi_p^{m*}$

$\psi_1^0 = 1$
$\psi_1^1 = e^{2\pi i/6}$
$\psi_1^2 = \psi_2^1 = e^{4\pi i/6}$
$\psi_1^3 = \psi_3^1 = -1$
$\psi_1^4 = \psi_4^1 = \psi_1^{-2} = e^{-4\pi i/6}$
$\psi_1^5 = \psi_5^1 = \psi_1^{-1} = e^{-2\pi i/6}$

p = power (exponent)
or position point

m = momentum
or wave-number



$$\begin{array}{c|cccccc}
{}_6\,\text{ring} & \mathbf{P}^{(0)} & \mathbf{P}^{(1)} & \mathbf{P}^{(2)} & \mathbf{P}^{(3)} & \mathbf{P}^{(4)} & \mathbf{P}^{(5)} \\
\hline
^{(0)} & \mathbf{P}^{(0)} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\mathbf{P}^{(1)} & \cdot & \mathbf{P}^{(1)} & \cdot & \cdot & \cdot & \cdot \\
\mathbf{P}^{(2)} & \cdot & \cdot & \mathbf{P}^{(2)} & \cdot & \cdot & \cdot \\
\mathbf{P}^{(3)} & \cdot & \cdot & \cdot & \mathbf{P}^{(3)} & \cdot & \cdot \\
\mathbf{P}^{(4)} & \cdot & \cdot & \cdot & \cdot & \mathbf{P}^{(4)} & \cdot \\
\mathbf{P}^{(5)} & \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{P}^{(5)}
\end{array}$$

$$\mathbf{r}^p = \chi_p^0\,\mathbf{P}^{(0)} + \chi_p^1\,\mathbf{P}^{(1)} + \chi_p^2\,\mathbf{P}^{(2)} + \chi_p^3\,\mathbf{P}^{(3)} + \chi_p^4\,\mathbf{P}^{(4)} + \chi_p^5\,\mathbf{P}^{(5)}$$

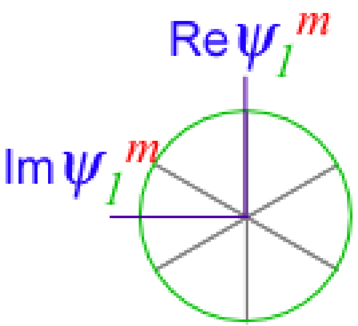
$$\begin{pmatrix}\chi_p^0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \chi_p^1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \chi_p^2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \chi_p^3 & \cdot & \cdot \end{pmatrix} = \chi_p^0\begin{pmatrix}1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + \chi_p^1\begin{pmatrix}\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + \chi_p^2\begin{pmatrix}\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} + \chi_p^3\begin{pmatrix}\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + \chi_p^4\begin{pmatrix}\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + \chi_p^5\begin{pmatrix}\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

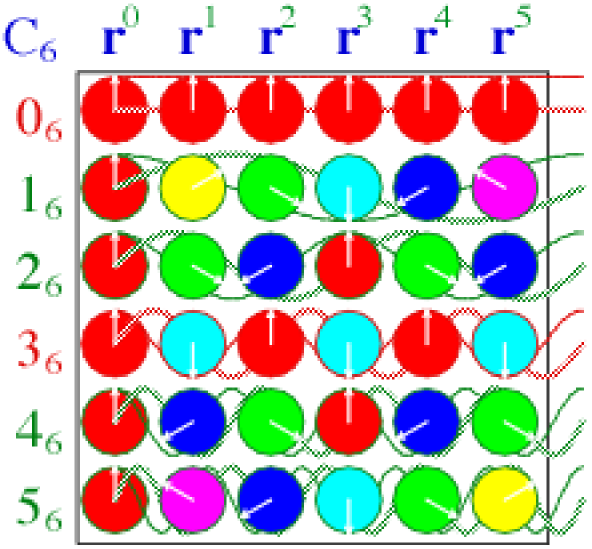
Inverse C_6 spectral resolution m-wave $\psi_p^m = D^{m*}(\mathbf{r}^p) = e^{+2\pi i m\cdot p/6}$:

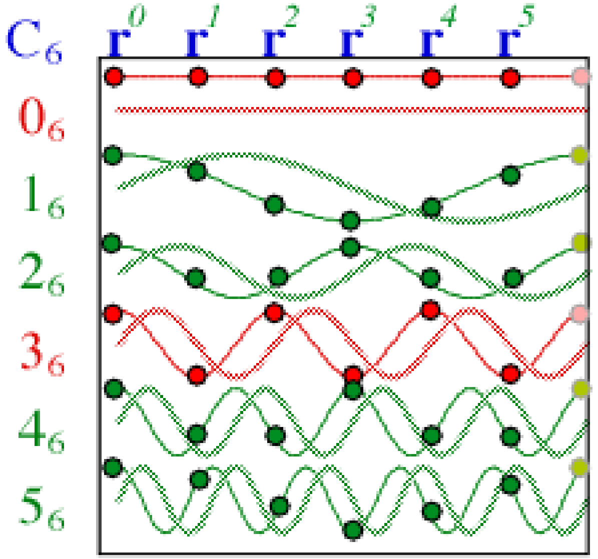
$$6\cdot\mathbf{P}^{(m)} = \psi_0^m\,\mathbf{r}^0 + \psi_1^m\,\mathbf{r}^1 + \psi_2^m\,\mathbf{r}^2 + \psi_3^m\,\mathbf{r}^3 + \psi_4^m\,\mathbf{r}^4 + \psi_5^m\,\mathbf{r}^5$$

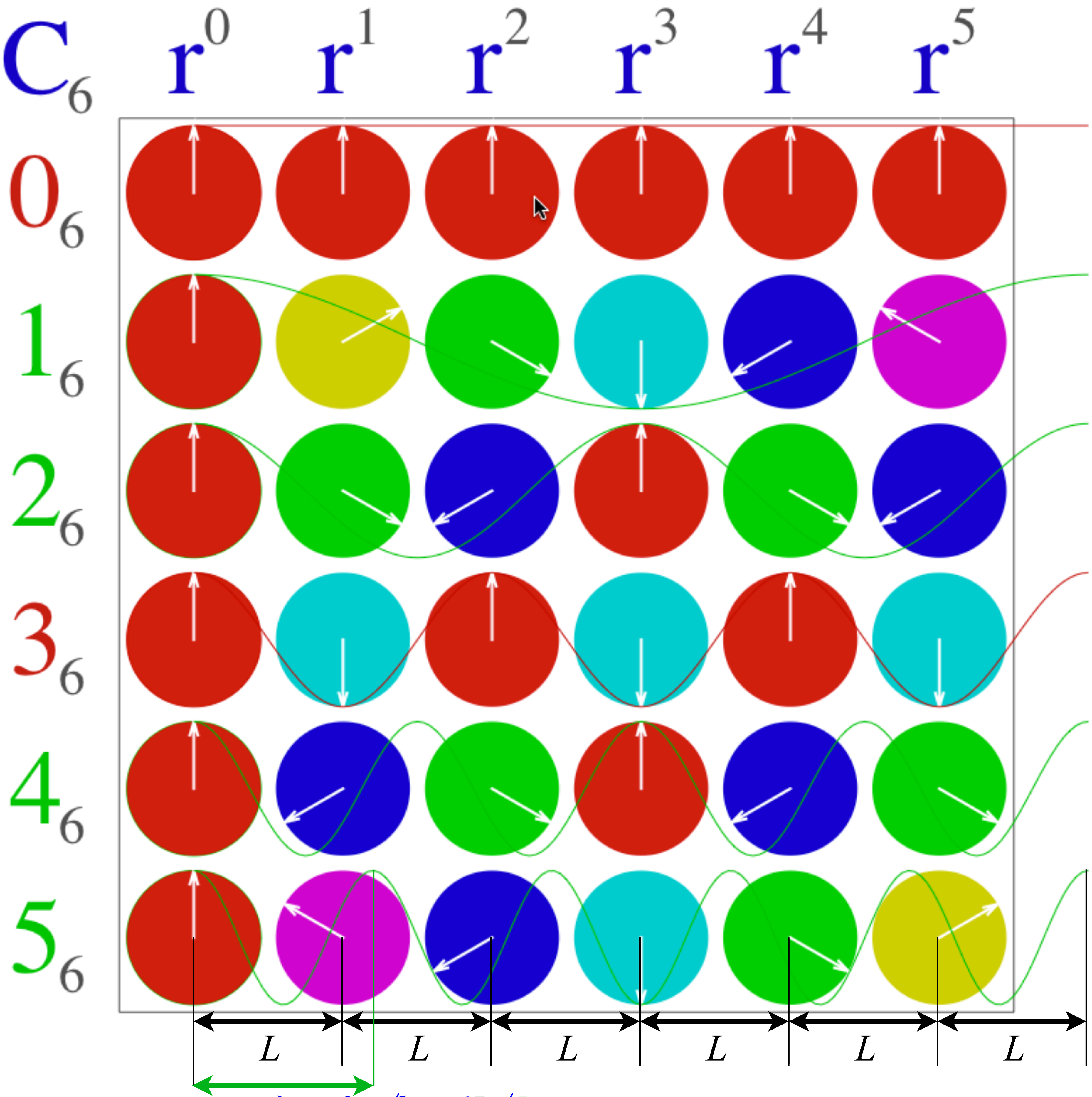
position p (or power of $\mathbf{r}^p$)

momentum m	p=0	1	2	3	4	5
m=0	ψ_0^0	ψ_1^0	ψ_2^0	ψ_3^0	ψ_4^0	ψ_5^0
m=1	ψ_0^1	ψ_1^1	ψ_2^1	ψ_3^1	ψ_4^1	ψ_5^1
m=2	ψ_0^2	ψ_1^2	ψ_2^2	ψ_3^2	ψ_4^2	ψ_5^2
m=3	ψ_0^3	ψ_1^3	ψ_2^3	ψ_3^3	ψ_4^3	ψ_5^3
m=4	ψ_0^4	ψ_1^4	ψ_2^4	ψ_3^4	ψ_4^4	ψ_5^4
m=5	ψ_0^5	ψ_1^5	ψ_2^5	ψ_3^5	ψ_4^5	ψ_5^5









$\lambda_5 = 2\pi/k_5 = 6L/5$

C_6 character

$$\chi_{mp} = e^{-imp2\pi/6}$$

is wave function conjugate

$$\psi^*_m(r_p) = \frac{e^{-imp2\pi/6}}{\sqrt{6}}$$ (with norm √6)

C_6 Plane wave function

$$\psi_m(r_p) = \frac{e^{ik_m \cdot r_p}}{\sqrt{6}}$$

$$= \frac{e^{imp2\pi/6}}{\sqrt{6}}$$

C_6 Lattice position vector

$$r_p = L \cdot p$$

Wavevector

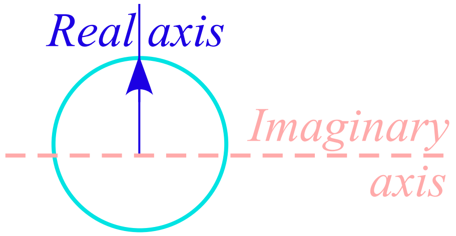
$$k_m = 2\pi m/6L = 2\pi/\lambda_m$$

Wavelength

$$\lambda_m = 2\pi/k_m = 6L/m$$

WaveIt App

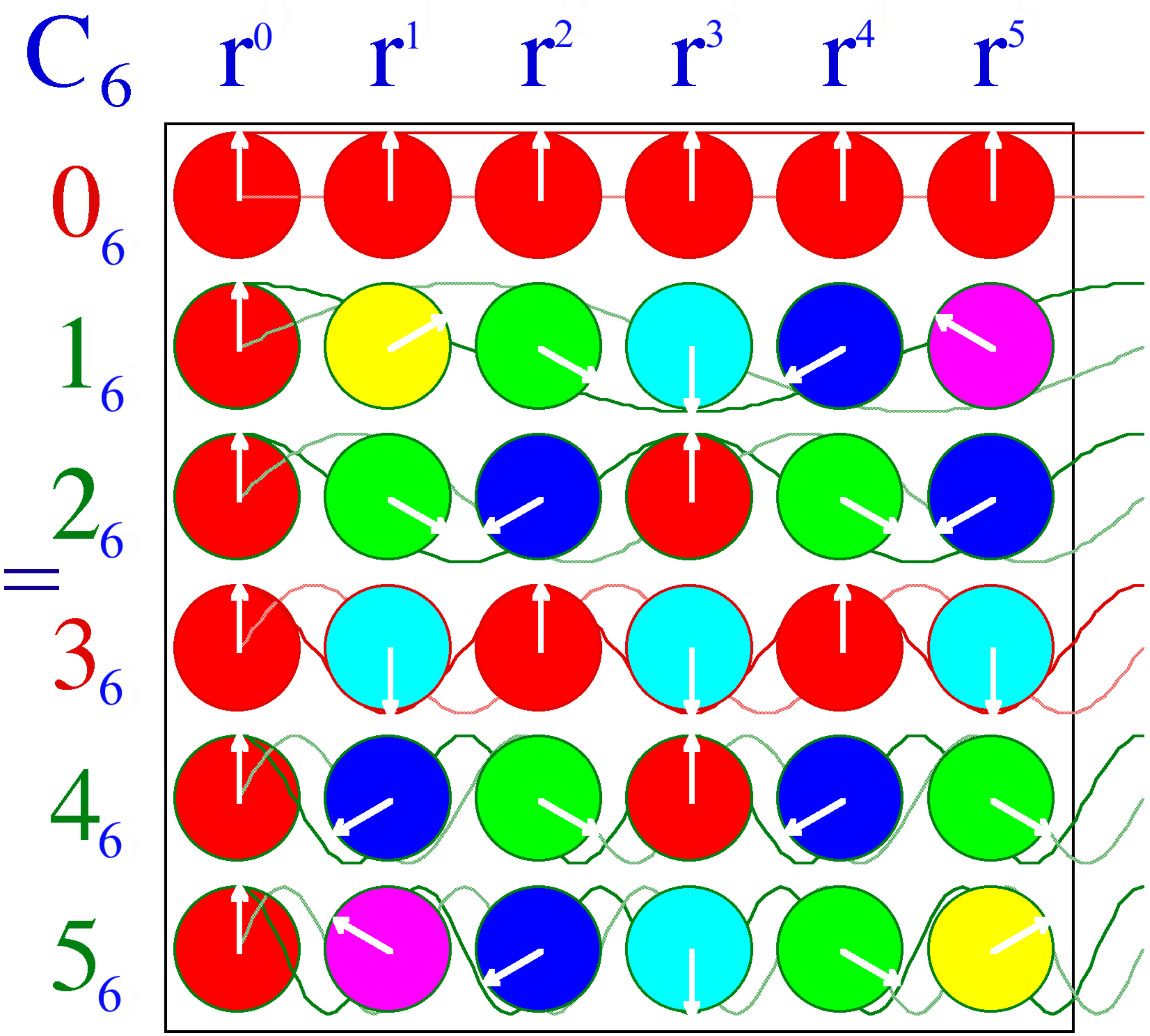
Backwards phasors
for
conjugate waves
(turn counter-clockwise)



$\chi^{m}_{p}(C_6)$	$\mathbf{r}^{p=0}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{r}^3$	$\mathbf{r}^4$	$\mathbf{r}^5$
$m=0_6$	1	1	1	1	1	1
1_6	1	ε^*	ε^{2*}	-1	ε^2	ε
2_6	1	ε^{2*}	ε^2	1	ε^{2*}	ε^2
$3_6=-3_6$	1	-1	1	-1	1	-1
$4_6=-2_6$	1	ε^2	ε^{2*}	1	ε^2	ε^{2*}
$5_6=-1_6$	1	ε	ε^2	-1	ε^{2*}	ε

$=$

$$\varepsilon=e^{i2\pi/6}$$

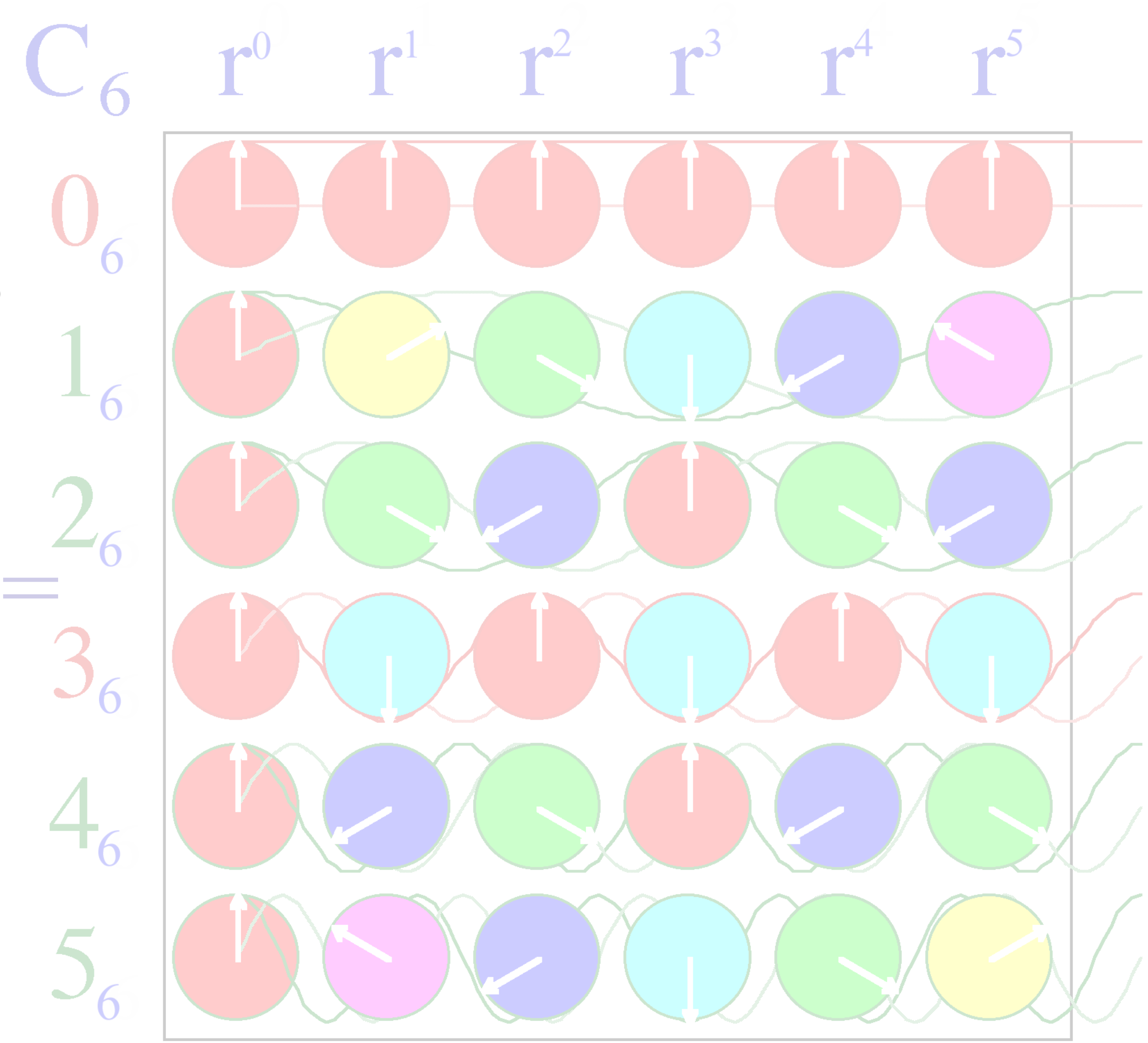


WaveIt App

	$0°$	$60°$	$120°$	$180°$	$-120°$	$-60°$
α	1	1	1	1	1	1
β	1	ε^{*}	ε^{2*}	-1	ε^{2}	ε
γ	1	ε^{2*}	ε^{2}	1	ε^{2*}	ε^{2}
δ	1	-1	1	-1	1	-1
γ^{*}	1	ε^{2}	ε^{2*}	1	ε^{2}	ε^{2*}
β^{*}	1	ε	ε^{2}	-1	ε^{2*}	ε

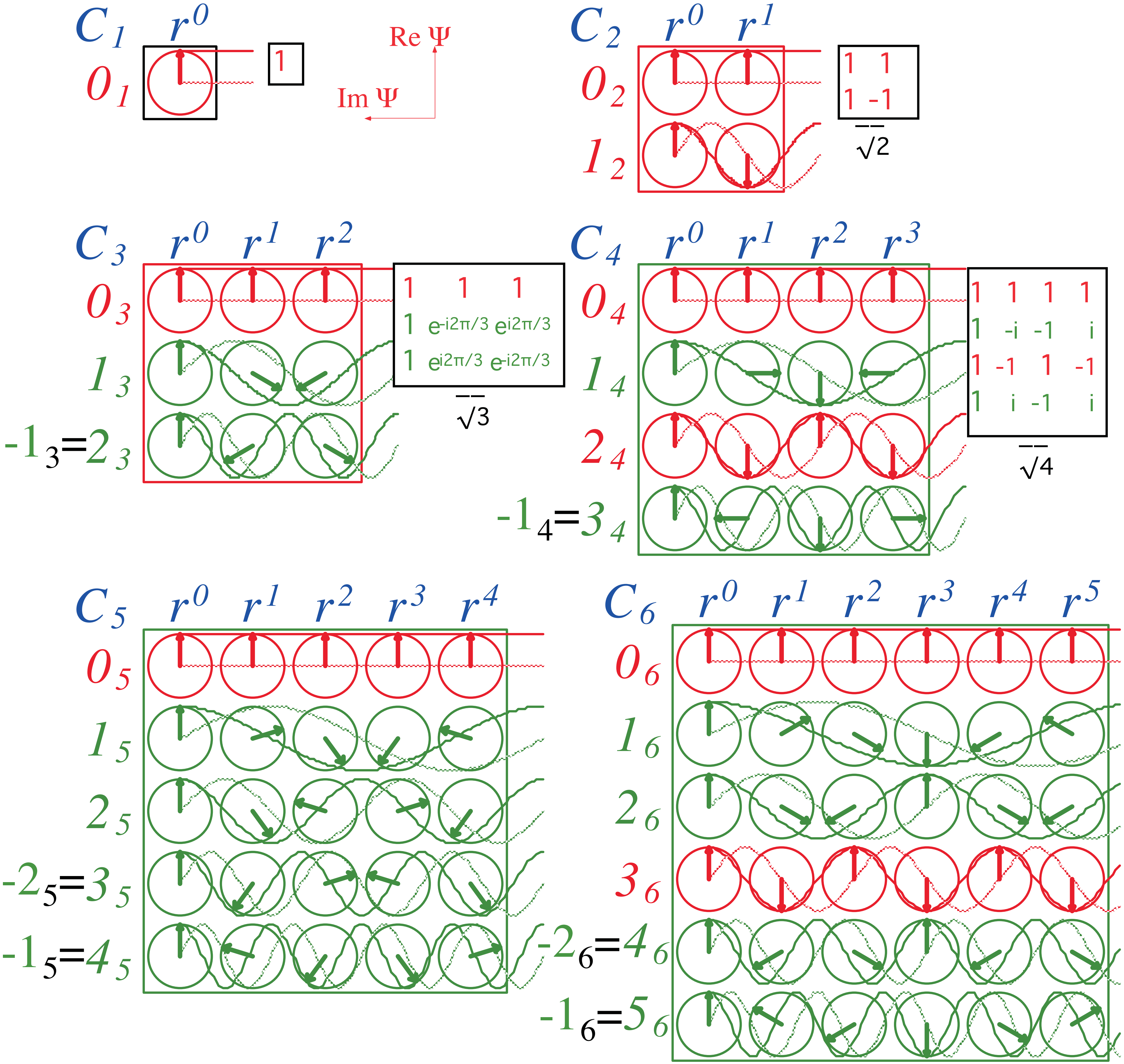
$$\varepsilon = e^{i2\pi/6}$$

What you'll get
if you look up
C_6 characters in library



Wave phasor stuff? FUGggedd-aboudit!

WaveIt App



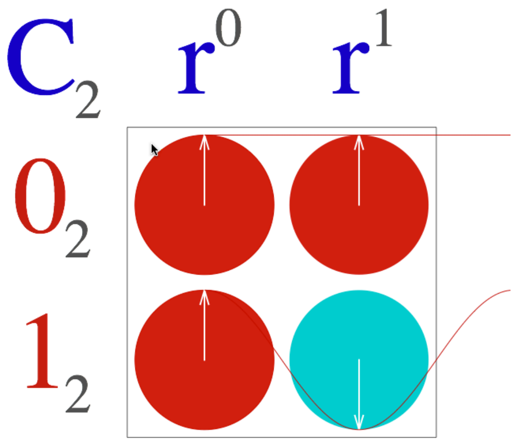
$$\boxed{1}$$

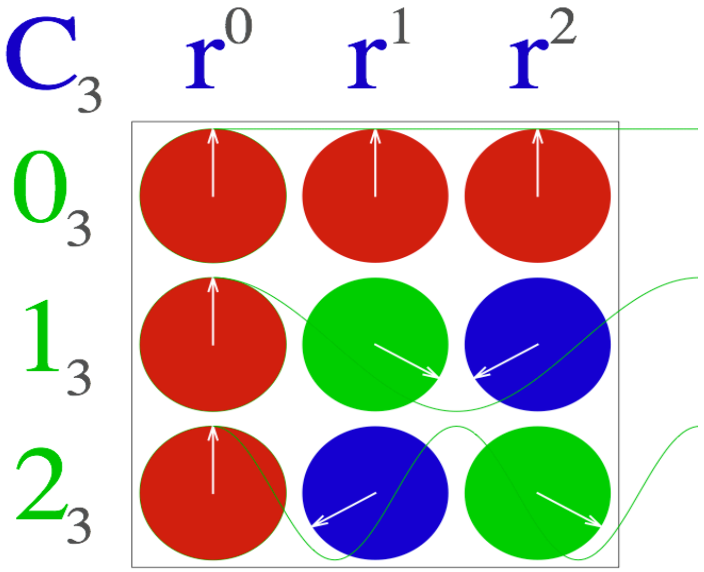
$$\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\quad \frac{\quad}{\sqrt{2}}$$

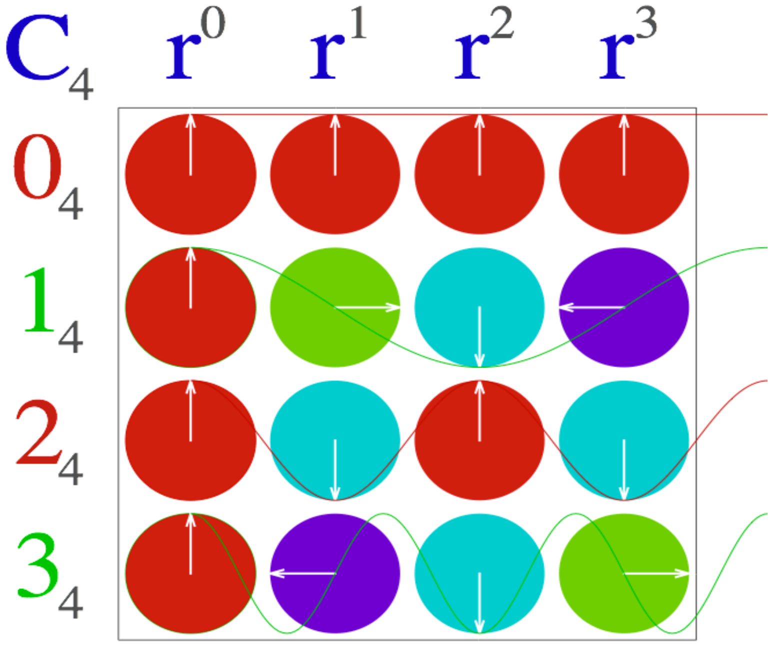
$$\begin{pmatrix}1 & 1 & 1\\ 1 & e^{-i2\pi/3} & e^{i2\pi/3}\\ 1 & e^{i2\pi/3} & e^{-i2\pi/3}\end{pmatrix}\quad \frac{\quad}{\sqrt{3}}$$

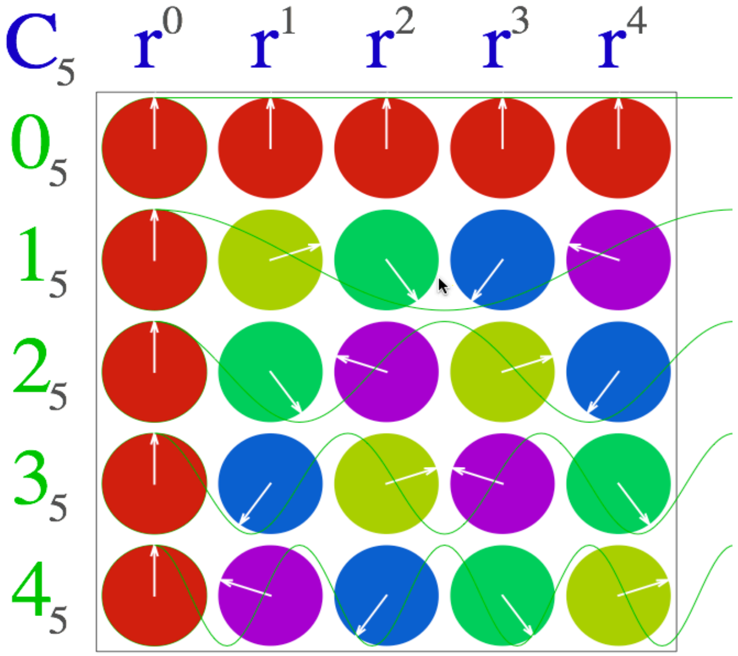
$$\begin{pmatrix}1 & 1 & 1 & 1\\ 1 & -i & -1 & i\\ 1 & -1 & 1 & -1\\ 1 & i & -1 & i\end{pmatrix}\quad \frac{\quad}{\sqrt{4}}$$

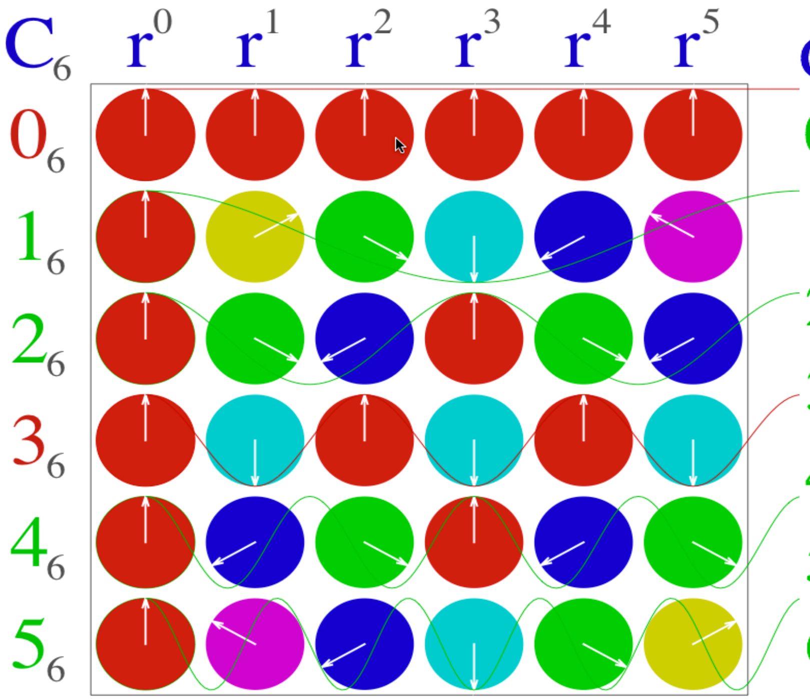
WaveIt App

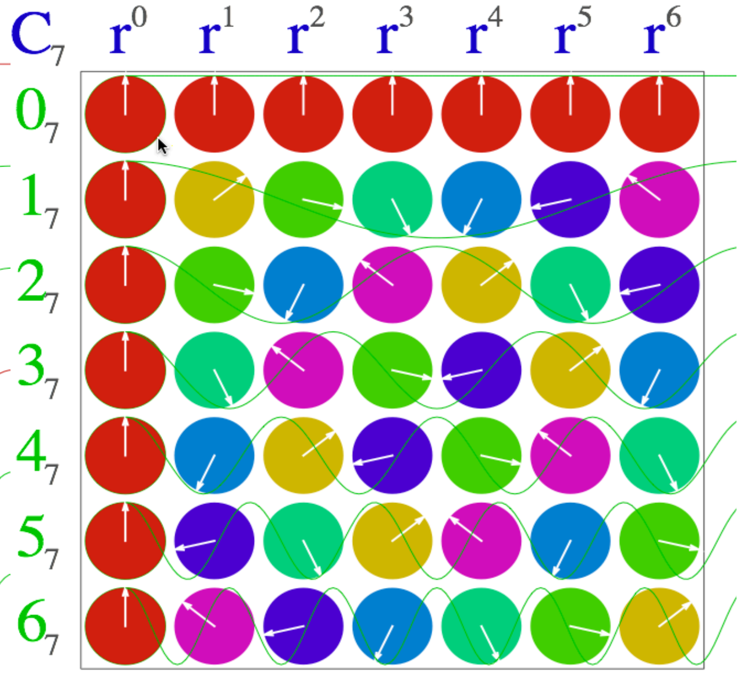

C_2
r^0
r^1
0_2
1_2


C_3
r^0
r^1
r^2
0_3
1_3
2_3

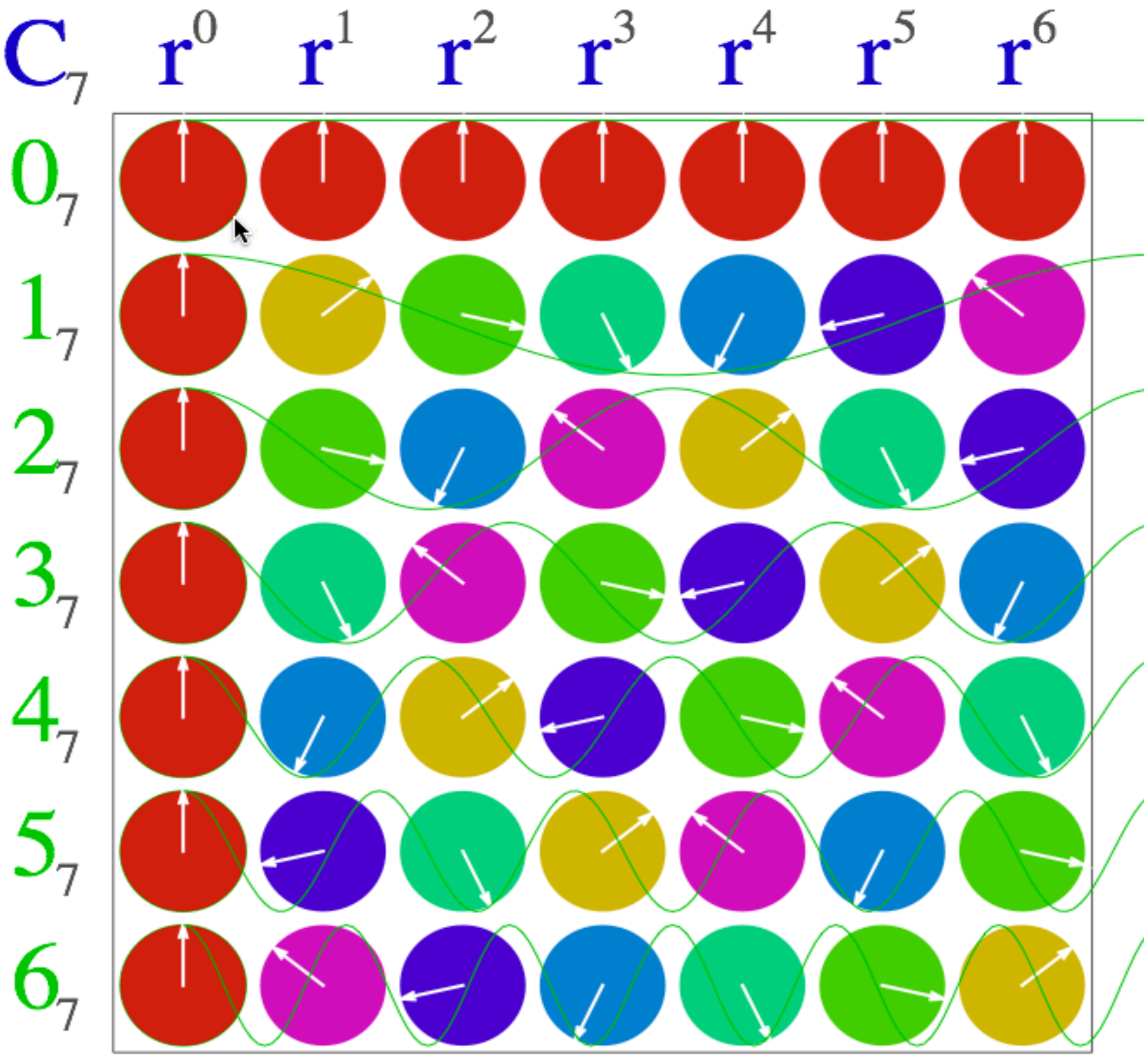

C_4
r^0
r^1
r^2
r^3
0_4
1_4
2_4
3_4


C_5
r^0
r^1
r^2
r^3
r^4
0_5
1_5
2_5
3_5
4_5


C_6
r^0
r^1
r^2
r^3
r^4
r^5
0_6
1_6
2_6
3_6
4_6
5_6


C_7
r^0
r^1
r^2
r^3
r^4
r^5
r^6
0_7
1_7
2_7
3_7
4_7
5_7
6_7

WaveIt App



WaveIt App

C_N *Lattice position vector*

$r_p = L \cdot p$

Wavevector

$k_m = 2\pi / \lambda_m$

$= 2\pi m / NL$

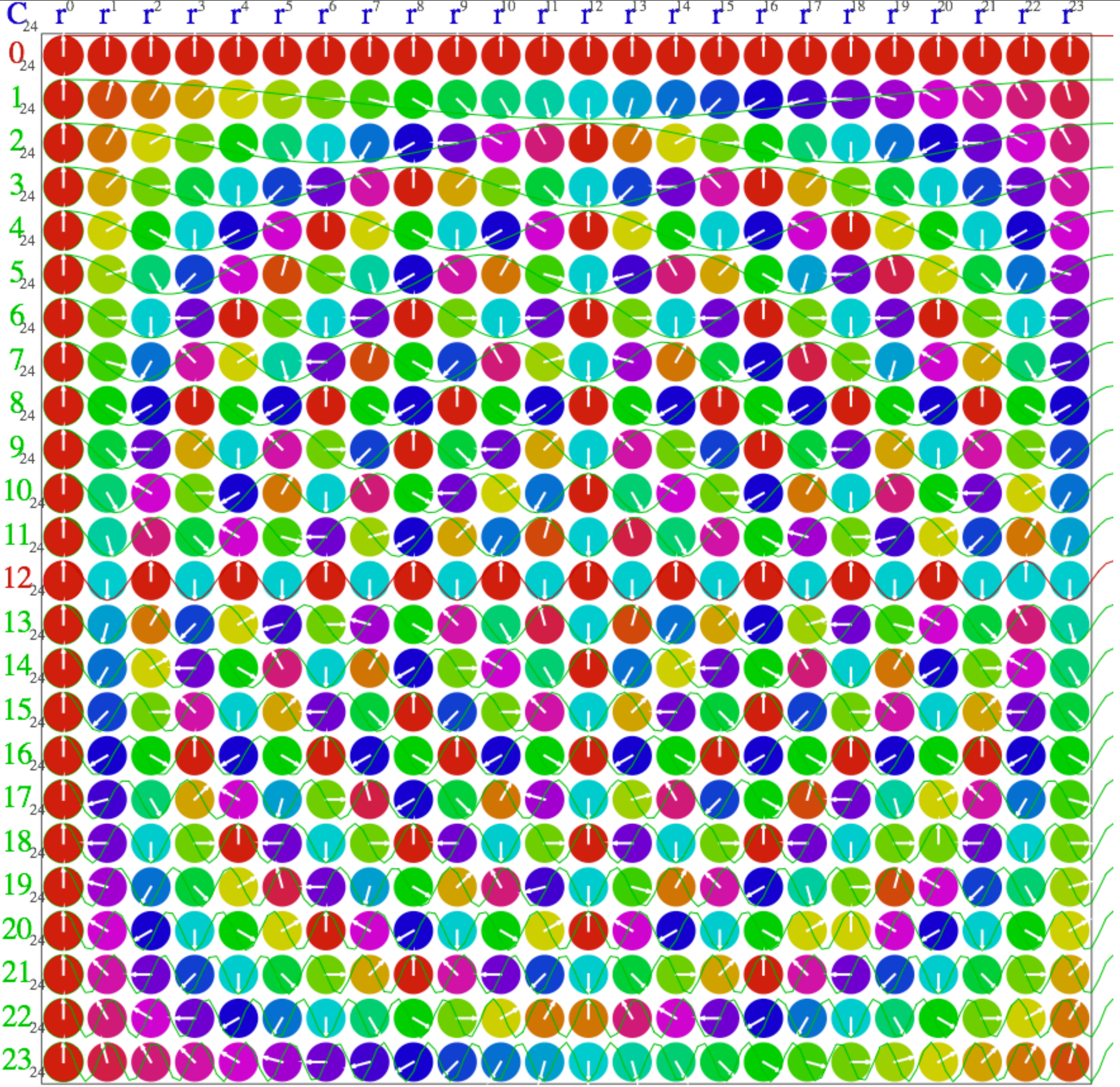
Wavelength

$\lambda_m = 2\pi / k_m$

$= NL / m$

C_N *Plane wave function*

$$\psi_m(x_p) = \frac{e^{ik_m \cdot x_p}}{\sqrt{N}} = \frac{e^{imp2\pi/N}}{\sqrt{N}}$$



$N=72$

C_{72} Fourier transformation matrix

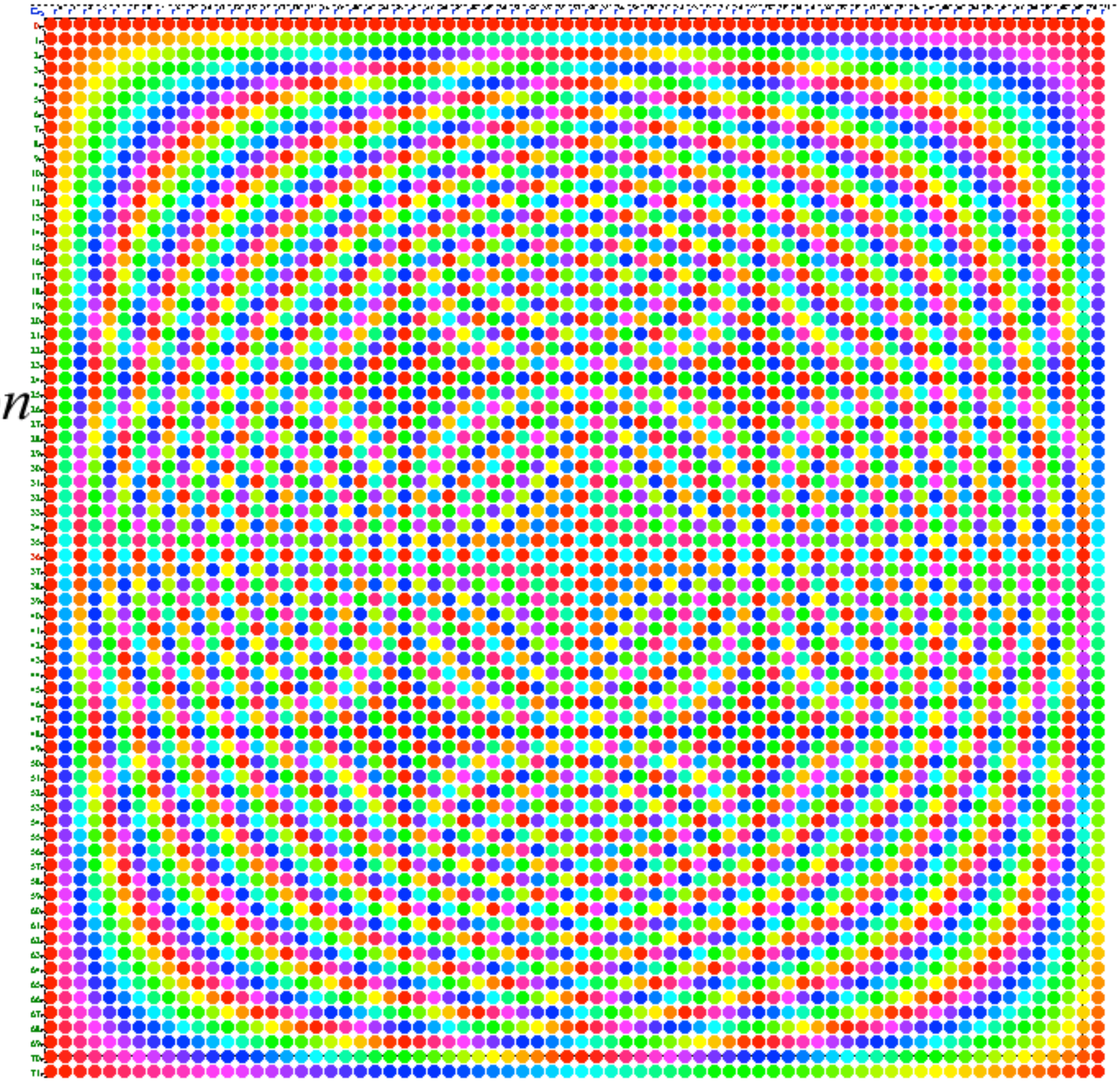
C_N Lattice position vector
$r_p = L\cdot p$

Wavevector
$k_m = 2\pi/\lambda_m$
$= 2\pi m/NL$

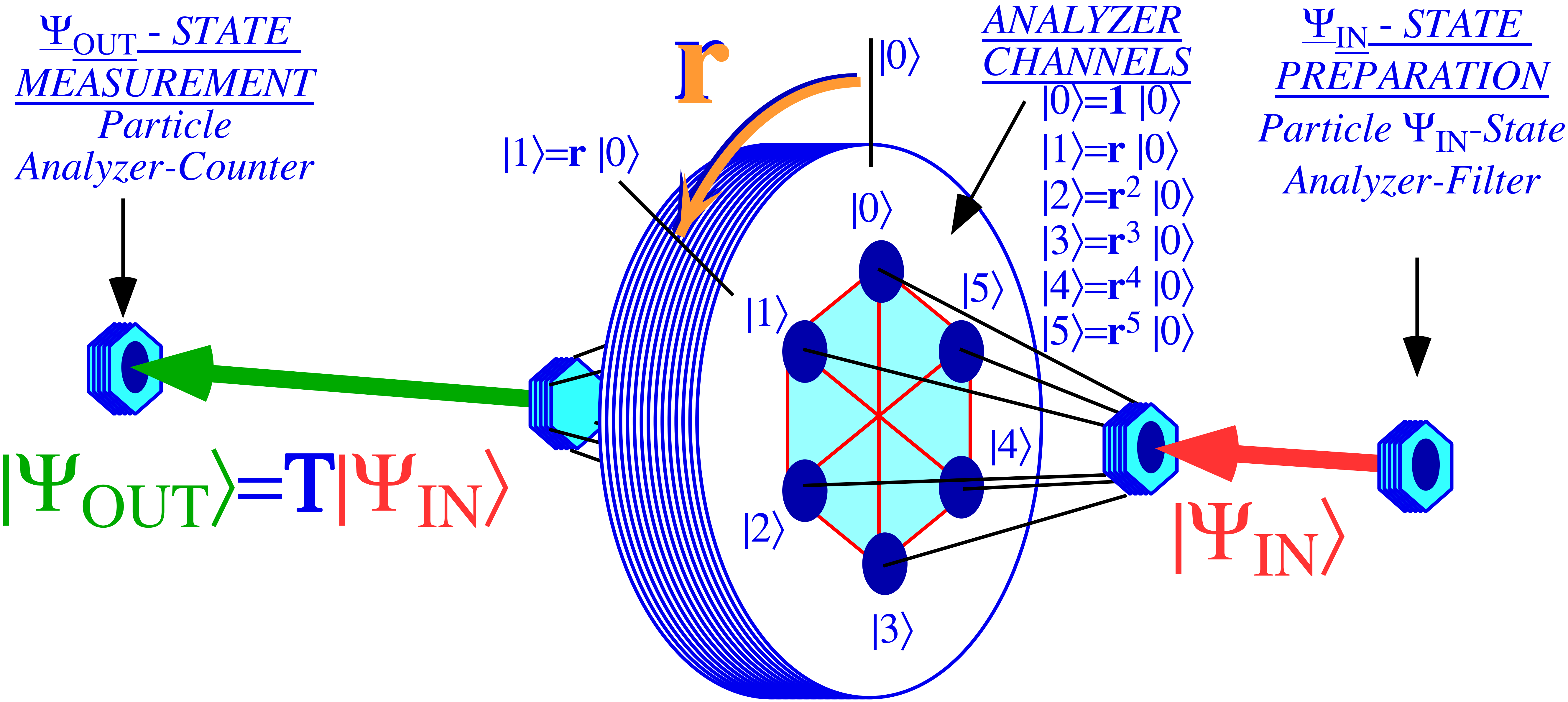
Wavelength
$\lambda_m = 2\pi/k_m$
$= NL/m$

C_N Plane wave function

$$\psi_m(x_p) = \frac{e^{ik_m\cdot x_p}}{\sqrt{N}} = \frac{e^{imp2\pi/N}}{\sqrt{N}}$$



C_6 Beam analyzer used in Unit 3 Ch. 8 thru Ch. 9



Ψ_{OUT} - STATE MEASUREMENT
Particle Analyzer-Counter

$|\Psi_{OUT}\rangle = \mathbf{T}|\Psi_{IN}\rangle$

ANALYZER CHANNELS
$|0\rangle = \mathbf{1}\ |0\rangle$
$|1\rangle = \mathbf{r}\ |0\rangle$
$|2\rangle = \mathbf{r}^2\ |0\rangle$
$|3\rangle = \mathbf{r}^3\ |0\rangle$
$|4\rangle = \mathbf{r}^4\ |0\rangle$
$|5\rangle = \mathbf{r}^5\ |0\rangle$

Ψ_{IN} - STATE PREPARATION
Particle Ψ_{IN}-State Analyzer-Filter

$|\Psi_{IN}\rangle$

Fig. 8.1.1

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: 3rd roots of unity and ortho-completeness relations
C_3 character table and modular labeling

Ortho-completeness inversion for operators and states
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: 6th roots of unity and higher
➡ *Complete sets of coupling parameters and Fourier dispersion*
Gauge shifts due to complex coupling

3rd Step *Display all eigensolutions of all possible C_6 symmetric real H*

$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

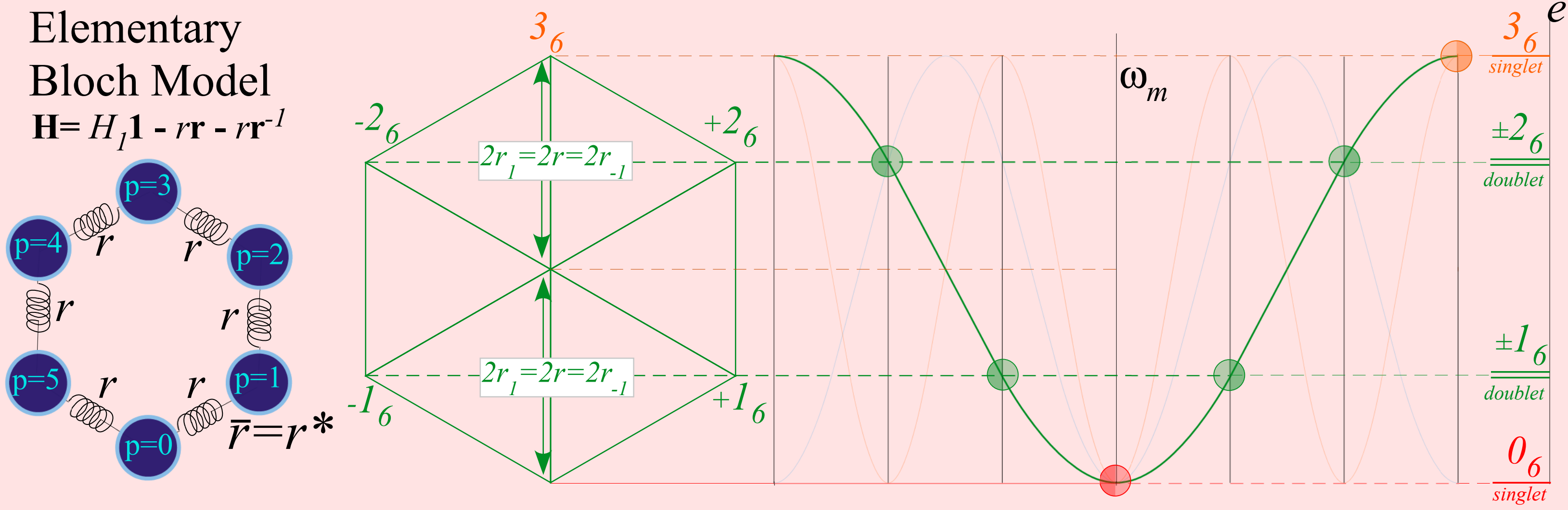
(Dispersion functions)

3^{rd} Step *Display all eigensolutions of all possible C_6 symmetric real H*

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p=\sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)}=\sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)}=\sum_{p=0}^{n-1} r_p \chi_p^m=\omega(k_m)$$

(Dispersion functions)

Elementary
Bloch Model
H= $H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$



eigenvalues of $\mathbf{H}^{B1(6)}$

$$\begin{array}{c|cccccc} & p=0 & 1 & 2 & 3 & 4 & 5 \\ \hline 0 & H_1 & -r & \cdot & \cdot & \cdot & -r \\ 1 & -r & H_1 & -r & \cdot & \cdot & \cdot \\ 2 & \cdot & -r & H_1 & -r & \cdot & \cdot \\ 3 & \cdot & \cdot & -r & H_1 & -r & \cdot \\ 4 & \cdot & \cdot & \cdot & -r & H_1 & -r \\ 5 & -r & \cdot & \cdot & \cdot & -r & H_1 \end{array}$$

$$\omega^{B1(n)}(k_m)$$
$$=r_0\chi_0^m+r_1\chi_1^m+r_{-1}\chi_{-1}^m$$
$$=H_1-2r\,cos(2\pi m/6)$$

r_1 equals conjugate of r_5: ($r_1=r_5^*=-r$)

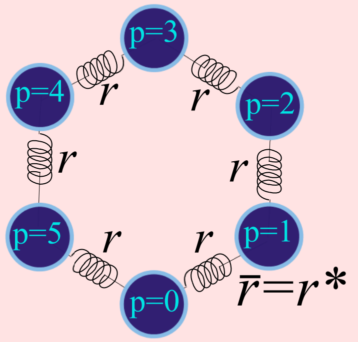
3rd Step *Display all eigensolutions of all possible C_6 symmetric real H*

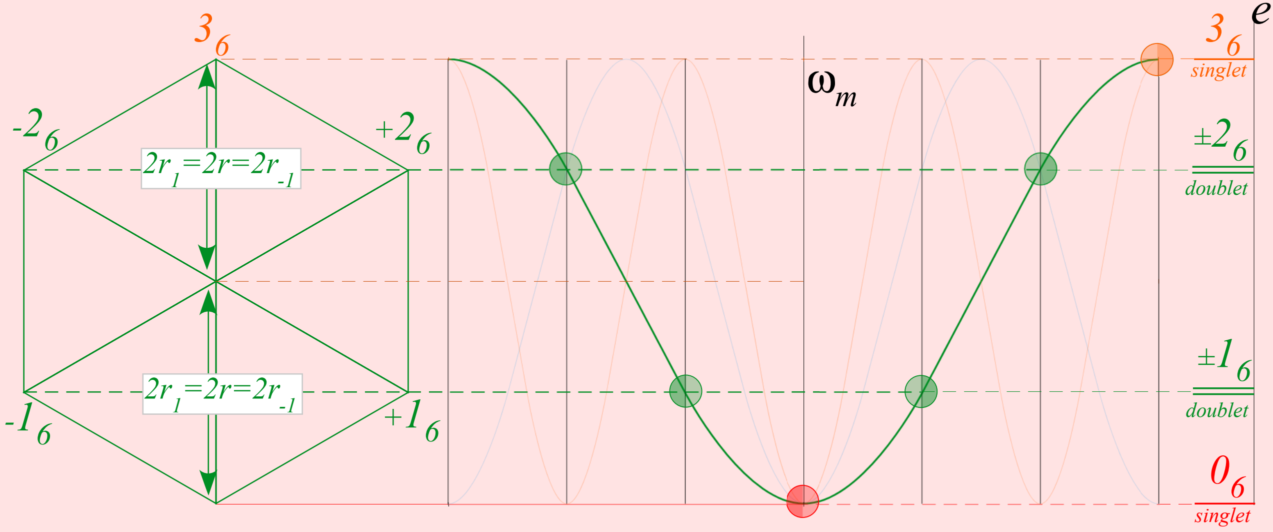
$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where:\ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

(Dispersion functions)

Elementary
Bloch Model

H= $H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$





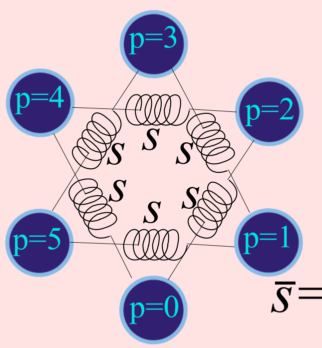
eigenvalues of $\mathbf{H}^{B1(6)}$

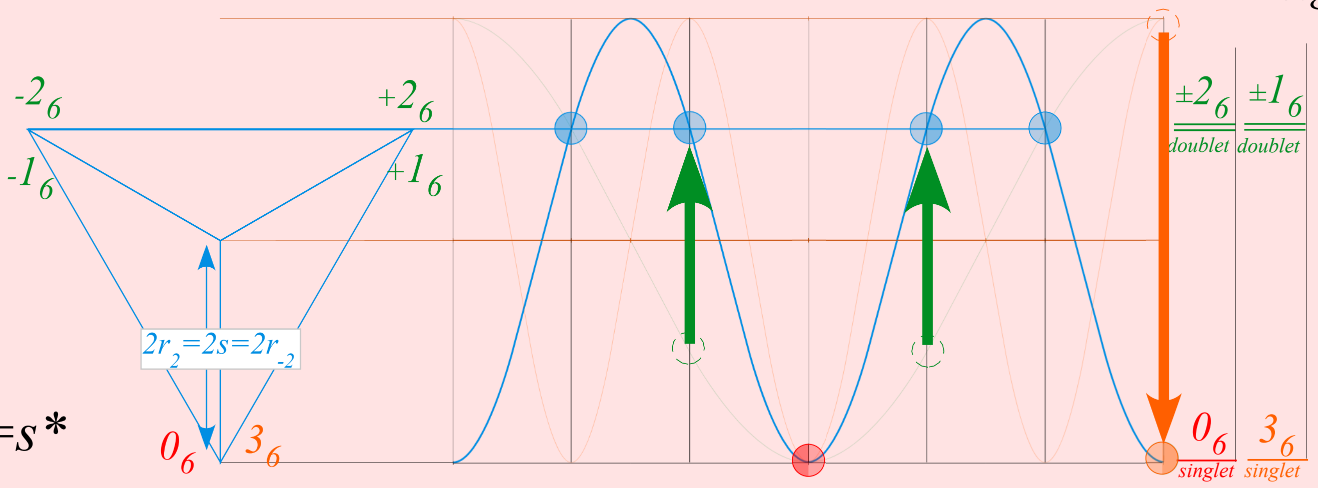
$$\begin{array}{cccccc c} p=0 & 1 & 2 & 3 & 4 & 5 & \\ H_1 & -r & \cdot & \cdot & \cdot & -r & 0 \\ -r & H_1 & -r & \cdot & \cdot & \cdot & 1 \\ \cdot & -r & H_1 & -r & \cdot & \cdot & 2 \\ \cdot & \cdot & -r & H_1 & -r & \cdot & 3 \\ \cdot & \cdot & \cdot & -r & H_1 & -r & 4 \\ -r & \cdot & \cdot & \cdot & -r & H_1 & 5 \end{array}$$

$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\,cos(2\pi m/6)$$

2nd Neighbor
coupling

H= $H_2\mathbf{1} - s\mathbf{r}^2 - s\mathbf{r}^{-2}$





eigenvalues of $\mathbf{H}^{B2(6)}$

$$\begin{array}{cccccc c} p=0 & 1 & 2 & 3 & 4 & 5 & \\ H_2 & \cdot & -s & \cdot & -s & \cdot & 0 \\ \cdot & H_2 & \cdot & -s & \cdot & -s & 1 \\ -s & \cdot & H_2 & \cdot & -s & \cdot & 2 \\ \cdot & -s & \cdot & H_2 & \cdot & -s & 3 \\ -s & \cdot & -s & \cdot & H_2 & \cdot & 4 \\ \cdot & -s & \cdot & -s & \cdot & H_2 & 5 \end{array}$$

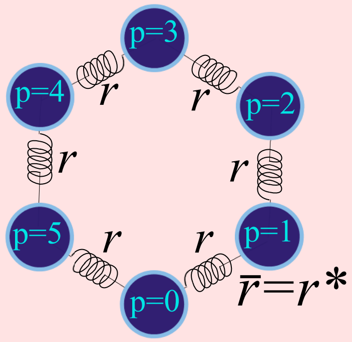
$$\omega^{B2(n)}(k_m) = r_0\chi_0^m + r_2\chi_2^m + r_{-2}\chi_{-2}^m = H_2 - 2s\,cos(4\pi m/6)$$

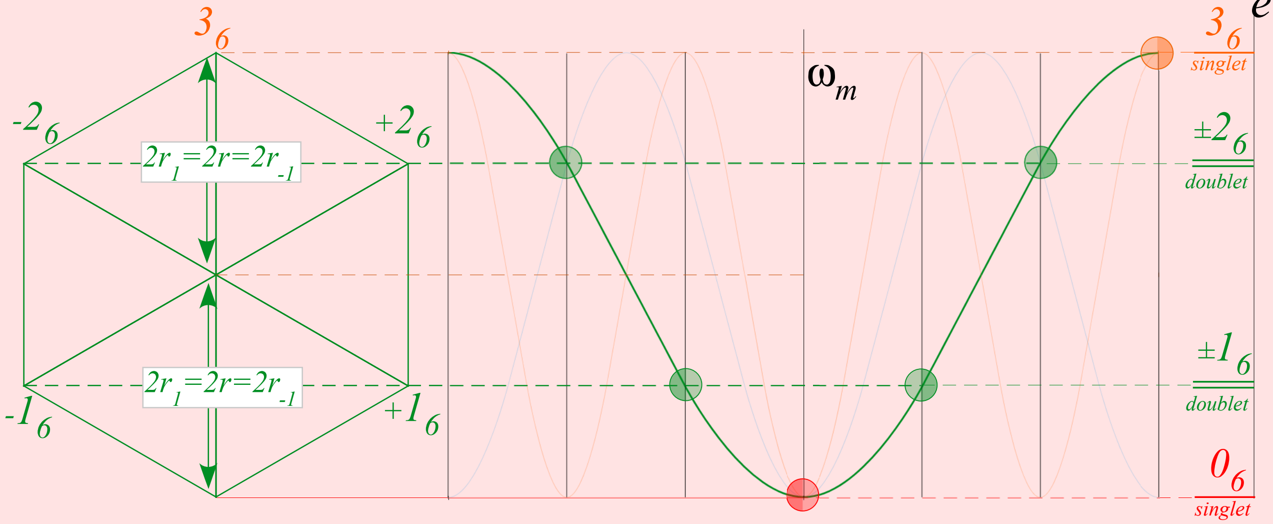
3rd Step *Display all eigensolutions of all possible C_6 symmetric real H*

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p=\sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1}\chi_p^m \mathbf{P}^{(m)}=\sum_{m=0}^{n-1}\omega^{(m)}\mathbf{P}^{(m)} \quad where:\ \omega^{(m)}=\sum_{p=0}^{n-1} r_p\chi_p^m=\omega(k_m)$$ *(Dispersion functions)*

Elementary Bloch Model

H= H_1**1** - *r***r** - *r***r**$^{-1}$





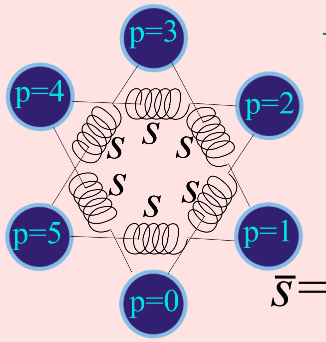
eigenvalues of $\mathbf{H}^{B1(6)}$

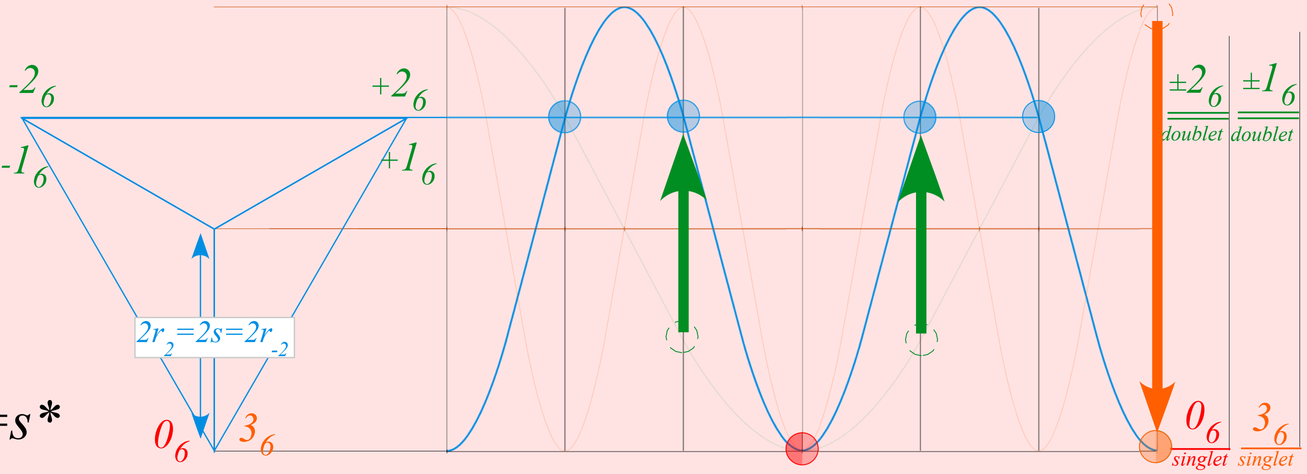
$$\begin{array}{c|cccccc} & p=0 & 1 & 2 & 3 & 4 & 5 \\ \hline 0 & H_1 & -r & \cdot & \cdot & \cdot & -r \\ 1 & -r & H_1 & -r & \cdot & \cdot & \cdot \\ 2 & \cdot & -r & H_1 & -r & \cdot & \cdot \\ 3 & \cdot & \cdot & -r & H_1 & -r & \cdot \\ 4 & \cdot & \cdot & \cdot & -r & H_1 & -r \\ 5 & -r & \cdot & \cdot & \cdot & -r & H_1 \end{array}$$

$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\,cos(2\pi m/6)$$

2nd Neighbor coupling

H= H_2**1** - *s***r**^{2} - *s***r**$^{-2}$





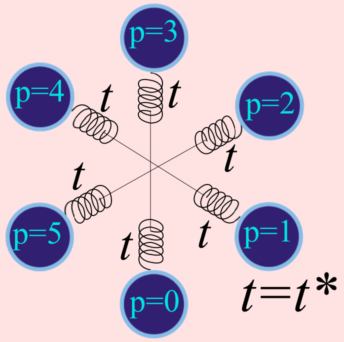
eigenvalues of $\mathbf{H}^{B2(6)}$

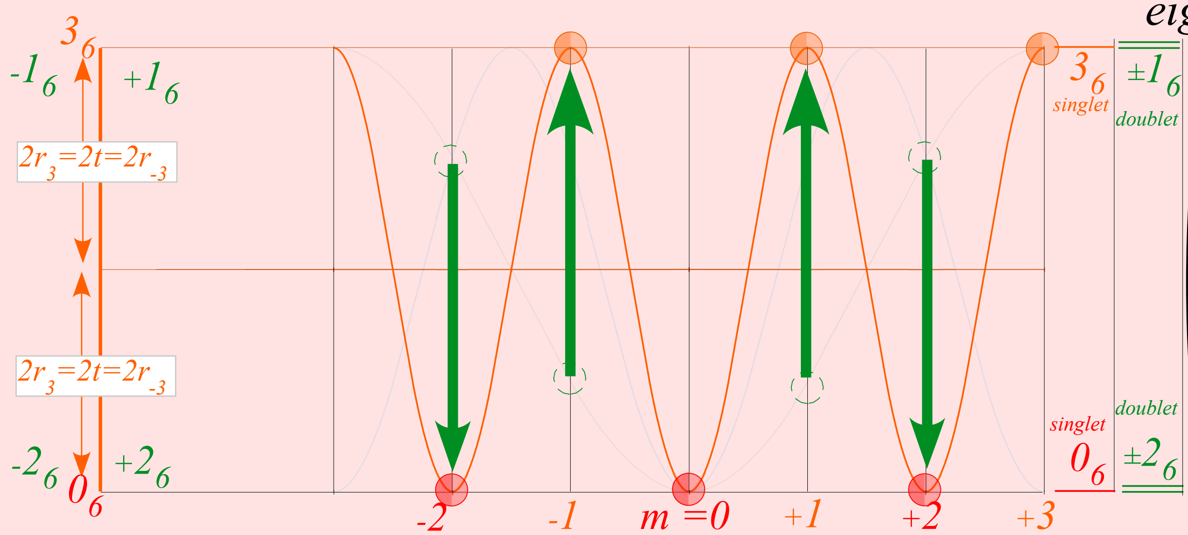
$$\begin{array}{c|cccccc} & p=0 & 1 & 2 & 3 & 4 & 5 \\ \hline 0 & H_2 & \cdot & -s & \cdot & -s & \cdot \\ 1 & \cdot & H_2 & \cdot & -s & \cdot & -s \\ 2 & -s & \cdot & H_2 & \cdot & -s & \cdot \\ 3 & \cdot & -s & \cdot & H_2 & \cdot & -s \\ 4 & -s & \cdot & -s & \cdot & H_2 & \cdot \\ 5 & \cdot & -s & \cdot & -s & \cdot & H_2 \end{array}$$

$$\omega^{B2(n)}(k_m) = r_0\chi_0^m + r_2\chi_2^m + r_{-2}\chi_{-2}^m = H_2 - 2s\,cos(4\pi m/6)$$

3rd Neighbor coupling

H= H_3**1** - *t***r**^{3} - *t***r**$^{-3}$





eigenvalues of $\mathbf{H}^{B3(6)}$

$$\begin{array}{c|cccccc} & p=0 & 1 & 2 & 3 & 4 & 5 \\ \hline 0 & H_3 & \cdot & \cdot & -t & \cdot & \cdot \\ 1 & \cdot & H_3 & \cdot & \cdot & -t & \cdot \\ 2 & \cdot & \cdot & H_3 & \cdot & \cdot & -t \\ 3 & -t & \cdot & \cdot & H_3 & \cdot & \cdot \\ 4 & \cdot & -t & \cdot & \cdot & H_3 & \cdot \\ 5 & \cdot & \cdot & -t & \cdot & \cdot & H_3 \end{array}$$

$$\omega^{B3(n)}(k_m) = r_0\chi_0^m + r_3\chi_3^m + r_{-3}\chi_{-3}^m = H_3 - 2t\,(-1)^m$$

Complete sets of C_6 coupling parameters and Fourier dispersion

$$\omega_m(\mathbf{H}^{GB(N)}) = \langle m| \sum_{p=0} r_p \mathbf{r}^p |m\rangle = \sum_{p=0} r_p \langle m|\mathbf{r}^p|m\rangle = \sum_{p=0} r_p e^{-i2\pi\frac{m\cdot p}{N}} = \sum_{p=0} |r_p| e^{-i(2\pi\frac{m\cdot p}{N}-\phi_p)}$$

Real C_6 Bloch **H** $^{GB(N)}$ eigenvalues are Fourier series with 4 (for N=6) Fourier parameters

$\{ r_0 = H,\quad r_1 = r = r_{-1}\ ,\ r_2 = s = r_{-2},\quad r_3 = t = r_{-3} \}$

$$\omega_m(\mathbf{H}^{GB(6)}_{real}) = r_0 + r_1(e^{i\pi\frac{m\cdot 1}{3}} + e^{-i\pi\frac{m\cdot 1}{3}}) \quad + r_2(e^{i\pi\frac{m\cdot 2}{3}} + e^{-i\pi\frac{m\cdot 2}{3}}) \quad + r_3(e^{i\pi\frac{m\cdot 3}{3}}) \qquad \text{(for real: } r_p = r_{-p} = r_p^*\text{)}$$

$$= H \ + \ 2r\cos\pi\frac{m\cdot 1}{3} \quad + \quad 2s\cos\pi\frac{m\cdot 2}{3} \quad + \ t(-1)^m$$

giving 4 ω_m-levels:

...in terms of 4 solvable r_p-parameters:

$$\omega_m = \begin{cases} \omega_0 = H + 2r + 2s + t \\ \omega_{\pm 1} = H + r - s - t \\ \omega_{\pm 2} = H - r - s + t \\ \omega_3 = H - 2r + 2s - t \end{cases}$$

$$r_p = \begin{cases} H = \frac{1}{4}(\omega_0 + \omega_1 + \omega_2 + \omega_3) \\ r = \frac{1}{6}(\omega_0 + \omega_1 - \omega_2 - \omega_3) \\ s = \frac{1}{6}(\omega_0 - \omega_1 - \omega_2 + \omega_3) \\ t = \frac{1}{6}(\omega_0 - 2\omega_1 + 2\omega_2 - \omega_3) \end{cases}$$

General Bloch **H** $^{GB(N)}$ eigenvalues are Fourier series with six (for N=6) Fourier parameters

$\{ r_0 = H,\quad r_1 = re^{i\phi_1},\quad r_{-1} = re^{-i\phi_1},\quad r_2 = se^{i\phi_2},\quad r_{-2} = se^{-i\phi_2},\quad r_3 = t = r_{-3} \}$

$$\omega_m(\mathbf{H}^{GZB(6)}_{complex}) = H + 2r\cos\left(\pi\frac{m\cdot 1}{3} - \phi_1\right) + 2s\cos\left(\pi\frac{m\cdot 2}{3} - \phi_2\right) + \ t(-1)^m \qquad \text{(for complex: } r_{-p} = r_p^*\text{)}$$

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

C_3 **H**-and-**r^p**-*matrix representations and conjugation symmetry*

C_3 Spectral resolution: 3rd roots of unity and ortho-completeness relations

C_3 *character table and modular labeling*

Ortho-completeness inversion for operators and states

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: 6th roots of unity and higher

Complete sets of coupling parameters and Fourier dispersion

→ *Gauge shifts due to complex coupling*

Complex sets of C_6 coupling parameters and gauge shifts

$$\omega_m(\mathbf{H}^{GB(N)}) = \langle m|\sum_{p=0} r_p\mathbf{r}^p|m\rangle = \sum_{p=0} r_p\langle m|\mathbf{r}^p|m\rangle = \sum_{p=0} r_p e^{-i2\pi\frac{m\cdot p}{N}} = \sum_{p=0}\left|r_p\right| e^{-i(2\pi\frac{m\cdot p}{N}-\phi_p)}$$

Complex Bloch matrix $\mathbf{H}^{GB(N)}$ eigenvalues are Fourier series with 6 (for N=6) Fourier parameters

$\{\ r_0 = H,\quad r_1 = re^{i\phi_1},\quad r_{-1} = re^{-i\phi_1},\quad r_2 = se^{i\phi_2},\quad r_{-2} = se^{-i\phi_2},\quad r_3 = t = r_{-3}\ \}$

$$\omega_m(\mathbf{H}^{GZB(6)}_{complex}) = r_0 + r_1 e^{i\pi\frac{m\cdot 1}{3}} + r_{-1}e^{-i\pi\frac{m\cdot 1}{3}} + r_2 e^{i\pi\frac{m\cdot 2}{3}} + r_{-2}e^{-i\pi\frac{m\cdot 2}{3}} + r_3 e^{i\pi\frac{m\cdot 3}{3}} \qquad (\text{for complex: } r_{-p} = r_p^*)$$

giving 6 ω_m-levels:

...in terms of 6 solvable r_p-parameters:

$$\omega_m = \begin{cases} \omega_0 = r_0 + r_1 + r_{-1} + r_2 + r_{-2} + r_3 \\ \omega_{+1} = r_0 + r_1 e^{\frac{i\pi}{3}} + r_{-1}e^{\frac{-i\pi}{3}} + r_2 e^{\frac{i2\pi}{3}} + r_{-2}e^{\frac{-i2\pi}{3}} - r_3 \\ \omega_{-1} = r_0 + r_1 e^{\frac{-i\pi}{3}} + r_{-1}e^{\frac{i\pi}{3}} + r_2 e^{\frac{-i2\pi}{3}} + r_{-2}e^{\frac{i2\pi}{3}} - r_3 \\ \omega_{+2} = r_0 + r_1 e^{\frac{i2\pi}{3}} + r_{-1}e^{\frac{-i2\pi}{3}} - r_2 e^{\frac{i\pi}{3}} - r_{-2}e^{\frac{-i\pi}{3}} + r_3 \\ \omega_{-2} = r_0 + r_1 e^{\frac{-i2\pi}{3}} + r_{-1}e^{\frac{i2\pi}{3}} - r_2 e^{\frac{-i\pi}{3}} - r_{-2}e^{\frac{i\pi}{3}} + r_3 \\ \omega_3 = r_0 - r_1 - r_{-1} + r_2 + r_{-2} - r_3 \end{cases}$$

$$r_p = \begin{cases} r_0 = ? \\ r_1 = ? \\ r_{-1} = ? \\ r_2 = ? \\ r_{-2} = ? \\ r_3 = ? \end{cases}$$

Left as an exercise...

Geometric solution shown next...

$$\omega_m(\mathbf{H}^{GZB(6)}_{complex}) = H + 2r\cos\left(\pi\frac{m\cdot 1}{3} - \phi_1\right) + 2s\cos\left(\pi\frac{m\cdot 2}{3} - \phi_2\right) + t(-1)^m \qquad (\text{for complex: } r_{-p} = r_p^*)$$

3^{rd} Step (contd.)

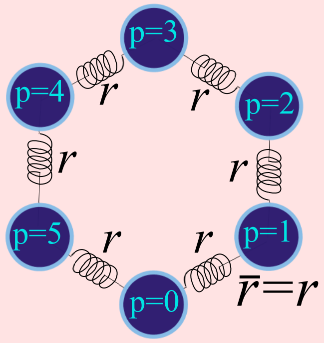
...eigensolutions for all possible C_6 symmetric complex H

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where:\ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

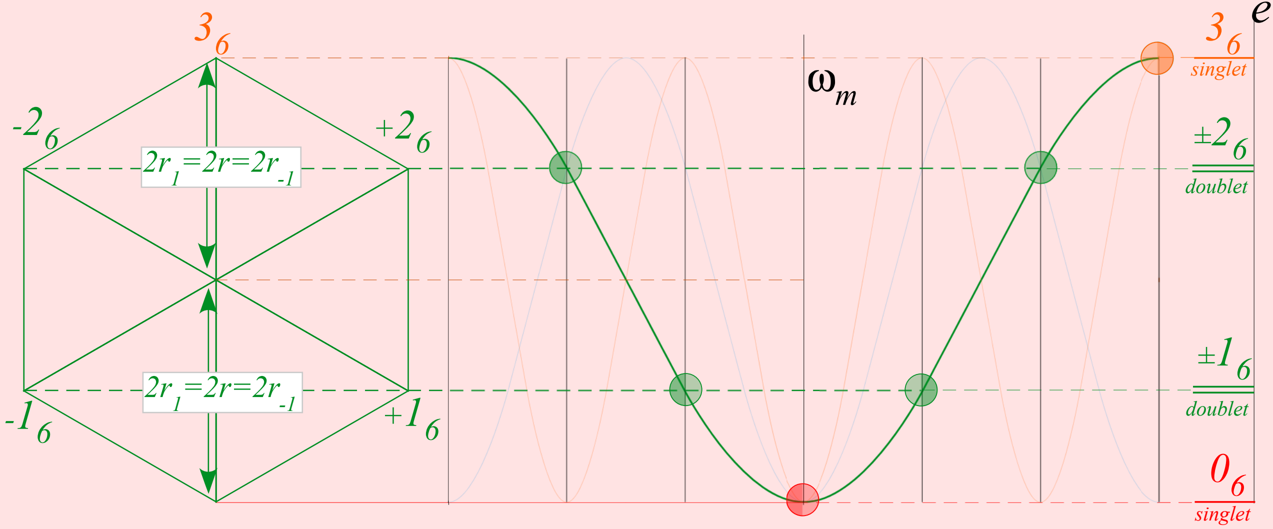
(Dispersion function)

Elementary
Bloch Model

$\mathbf{H}= H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$



$\bar{r}=r^*$



eigenvalues of $\mathbf{H}^{B1(6)}$

$$\begin{array}{cccccccc}
p=0 & 1 & 2 & 3 & 4 & 5 & \\
H_1 & r_{-1} & \cdot & \cdot & \cdot & r_1 & 0 \\
r_1 & H_1 & r_{-1} & \cdot & \cdot & \cdot & 1 \\
\cdot & r_1 & H_1 & r_{-1} & \cdot & \cdot & 2 \\
\cdot & \cdot & r_1 & H_1 & r_{-1} & \cdot & 3 \\
\cdot & \cdot & \cdot & r_1 & H_1 & r_{-1} & 4 \\
r_{-1} & \cdot & \cdot & \cdot & r_1 & H_1 & 5
\end{array}$$

$$\begin{aligned} &\omega^{B1(n)}(k_m) \\ &= r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m \\ &= H_1 - 2r\,cos(2\pi m/6) \end{aligned}$$

Nearest neighbor coupling

$$\begin{pmatrix}
r_0 & r_{-1} & & & & r_1 \\
r_1 & r_0 & r_{-1} & & & \\
& r_1 & r_0 & r_{-1} & & \\
& & r_1 & r_0 & r_{-1} & \\
& & & r_1 & r_0 & r_{-1} \\
r_{-1} & & & & r_1 & r_0
\end{pmatrix}$$

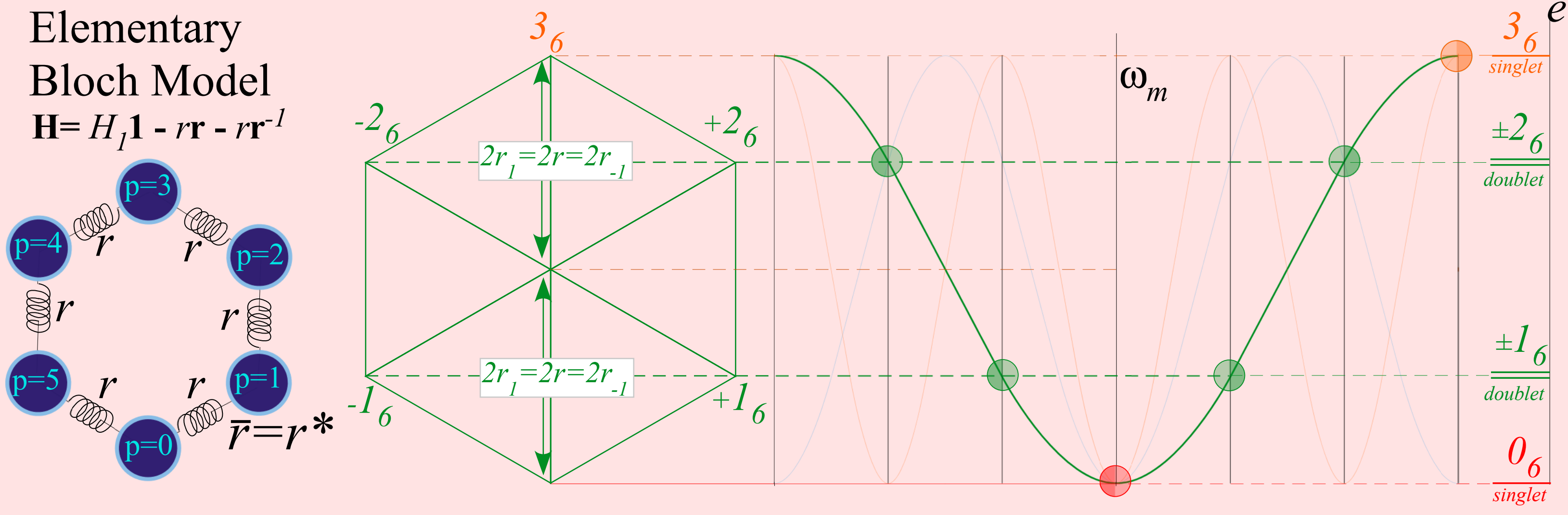
3^{rd} Step (contd.)

...eigensolutions for all possible C_6 symmetric complex H

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p\mathbf{r}^p=\sum_{p=0}^{n-1} r_p\sum_{m=0}^{n-1}\chi_p^m\mathbf{P}^{(m)}=\sum_{m=0}^{n-1}\omega^{(m)}\mathbf{P}^{(m)}\quad where:\ \omega^{(m)}=\sum_{p=0}^{n-1} r_p\chi_p^m=\omega(k_m)$$

(Dispersion function)

Elementary Bloch Model
$\mathbf{H}= H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$



eigenvalues of $\mathbf{H}^{B1(6)}$

$$\begin{array}{cccccc|c} p=0 & 1 & 2 & 3 & 4 & 5 & \\ H_1 & r_{-1} & \cdot & \cdot & \cdot & r_1 & 0 \\ r_1 & H_1 & r_{-1} & \cdot & \cdot & \cdot & 1 \\ \cdot & r_1 & H_1 & r_{-1} & \cdot & \cdot & 2 \\ \cdot & \cdot & r_1 & H_1 & r_{-1} & \cdot & 3 \\ \cdot & \cdot & \cdot & r_1 & H_1 & r_{-1} & 4 \\ r_{-1} & \cdot & \cdot & \cdot & r_1 & H_1 & 5 \end{array}$$

$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\cos(2\pi m/6)$$

Nearest neighbor coupling

$$\mathbf{H}^{B1(6)}=\begin{pmatrix} r_0 & r_{-1} & & & & r_1 \\ r_1 & r_0 & r_{-1} & & & \\ & r_1 & r_0 & r_{-1} & & \\ & & r_1 & r_0 & r_{-1} & \\ & & & r_1 & r_0 & r_{-1} \\ r_{-1} & & & & r_1 & r_0 \end{pmatrix}$$

For Hermitian $\mathbf{H}^{B1(6)}=(\mathbf{H}^{B1(6)})^\dagger$
complex components
$r_1=-re^{i\phi}$ *imply*
conjugate components
$r^*_1=r_{-1}=-re^{-i\phi}$

3^{rd} Step (contd.)

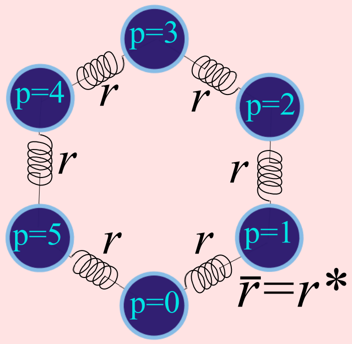
...eigensolutions for all possible C_6 symmetric complex H

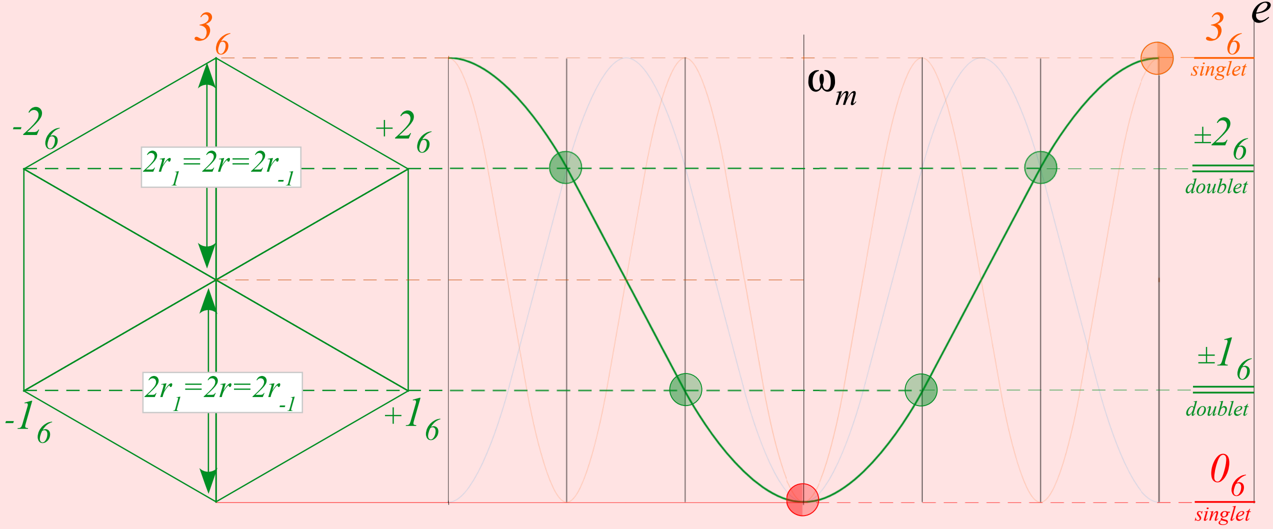
$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where:\ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

(Dispersion function)

Elementary Bloch Model

$\mathbf{H}= H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$





eigenvalues of $\mathbf{H}^{B1(6)}$

$$\begin{array}{c|cccccc|}
 & p=0 & 1 & 2 & 3 & 4 & 5 \\
0 & H_1 & r_{-1} & \cdot & \cdot & \cdot & r_1 \\
1 & r_1 & H_1 & r_{-1} & \cdot & \cdot & \cdot \\
2 & \cdot & r_1 & H_1 & r_{-1} & \cdot & \cdot \\
3 & \cdot & \cdot & r_1 & H_1 & r_{-1} & \cdot \\
4 & \cdot & \cdot & \cdot & r_1 & H_1 & r_{-1} \\
5 & r_{-1} & \cdot & \cdot & \cdot & r_1 & H_1
\end{array}$$

$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\,cos(2\pi m/6)$$

Nearest neighbor coupling

$$\mathbf{H}^{B1(6)}=\begin{pmatrix} r_0 & r_{-1} & & & & r_1 \\ r_1 & r_0 & r_{-1} & & & \\ & r_1 & r_0 & r_{-1} & & \\ & & r_1 & r_0 & r_{-1} & \\ & & & r_1 & r_0 & r_{-1} \\ r_{-1} & & & & r_1 & r_0 \end{pmatrix}$$

For Hermitian $\mathbf{H}^{B1(6)}=(\mathbf{H}^{B1(6)})^\dagger$

complex components

$r_1=-re^{i\phi}$ *imply*

conjugate components

$r^*_1=r_{-1}=-re^{-i\phi}$

$$\omega^{B1(6)}(k_m) = r_0\chi^m{}_0 + r_1\chi^m{}_1 + r_{-1}\chi^m{}_{-1}$$

$$= r_0 - r\,e^{i\phi}e^{i2\pi m/6} - r\,e^{-i\phi}e^{-i2\pi m/6}$$

$$= r_0 - 2r\,cos(2\pi m/6 + \phi)$$

3^{rd} Step (contd.)

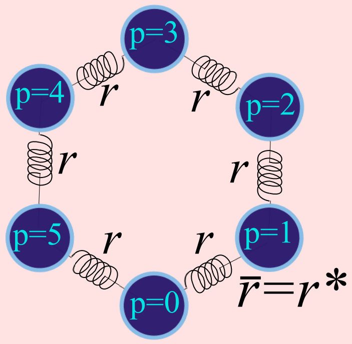
...eigensolutions for all possible C_6 symmetric complex H

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p\mathbf{r}^p=\sum_{p=0}^{n-1} r_p\sum_{m=0}^{n-1}\chi_p^m\mathbf{P}^{(m)}=\sum_{m=0}^{n-1}\omega^{(m)}\mathbf{P}^{(m)}\quad where:\ \omega^{(m)}=\sum_{p=0}^{n-1} r_p\chi_p^m=\omega(k_m)$$

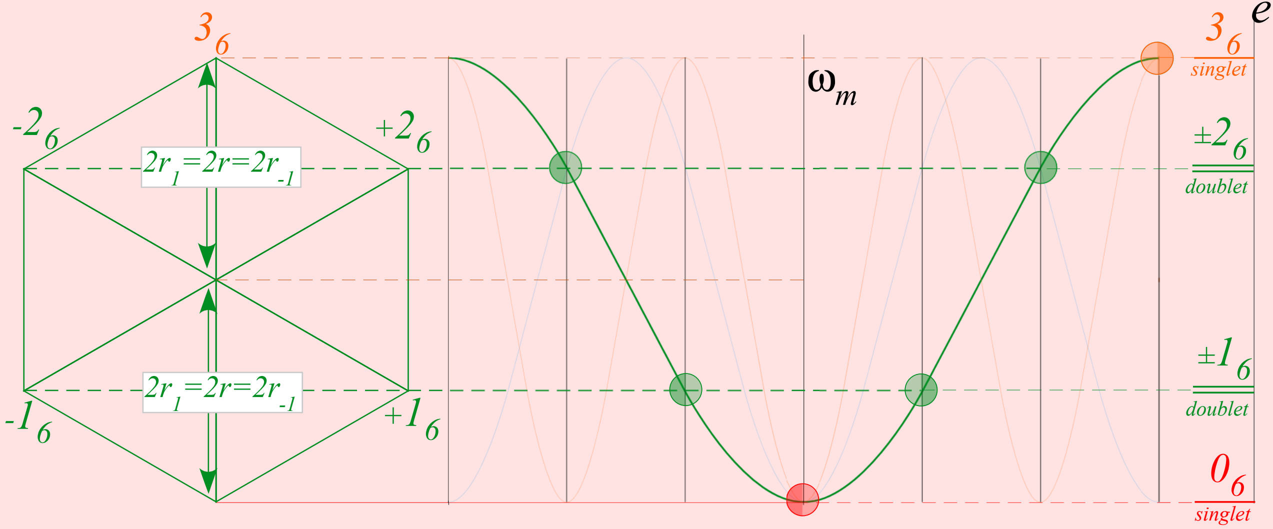
(Dispersion function)

Elementary
Bloch Model

$\mathbf{H}= H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$



$\bar{r}=r^*$



eigenvalues of $\mathbf{H}^{B1(6)}$

$$\begin{array}{c|cccccc|}
 & p=0 & 1 & 2 & 3 & 4 & 5 \\
\hline
0 & H_1 & r_{-1} & \cdot & \cdot & \cdot & r_1 \\
1 & r_1 & H_1 & r_{-1} & \cdot & \cdot & \cdot \\
2 & \cdot & r_1 & H_1 & r_{-1} & \cdot & \cdot \\
3 & \cdot & \cdot & r_1 & H_1 & r_{-1} & \cdot \\
4 & \cdot & \cdot & \cdot & r_1 & H_1 & r_{-1} \\
5 & r_{-1} & \cdot & \cdot & \cdot & r_1 & H_1
\end{array}$$

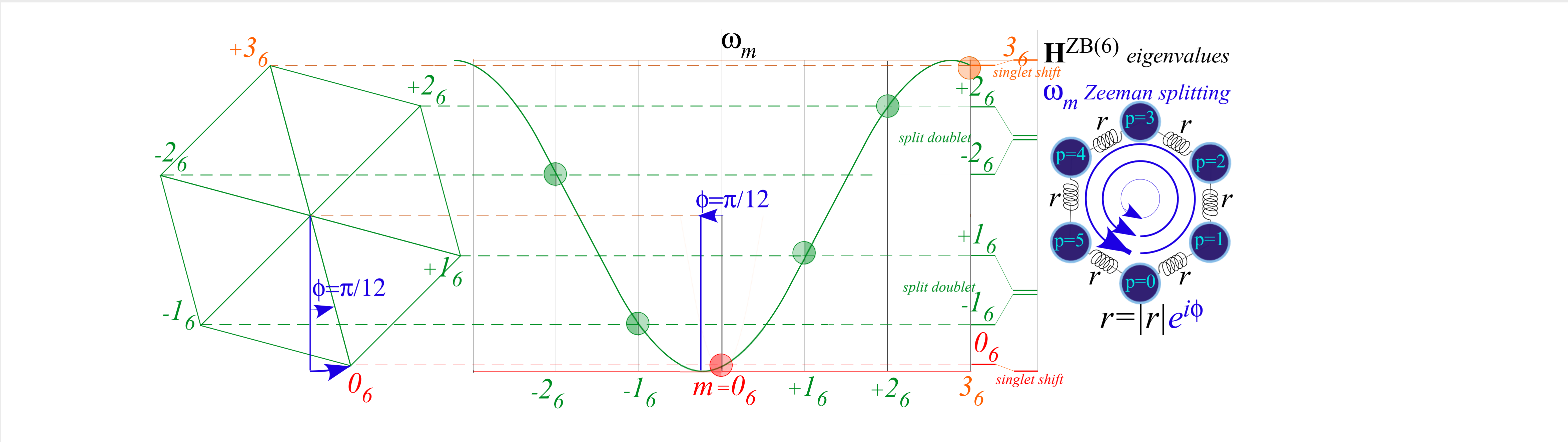
$$\omega^{B1(n)}(k_m)$$
$$=r_0\chi_0^m+r_1\chi_1^m+r_{-1}\chi_{-1}^m$$
$$=H_1-2r\,cos(2\pi m/6)$$

Nearest neighbor coupling

$$\mathbf{H}^{B1(6)}=\begin{pmatrix} r_0 & r_{-1} & & & & r_1 \\ r_1 & r_0 & r_{-1} & & & \\ & r_1 & r_0 & r_{-1} & & \\ & & r_1 & r_0 & r_{-1} & \\ & & & r_1 & r_0 & r_{-1} \\ r_{-1} & & & & r_1 & r_0 \end{pmatrix}$$

For Hermitian $\mathbf{H}^{B1(6)}=(\mathbf{H}^{B1(6)})^\dagger$
complex components
$r_1=-re^{i\phi}$ *imply*
conjugate components
$r^*_1=r_{-1}=-re^{-i\phi}$

$$\omega^{B1(6)}(k_m)=r_0\chi^m{}_0+\quad r_1\chi^m{}_1\quad+\quad r_{-1}\chi^m{}_{-1}$$
$$=\quad r_0\quad -r\,e^{i\phi}e^{i2\pi m/6}-r\,e^{-i\phi}e^{-i2\pi m/6}$$
$$=\quad r_0\quad -2r\,cos(2\pi m/6+\phi)$$



$\mathbf{H}^{ZB(6)}$ *eigenvalues*

ω_m *Zeeman splitting*

$r=|r|e^{i\phi}$

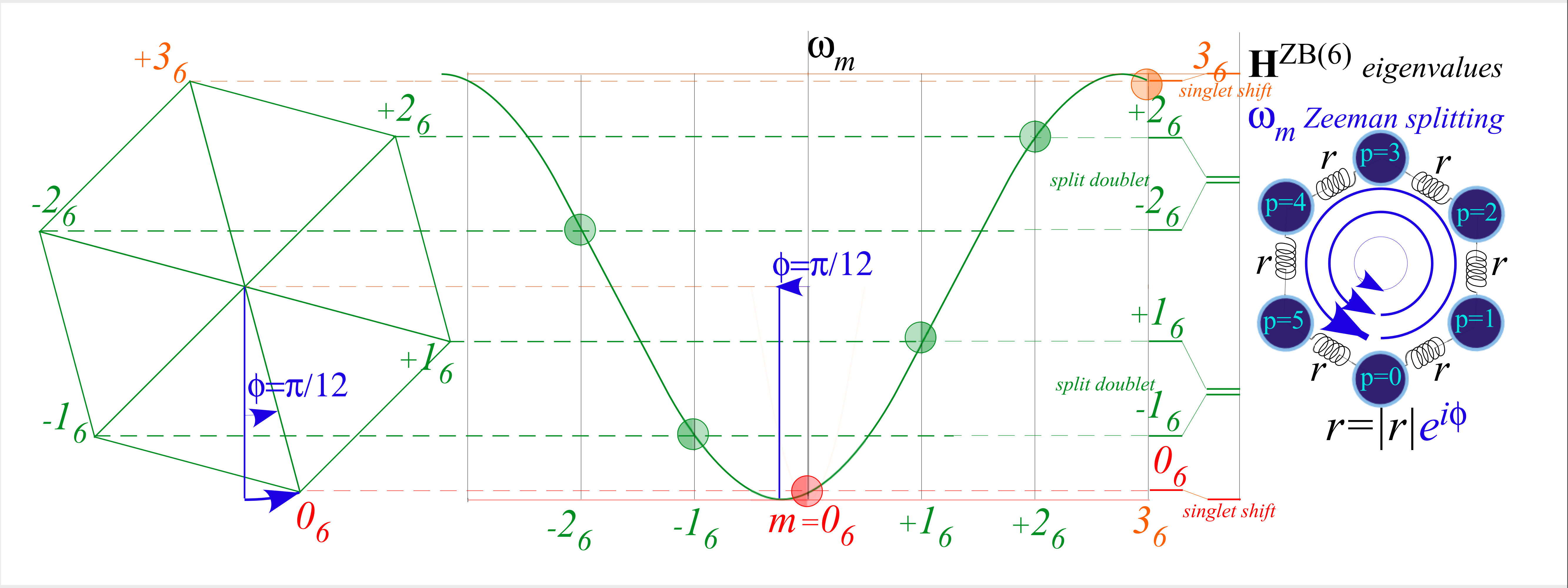
3rd Step (contd.)

...*eigensolutions for all possible C_6 symmetric complex H*

$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

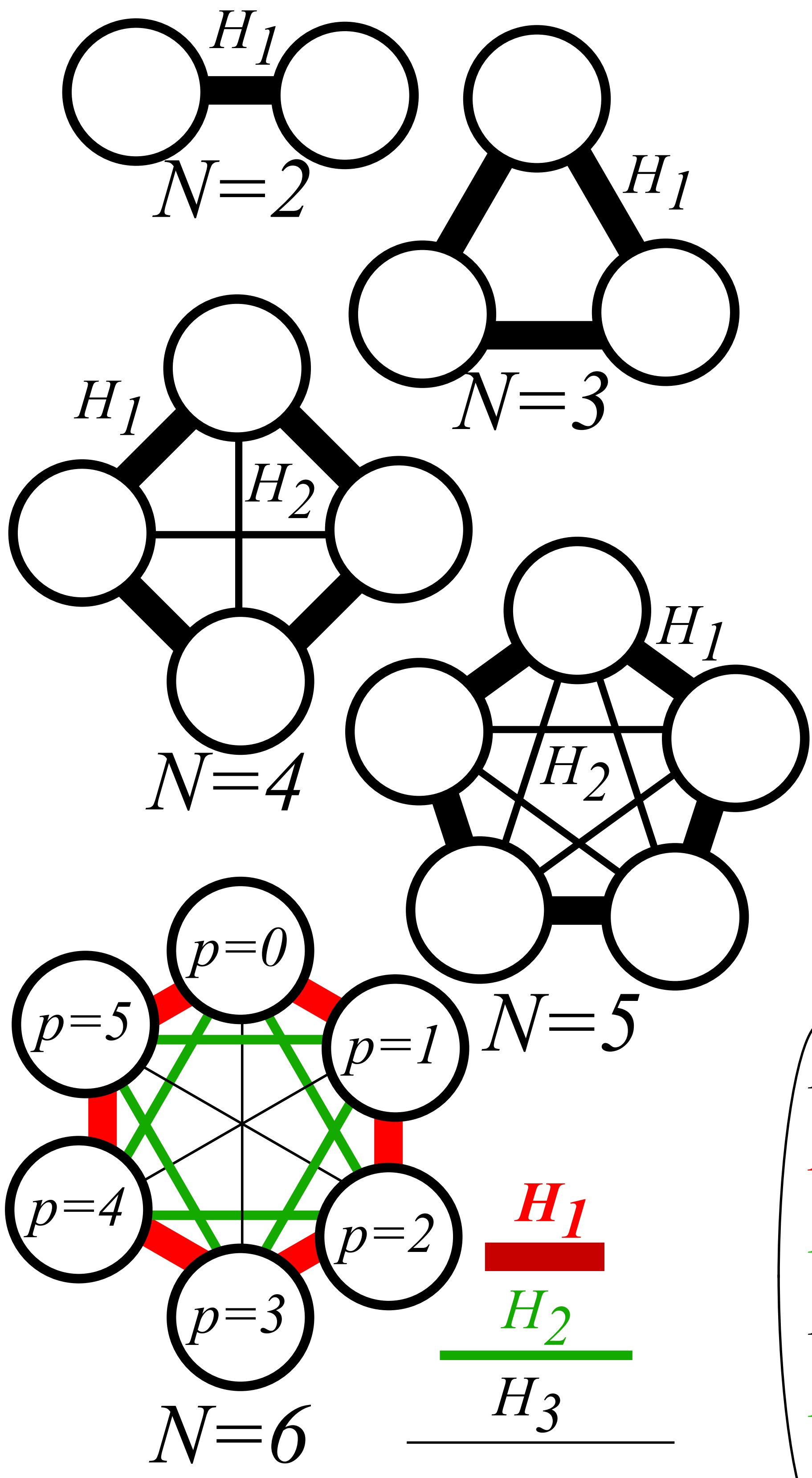
(Dispersion function)

In this C-Type situation m-eigenstates
are required to be moving waves $e^{ik_m \cdot x_p}$



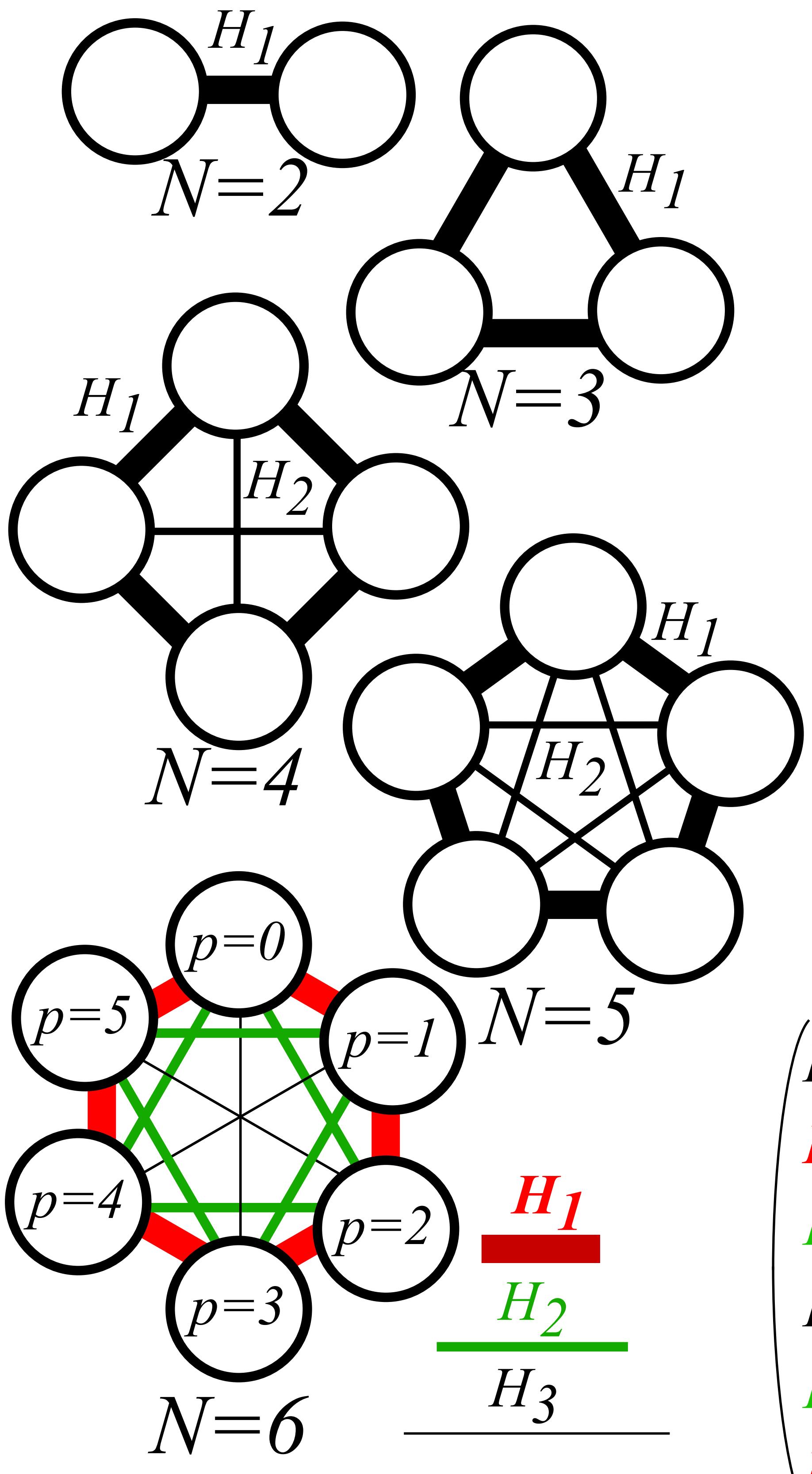
Simulating Complex Systems With Simpler Ones

Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots

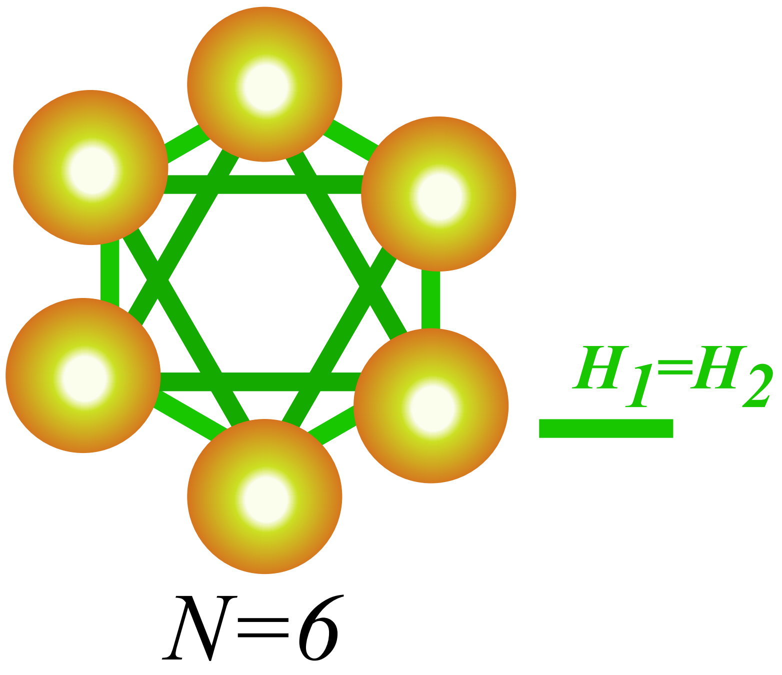


$$\begin{pmatrix} H_0 & \boldsymbol{H_1} & H_2 & H_3 & H_2 & \boldsymbol{H_1} \\ \mathbf{H1} & H_0 & \boldsymbol{H_1} & H_2 & H_3 & H_2 \\ H_2 & \boldsymbol{H_1} & H_0 & \boldsymbol{H_1} & H_2 & H_3 \\ H_3 & H_2 & \boldsymbol{H_1} & H_0 & \boldsymbol{H_1} & H_2 \\ H_2 & H_3 & H_2 & \boldsymbol{H_1} & H_0 & \boldsymbol{H_1} \\ \boldsymbol{H_1} & H_2 & H_3 & H_2 & \boldsymbol{H_1} & H_0 \end{pmatrix}$$

Simulating Complex Systems With Simpler Ones



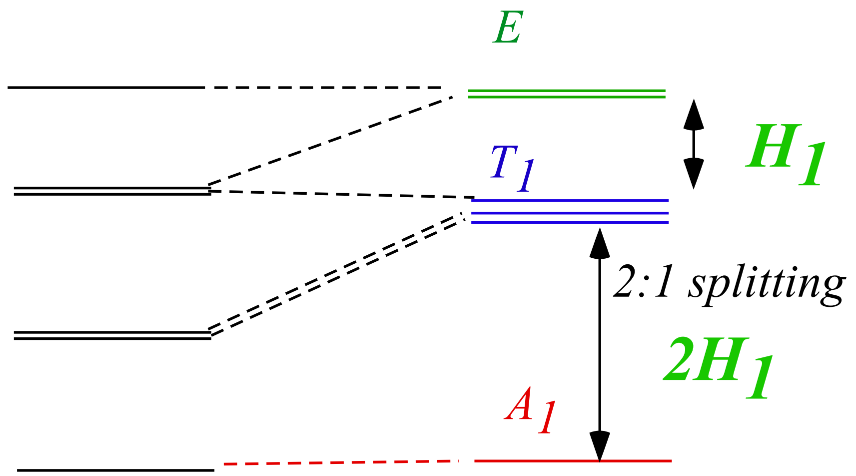
Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots



$$\begin{pmatrix} H_0 & H_1 & H_1 & 0 & H_1 & H_1 \\ H_1 & H_0 & H_1 & H_1 & 0 & H_1 \\ H_1 & H_1 & H_0 & H_1 & H_1 & 0 \\ 0 & H_1 & H_1 & H_0 & H_1 & H_1 \\ H_1 & 0 & H_1 & H_1 & H_0 & H_1 \\ H_1 & H_1 & 0 & H_1 & H_1 & H_0 \end{pmatrix}$$

Hexagonal becomes Octahedral

$$\begin{pmatrix} H_0 & H_1 & H_2 & H_3 & H_2 & H_1 \\ H1 & H_0 & H_1 & H_2 & H_3 & H_2 \\ H_2 & H_1 & H_0 & H_1 & H_2 & H_3 \\ H_3 & H_2 & H_1 & H_0 & H_1 & H_2 \\ H_2 & H_3 & H_2 & H_1 & H_0 & H_1 \\ H_1 & H_2 & H_3 & H_2 & H_1 & H_0 \end{pmatrix}$$



C_2 Fourier transformation matrix and dynamics