Group Theory in Quantum Mechanics

Lecture 10 *(2.19-26.13)*

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)

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

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

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

C_3 $\mathbf{g}^\dagger\mathbf{g}$-*product-table*
Pairs each operator $\mathbf{g}$ in the 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.

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

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

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

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

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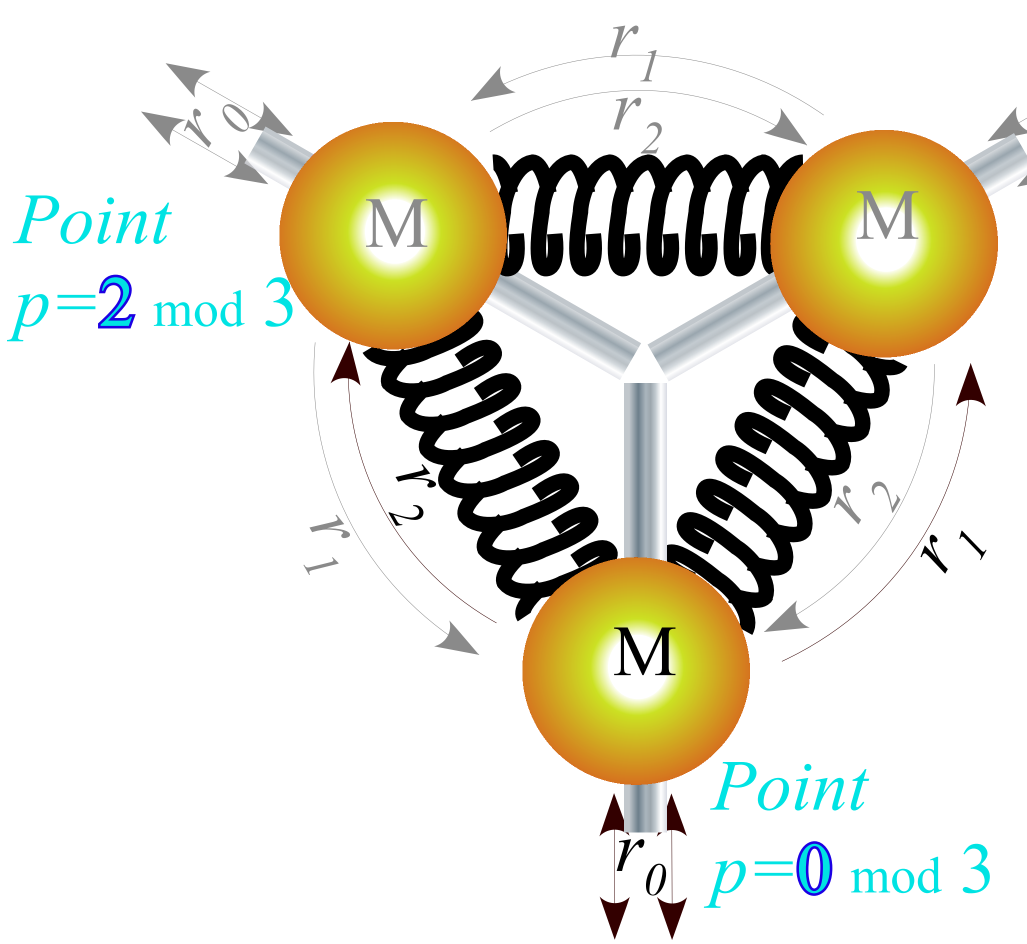
H-matrix coupling constants $\{r_0, r_1, r_2\}$
relate to particular operators $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$
that transmit a particular force or current.



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

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

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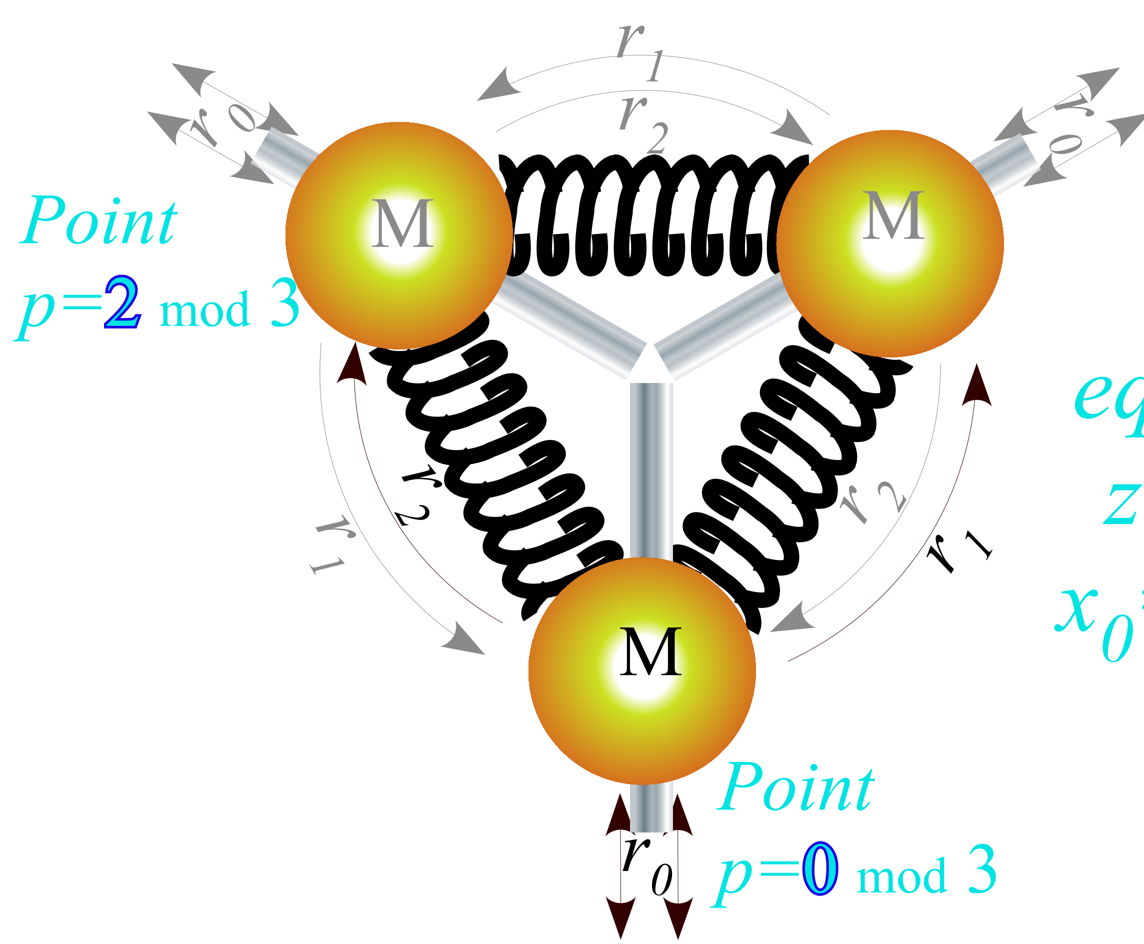

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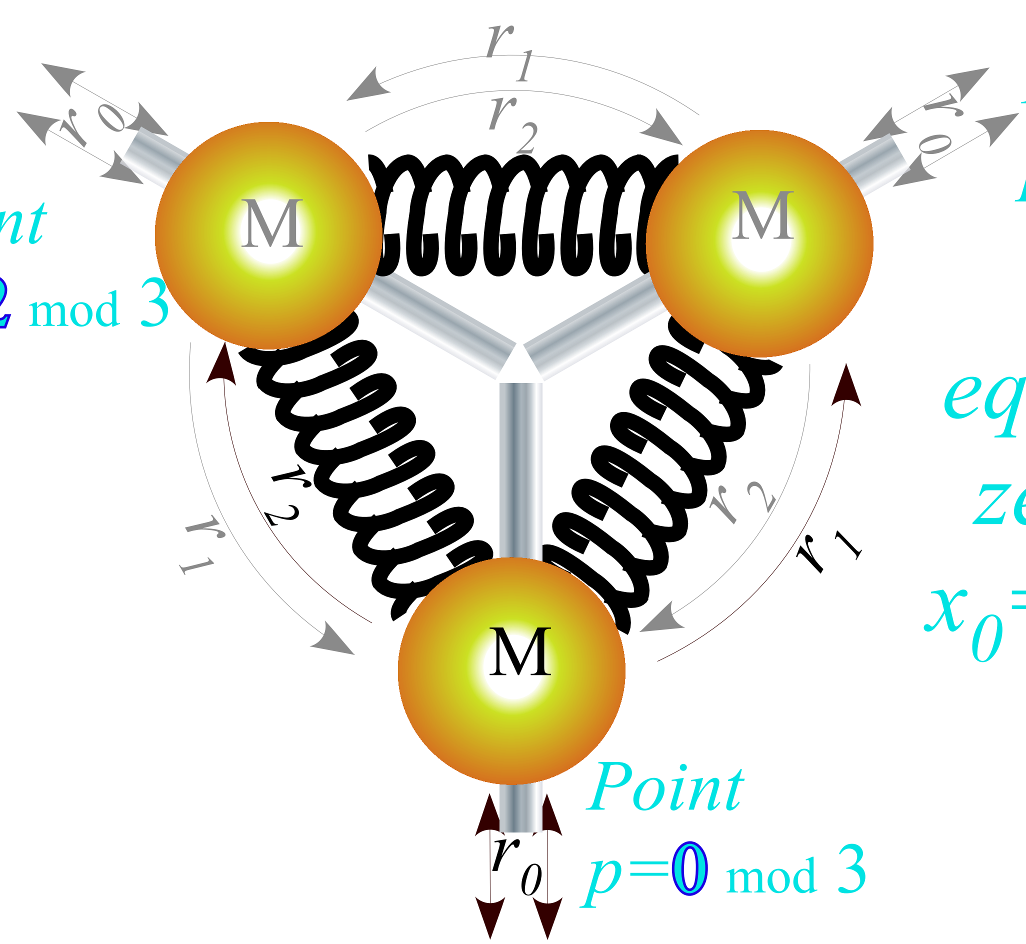
that transmit a particular force or current.

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



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

Constants r_k that are grayed-out
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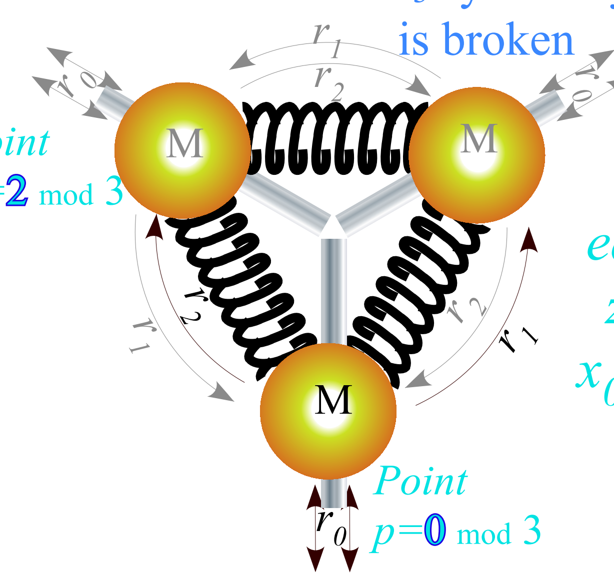

equilibrium
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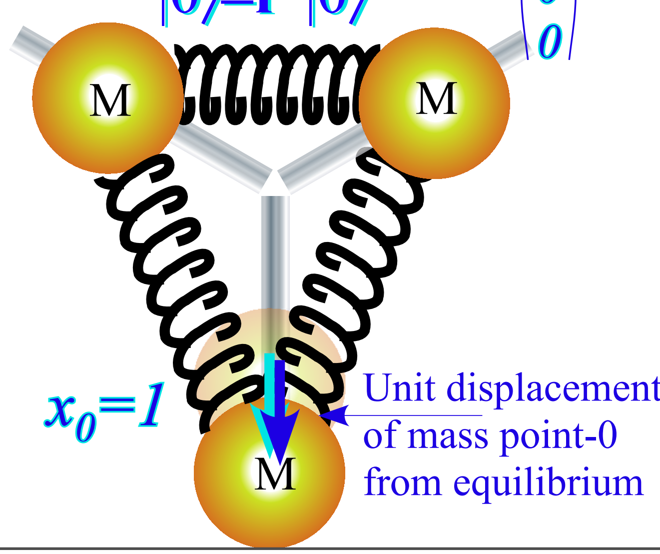
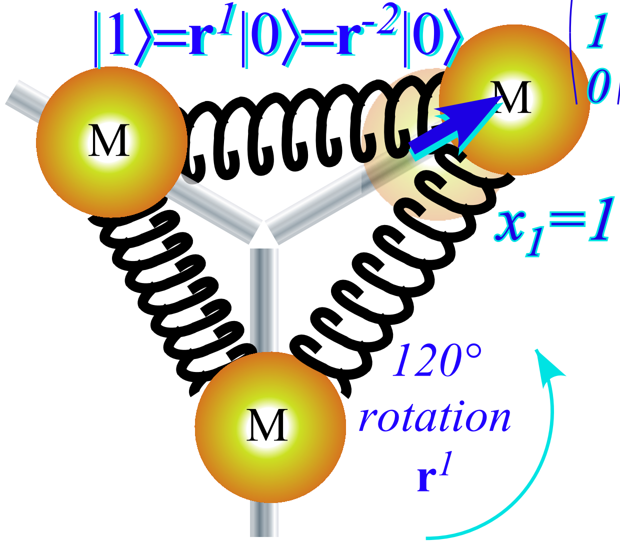
C_3 operators $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$
also label unit
base states:
$|0\rangle=\mathbf{r}^0|0\rangle$
$|1\rangle=\mathbf{r}^1|0\rangle$
$|2\rangle=\mathbf{r}^2|0\rangle$
modulo-3

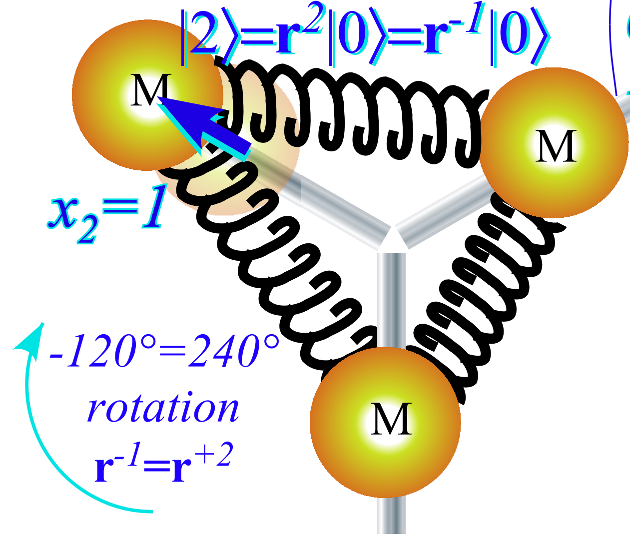
(p=0) unit base state
$|0\rangle=\mathbf{r}^0|0\rangle$ $\begin{pmatrix}1\\0\\0\end{pmatrix}$



(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***

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

Modular quantum number arithmetic

C_3-group jargon and structure of various tables

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Standing waves vs Moving waves

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Complete sets of coupling parameters and Fourier dispersion

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C_3 Spectral resolution: 3^{rd} roots of unity

We can spectrally resolve **H** if we resolve **r** since **H** is a combination of powers $\mathbf{r}^p$.

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

C_3 *Spectral resolution: 3rd roots of unity*

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

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"Chi"(χ) refers to *characters* or *characteristic* roots

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$\rho_0=e^{i0}=1,\quad \rho_1=e^{i2\pi/3},\quad \rho_2=e^{i4\pi/3}.$ $\mathbf{r}^1$*-Spectral-Decomp.* $\mathbf{r}^1 = \chi_0\,\mathbf{P}^{(0)} + \chi_1\,\mathbf{P}^{(1)} + \chi_2\,\mathbf{P}^{(2)}$

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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*

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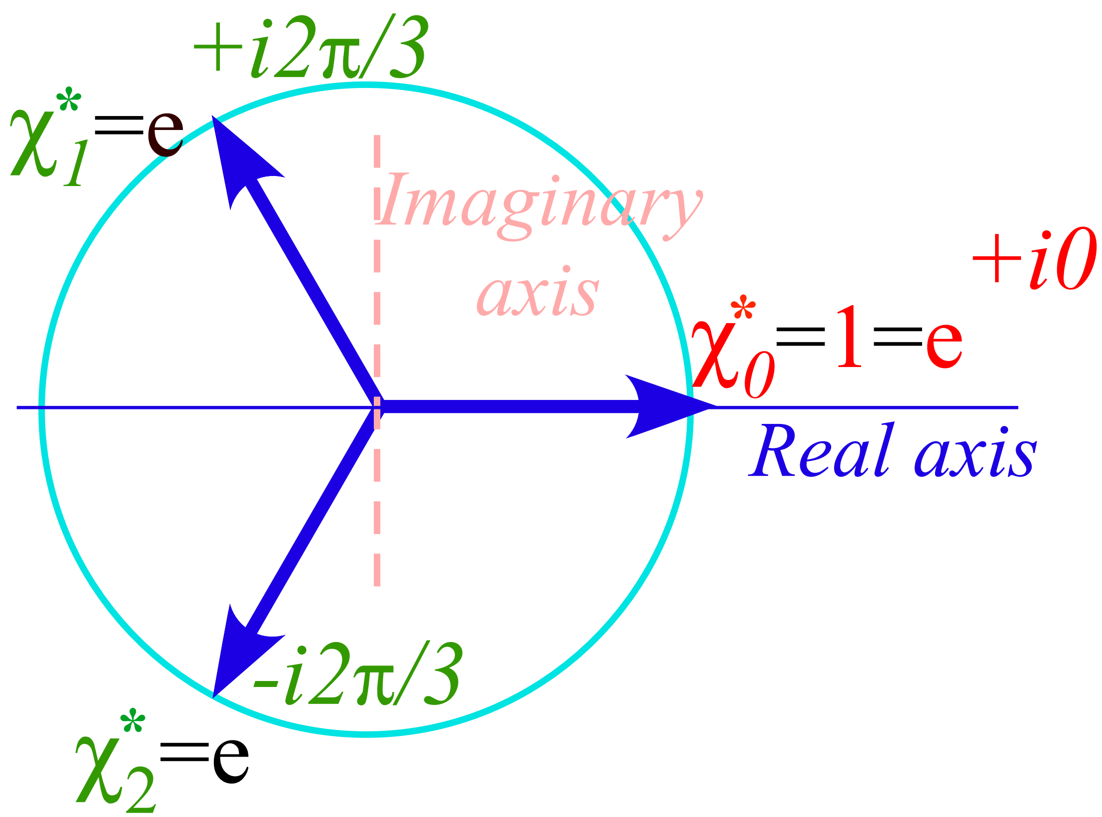

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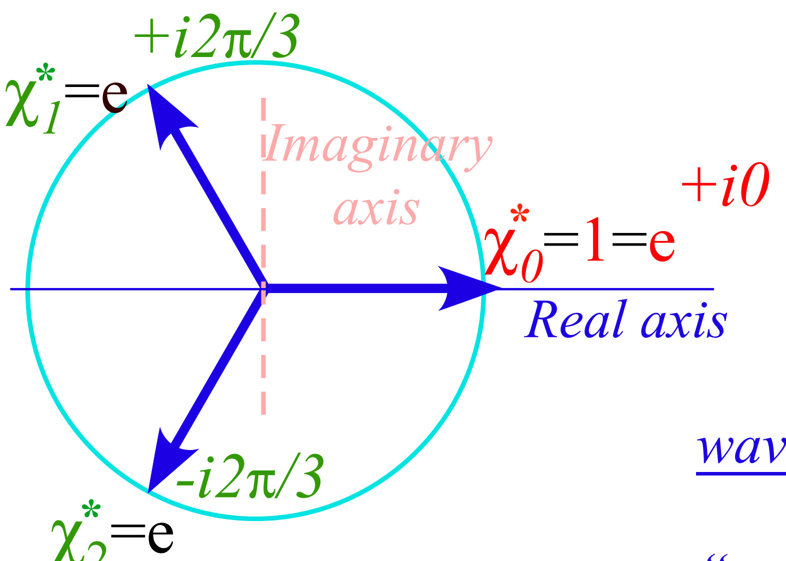

C_3 mode phase character table

wave-number $m=$ *"momentum"*

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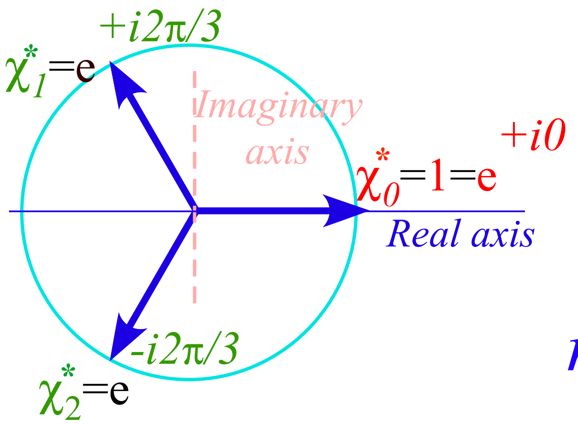

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C_3 character conjugate

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

is wave function

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

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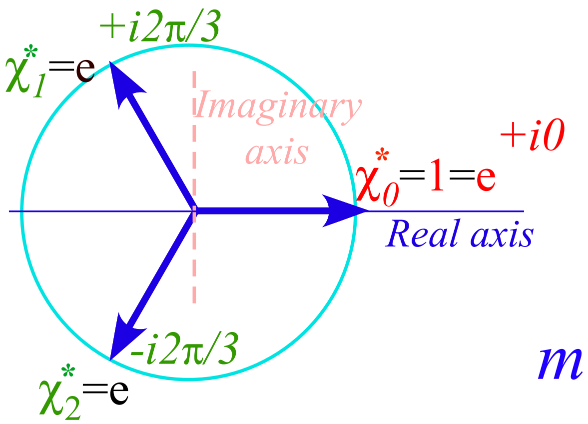

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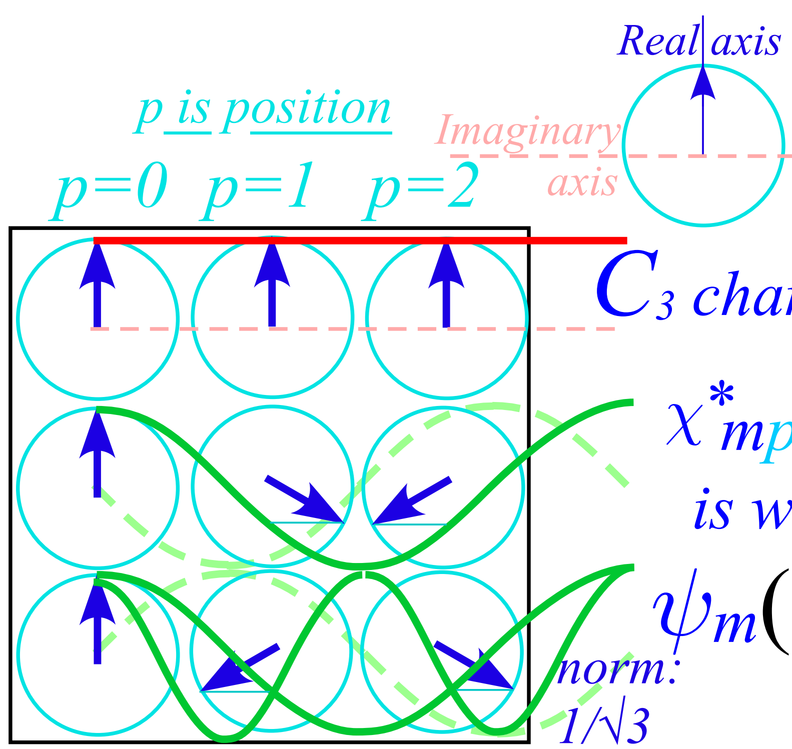
p is position



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norm: $1/\sqrt{3}$

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(or norm by $\sqrt{\frac{1}{3}}$)

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

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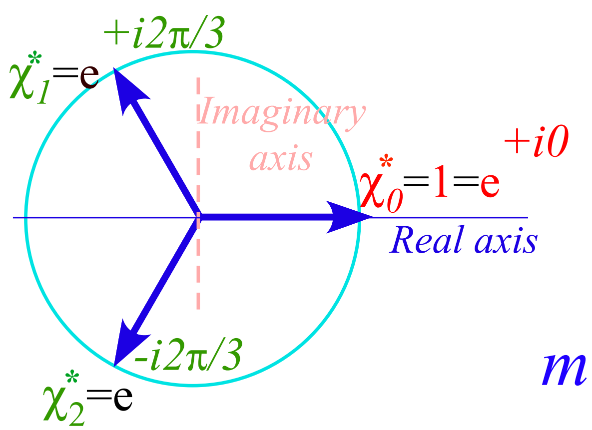

C_3 mode phase character table

	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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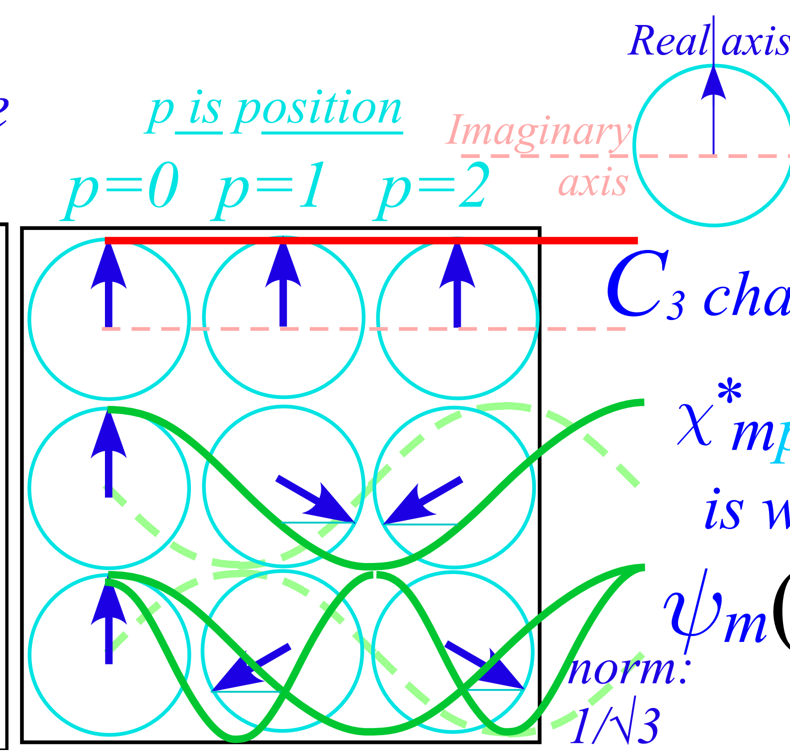
wave-number
m= "momentum"



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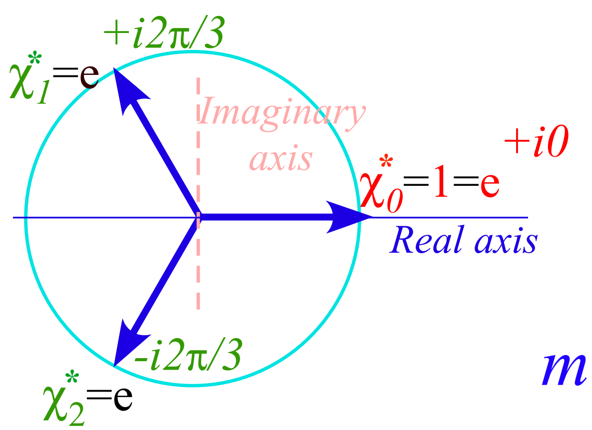

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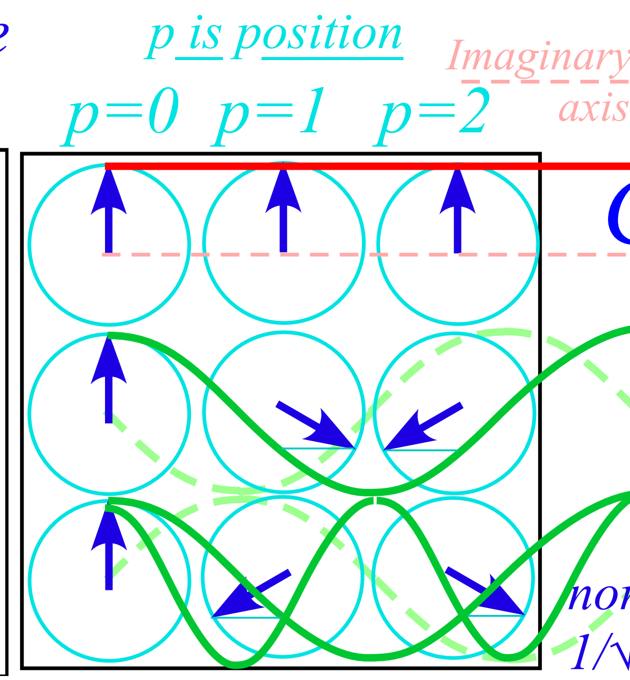

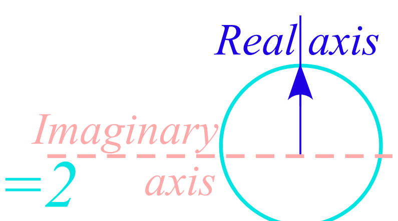

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norm:
1/√3

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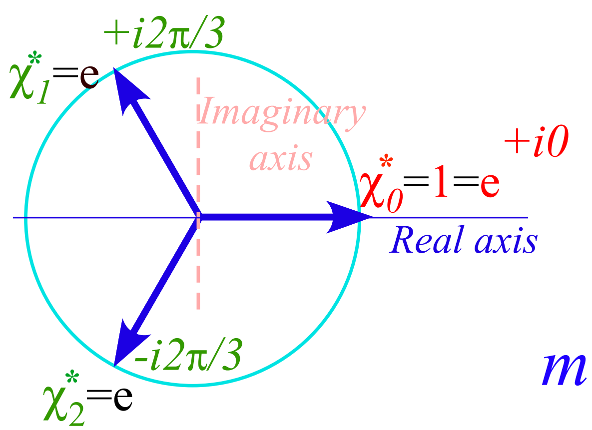

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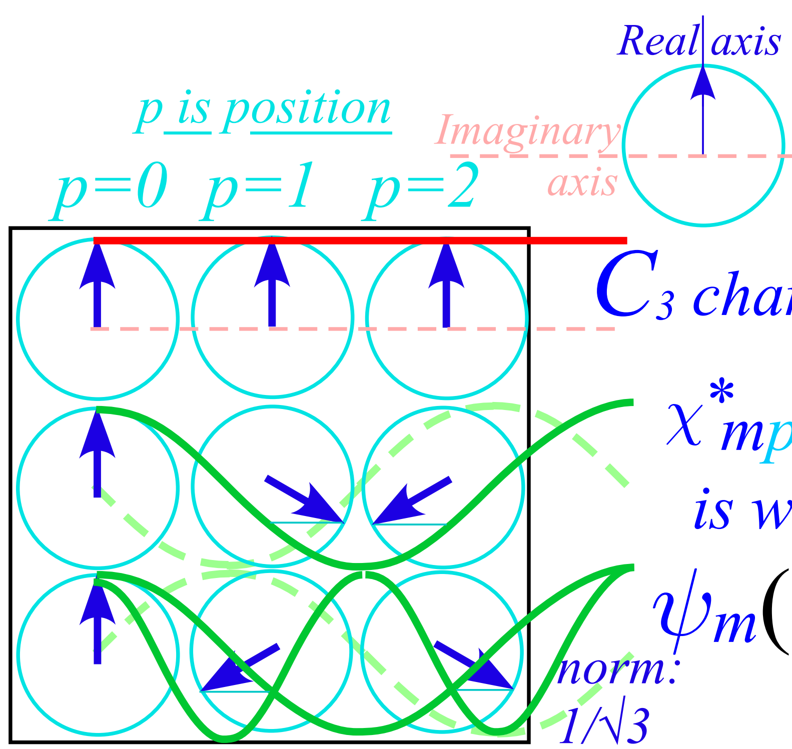

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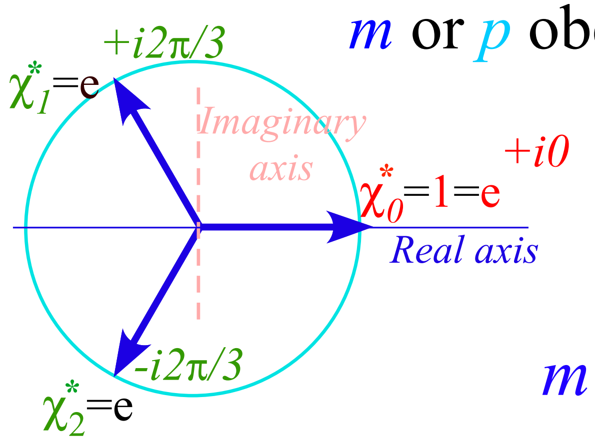

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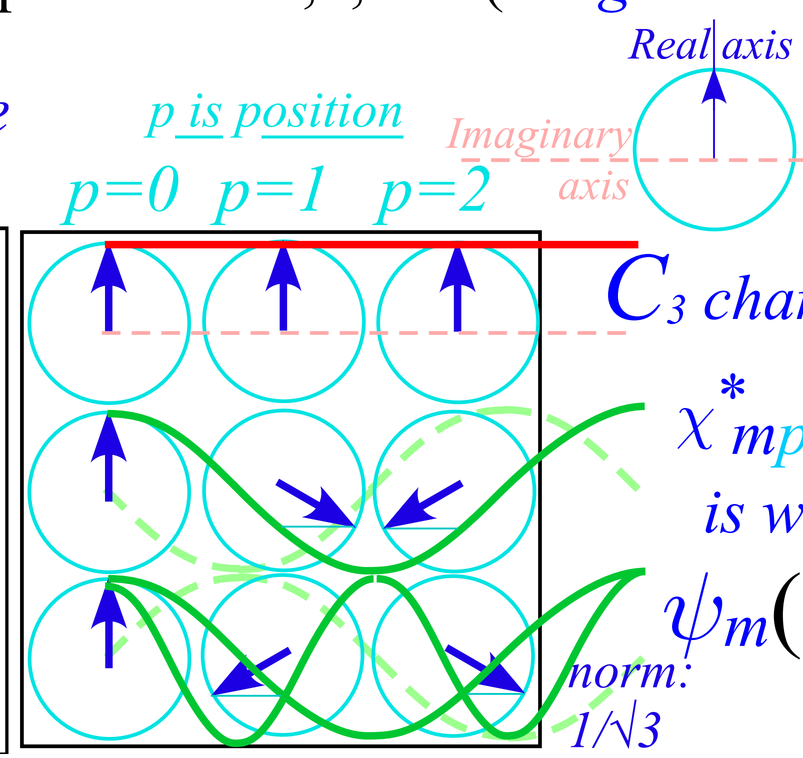

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C_3 *character table and modular labeling*

Ortho-completeness inversion for operators and states

Comparing wave function operator algebra to bra-ket algebra

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

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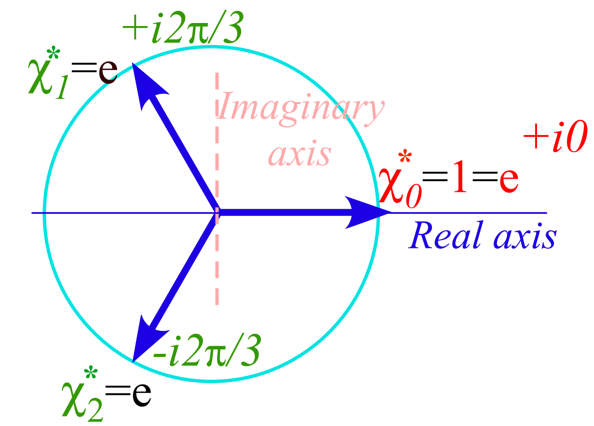

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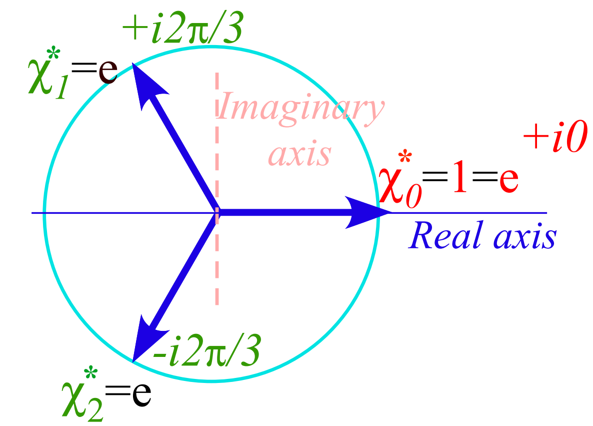
For example, for $m=2$ and $p=2$ the number $(\rho_m)^p=(e^{im2\pi/3})^p$ is $e^{imp\cdot 2\pi/3}= e^{i4\cdot 2\pi/3}= e^{i1\cdot 2\pi/3}\ e^{i3\cdot 2\pi/3}= e^{i2\pi/3}=\rho_1$.

Modular quantum number arithmetic



Two distinct types of modular "quantum" numbers:

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

$m=0,1$,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)*

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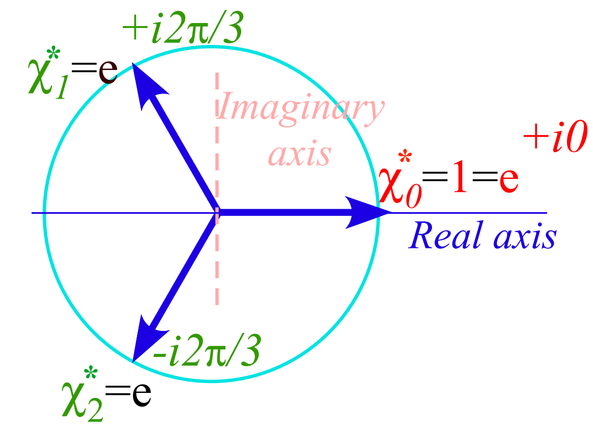

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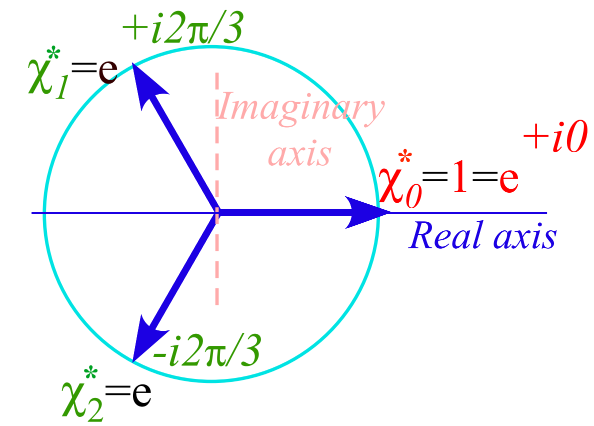
Modular quantum number arithmetic



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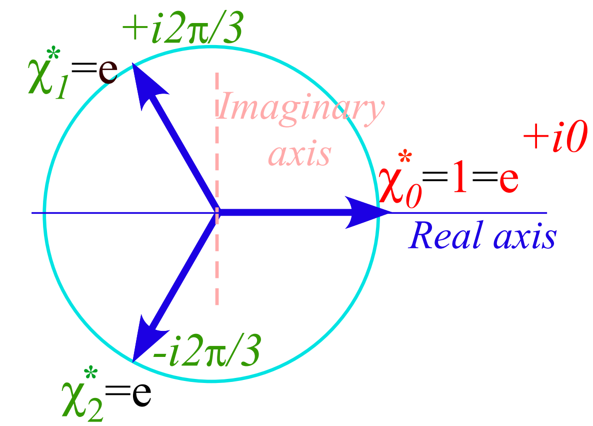
Modular quantum number arithmetic



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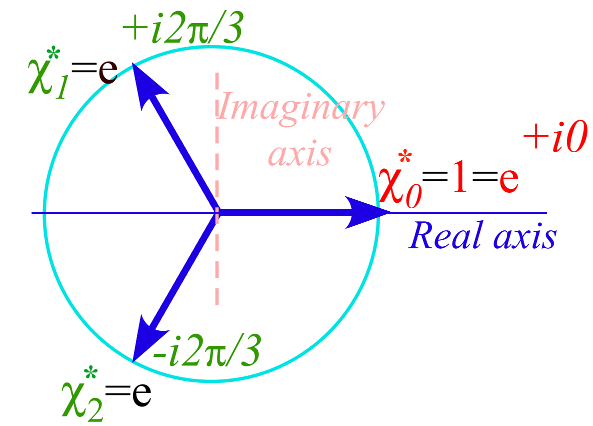
Imagine going around ring reading off address points p=... 0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2,....

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

Modular quantum number arithmetic



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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,....*

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

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

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

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

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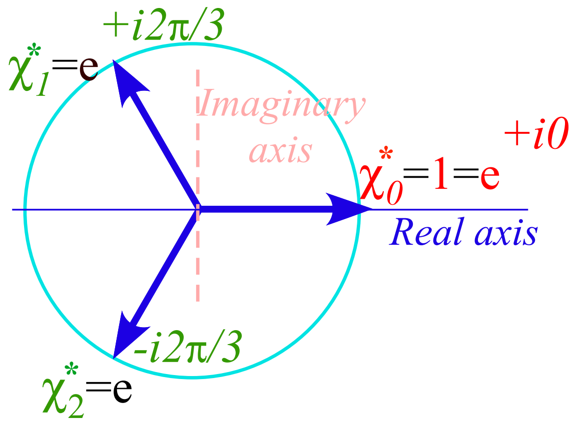
C_3-group $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$-table

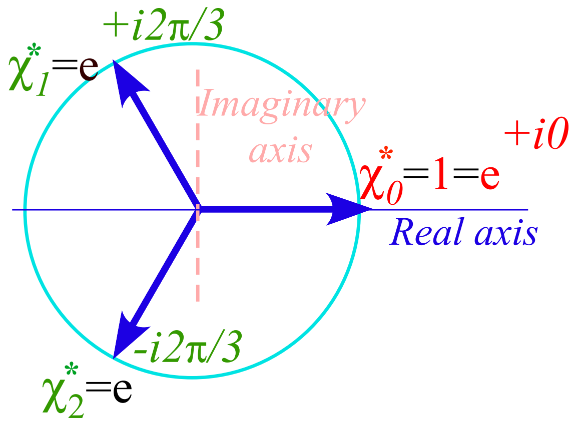
obeyed by $\{\chi_0=1,\ \chi_1=e^{-i2\pi/3},\ \chi_2=e^{+i2\pi/3}\}$



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

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

C_3-group jargon and structure of various tables



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

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

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

irreducible representation

(irrep) of C_3

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

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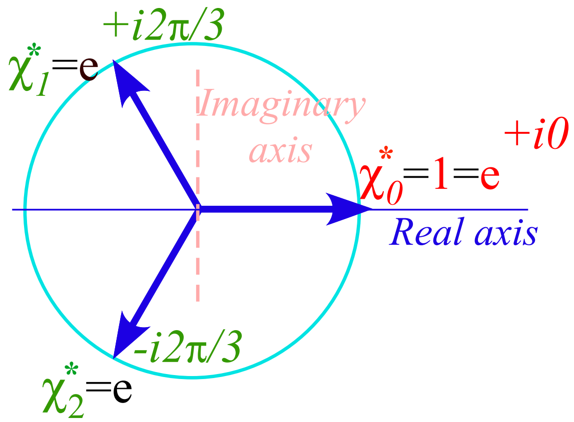

C_3-group $\{\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2\}$-table

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$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
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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	$e^{+\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$

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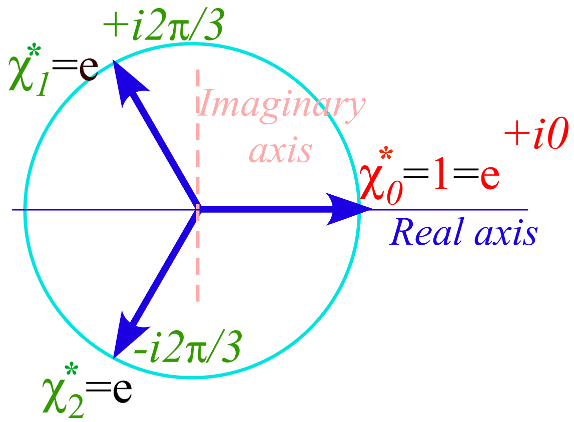

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$\mathbf{r}^2=\mathbf{r}^{-1}$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
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$D^{(2)}(\mathbf{g})$	$\chi_0^{(2)}$	$\chi_1^{(2)}$	$\chi_2^{(2)}$

=

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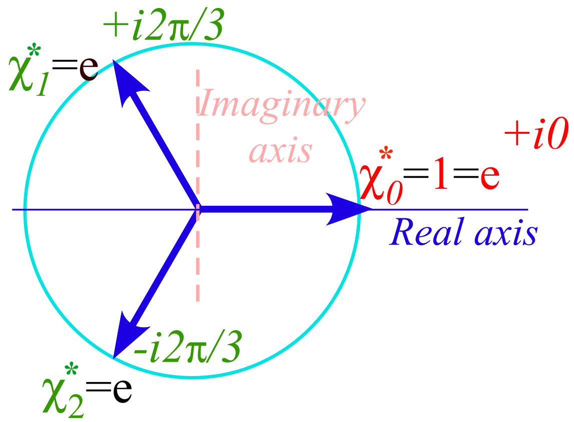
The *identity irrep* $D^{(0)}=\{1,1,1\}$ obeys *any* group table.

C_3-group jargon and structure of various tables



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=

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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 $D^{(1)}=\{1, e^{-i2\pi/3}, e^{+i2\pi/3}\}$

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

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Eigenvalues and wave dispersion functions

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

Eigenvalues and wave dispersion functions

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

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

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)

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

Eigenvalues and wave dispersion functions

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

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

Quantum **H**-values:

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

Eigenvalues and wave dispersion functions - Moving waves

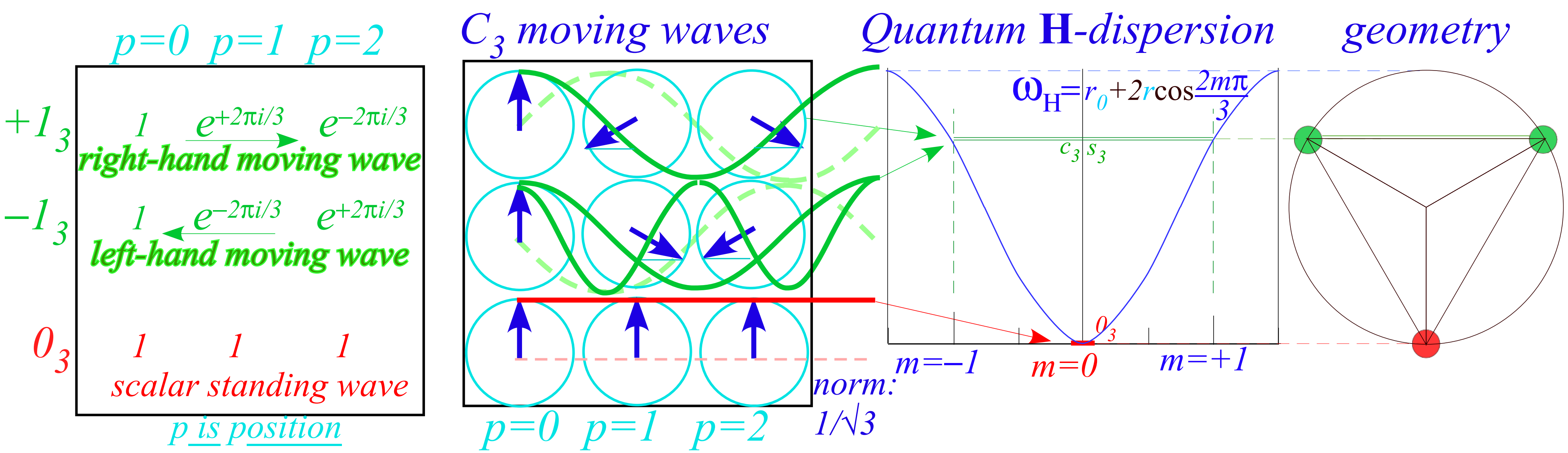
$$\langle m|\mathbf{H}|m\rangle = \langle m|r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2|m\rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

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

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

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

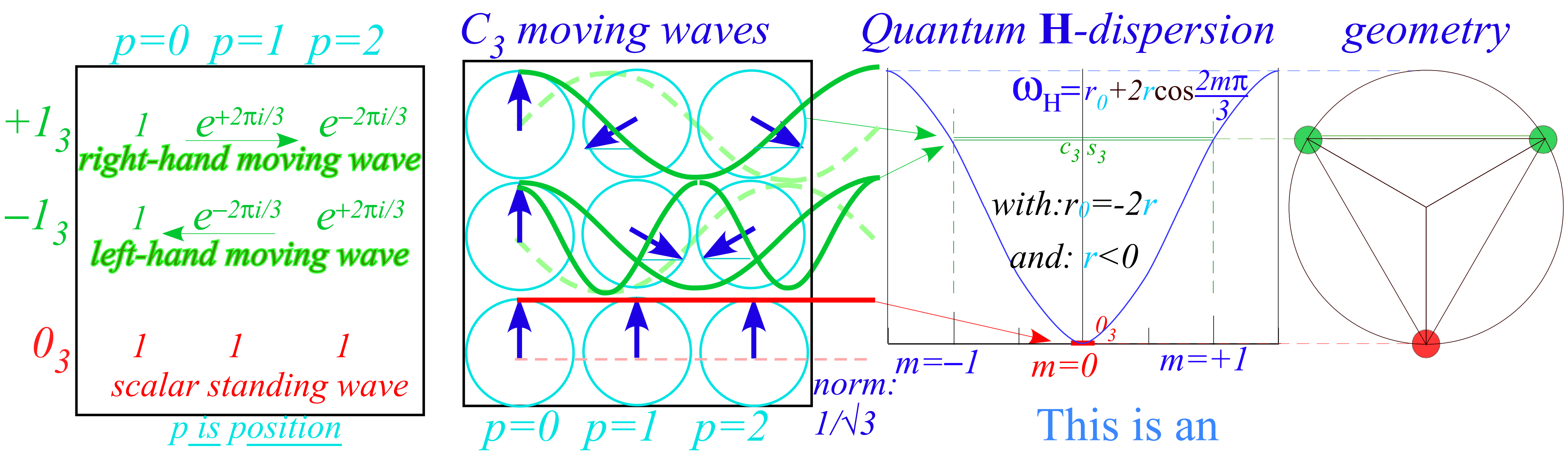
$$\langle m|\mathbf{H}|m\rangle = \langle m|r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2|m\rangle = r_0 e^{i0(m)\frac{2\pi}{3}} + r_1 e^{i1(m)\frac{2\pi}{3}} + r_2 e^{i2(m)\frac{2\pi}{3}}$$

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

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

Quantum **H**-values:

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



This is an

exciton-like

dispersion function

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

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

Eigenvalues and wave dispersion functions - Moving waves

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

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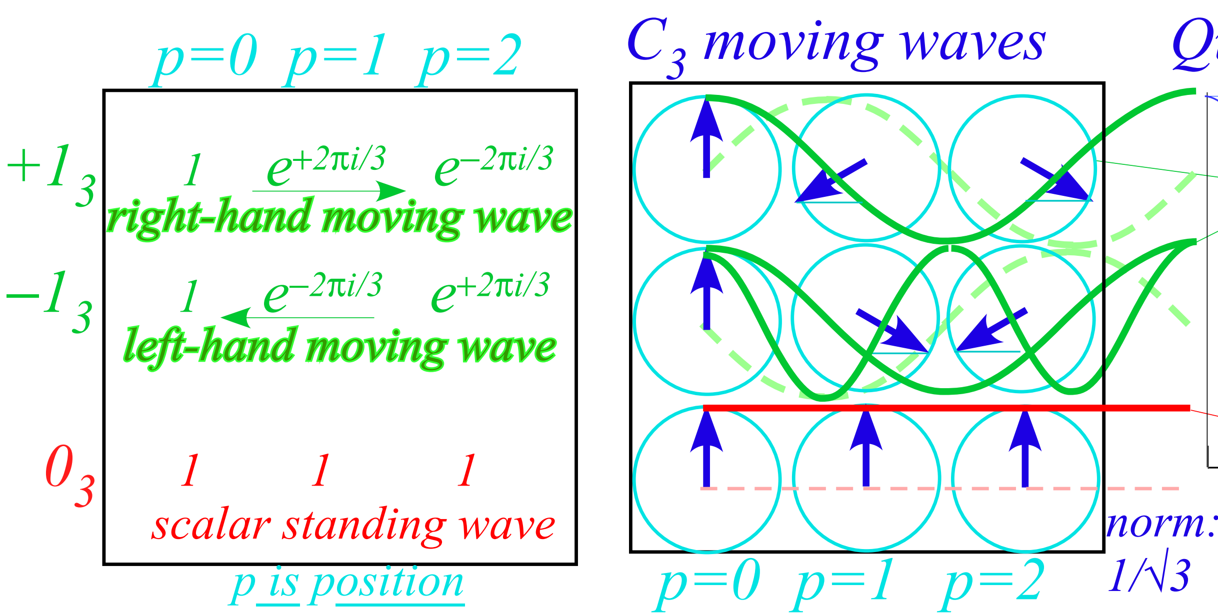
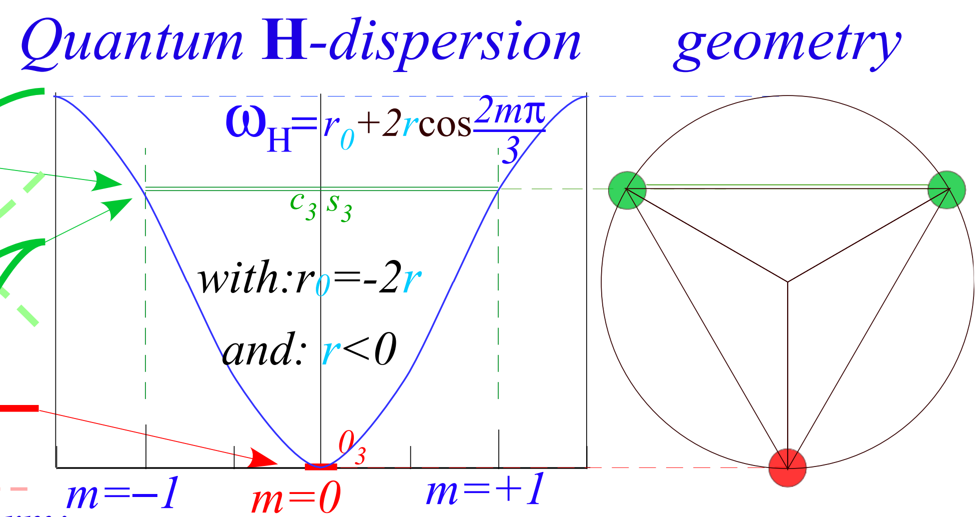
$$\begin{pmatrix} K & -k & -k \\ -k & K & -k \\ -k & -k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} = \left(K - 2k\cos\left(\tfrac{2m\pi}{3}\right)\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix}$$





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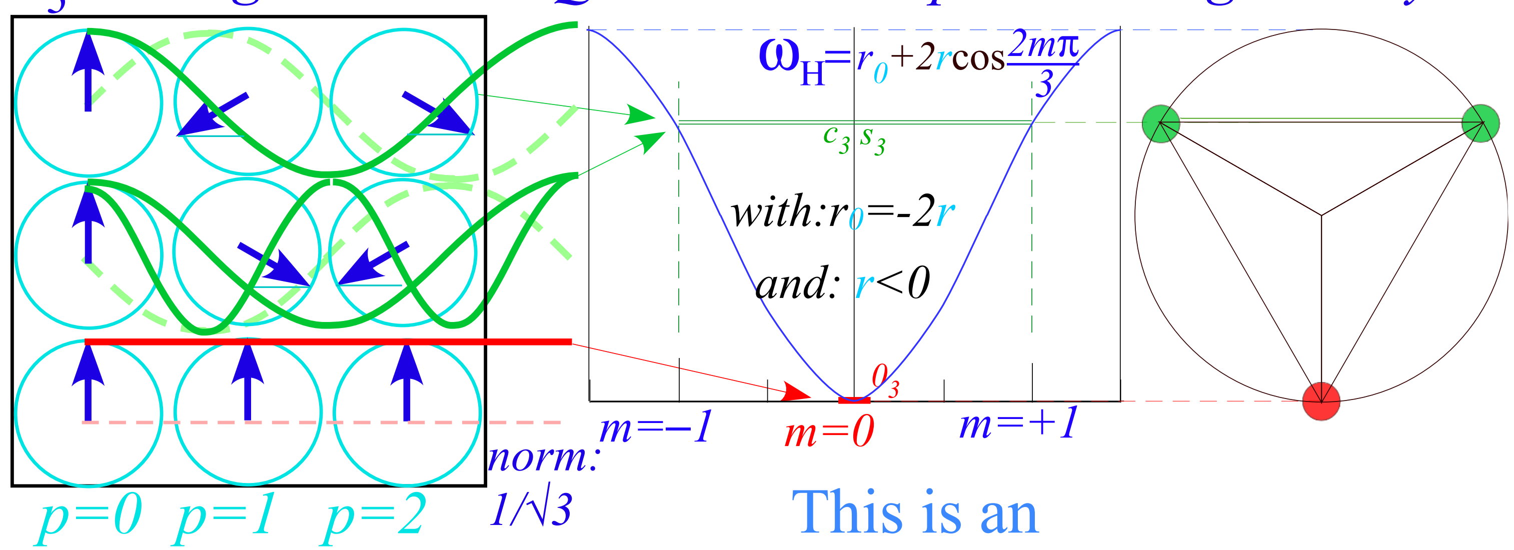
K-eigenvalue... needs *Square-Root* to be a *frequency*

p=0 p=1 p=2

	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*



This is an *exciton-like* dispersion function

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Eigenvalues and wave dispersion functions - Moving waves

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

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

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

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	p=0	*p=1*	*p=2*
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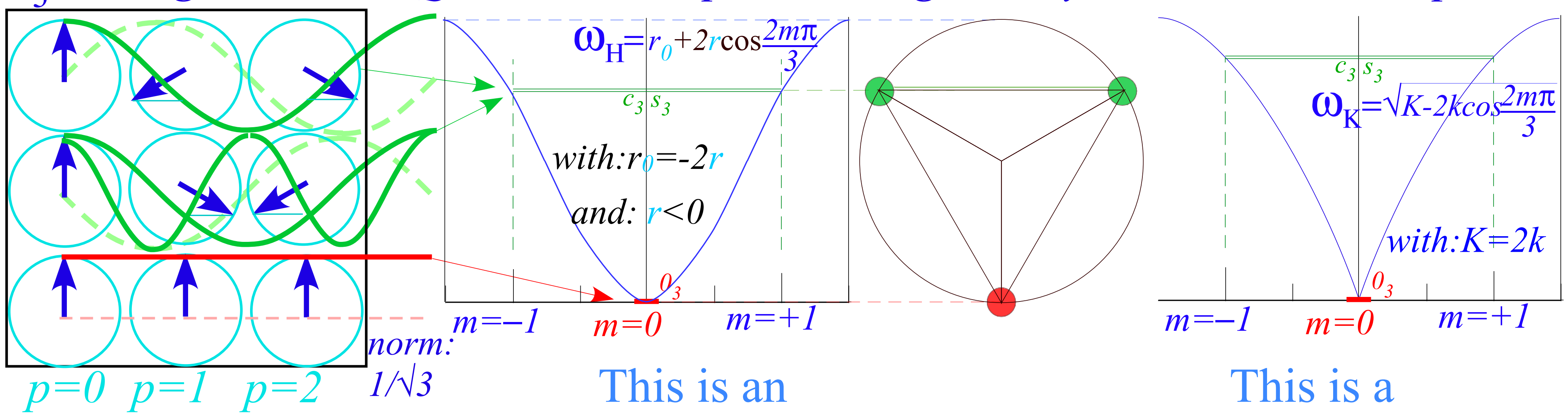
	left-hand moving wave		
0_3	*1*	*1*	*1*
	scalar standing wave		

p is position

C_3 moving waves — *Quantum* ***H****-dispersion* — *geometry* — *Classical* ***K****-dispersion*



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

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

(long wavelength λ)

This is a *phonon-like* dispersion function

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

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

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

(long wavelength λ)

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*

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

Eigenvalues and wave dispersion functions - Standing waves

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

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Classical **K**-values:

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

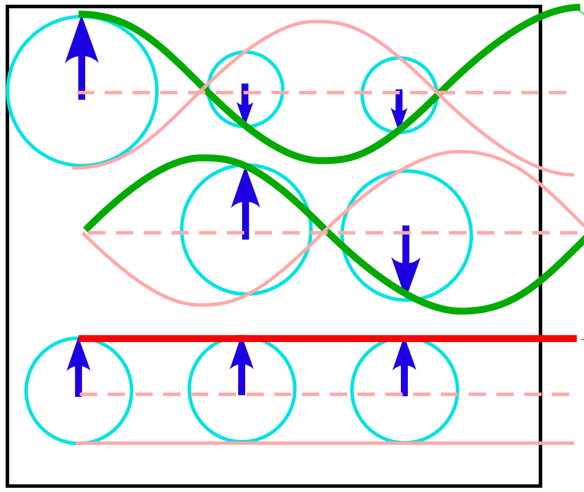
States $\lvert(+)\rangle$ and $\lvert(-)\rangle$ in *any mixtures* are still *stationary* due to $(\pm)$-*degeneracy* $(\cos(+x) = \cos(-x))$

Eigenvalues and wave dispersion functions - Standing waves

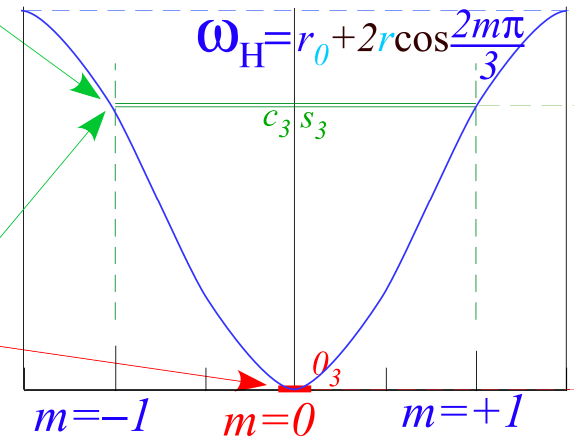
*(Possible if **H** is all-real)*

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

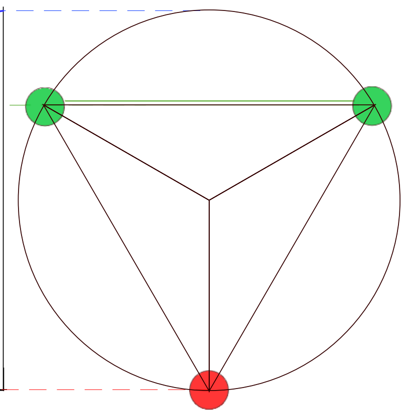
C_3 standing waves



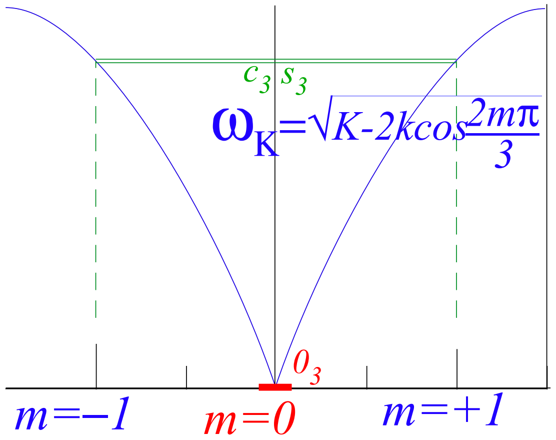
*Quantum **H**-dispersion*



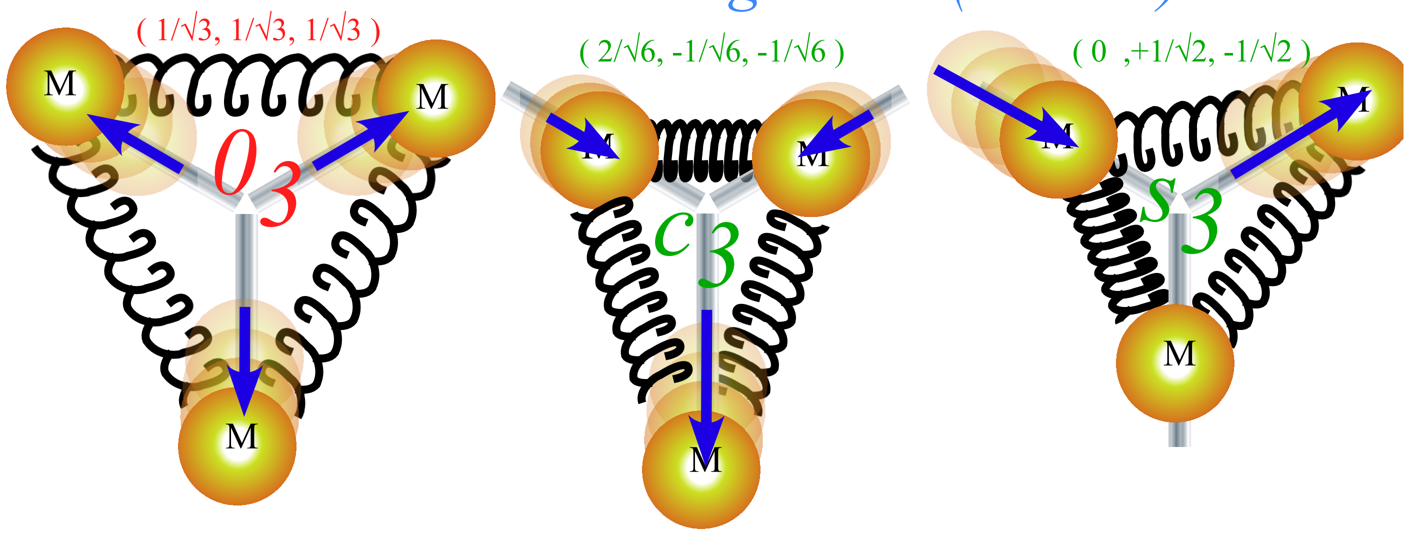
geometry



*Classical **K**-dispersion*



Radial standing waves (all-real)



Eigenvalues and wave dispersion functions - Standing waves

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

	$p=0$	$p=1$	$p=2$
c_3	$2/\sqrt{6}$	$-1/\sqrt{6}$	$-1/\sqrt{6}$
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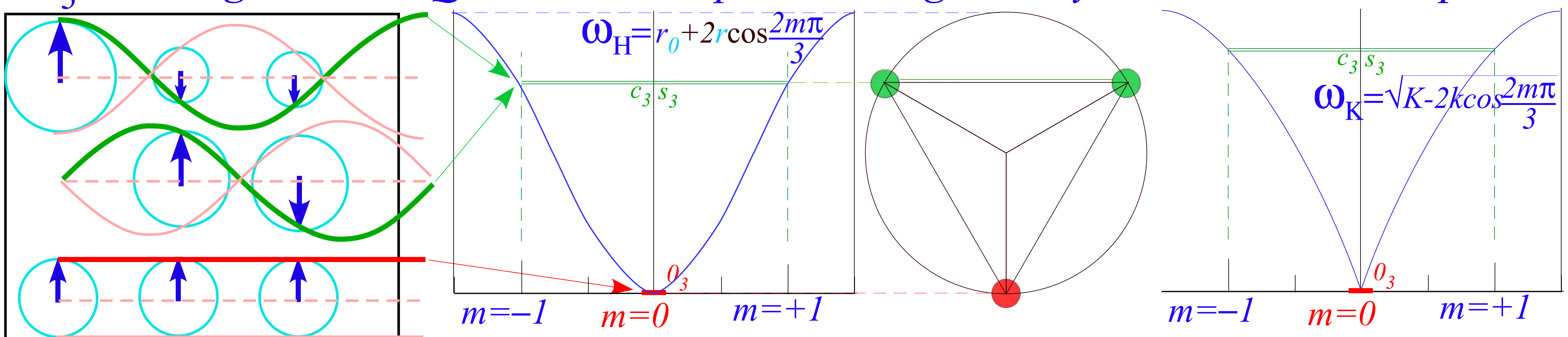
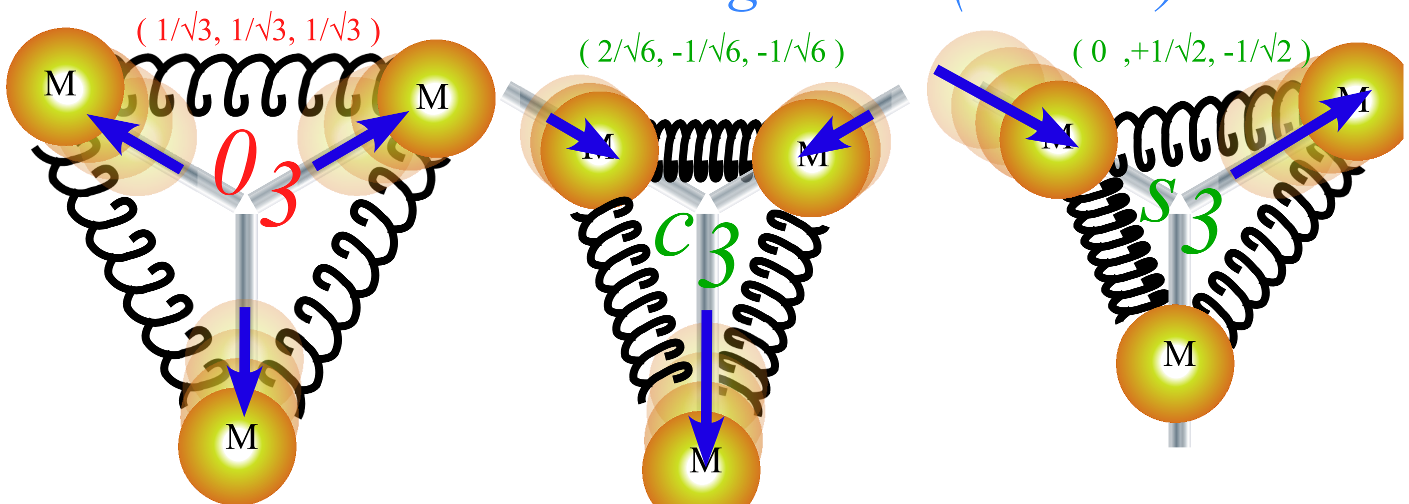
	scalar standing wave		

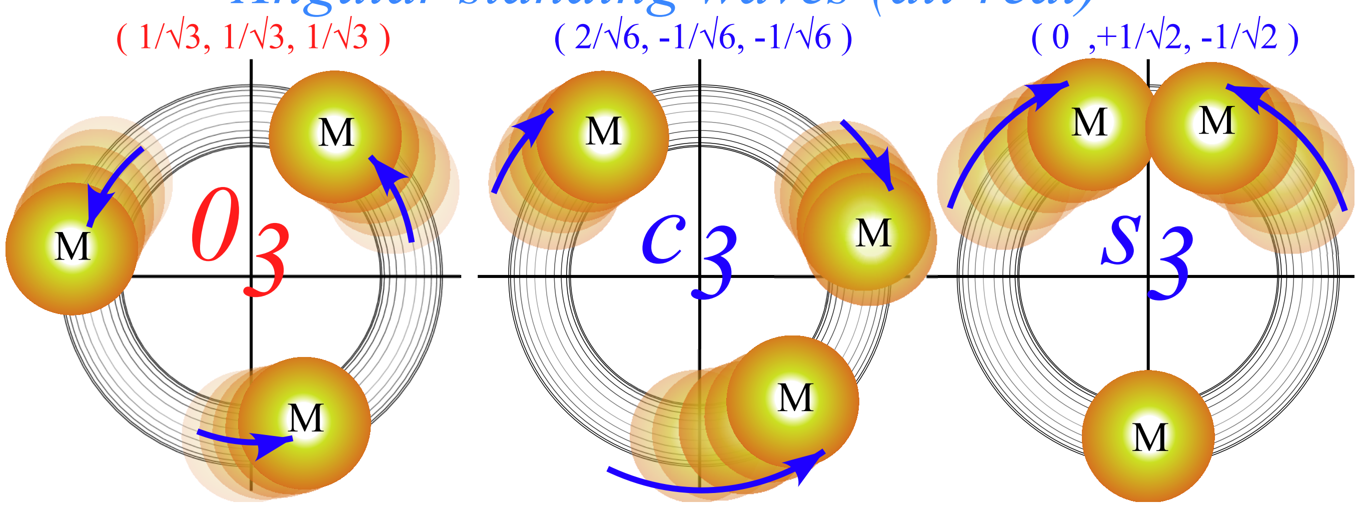
C_3 standing waves — *Quantum **H**-dispersion* — *geometry* — *Classical **K**-dispersion*



Radial standing waves (all-real)



Angular standing waves (all-real)



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*

Ortho-completeness inversion for operators and states

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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 $\mathbf{H}$ matrix using C_6 group table($\begin{smallmatrix} gg^\dagger \\ form \end{smallmatrix}$)

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

	$g^\dagger$					
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,...*

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

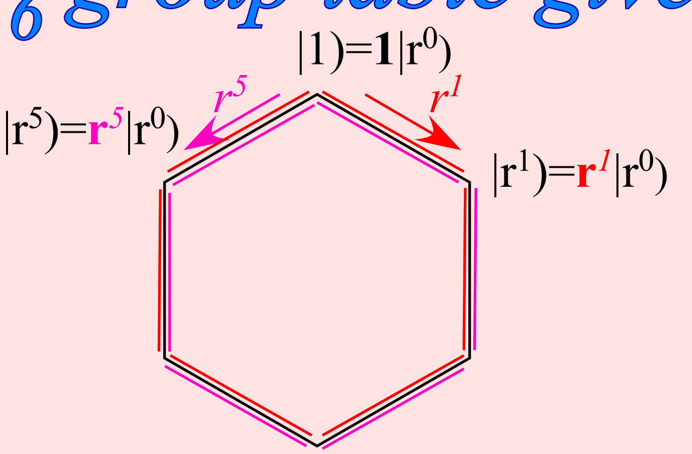
$$\mathbf{H}= r_0\mathbf{r}^0+r_1\mathbf{r}^1+r_2\mathbf{r}^2+\ldots+r_{n-1}\mathbf{r}^{n-1}=\Sigma\, r_q\mathbf{r}^k$$

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

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

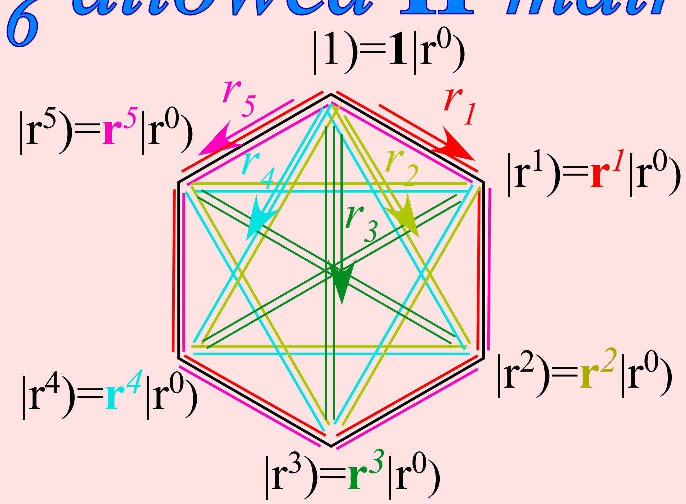
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \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 **r**-matrices,...C_6-allowed **H**-matrices...*



Nearest neighbor coupling

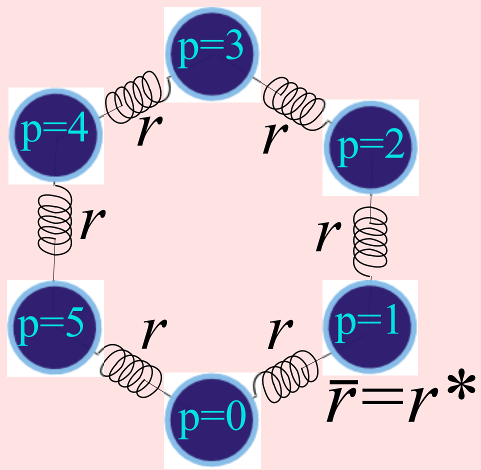
$$\begin{pmatrix} r_0 & r_5 & & & & r_1 \\ r_1 & r_0 & r_5 & & & \\ & r_1 & r_0 & r_5 & & \\ & & r_1 & r_0 & r_5 & \\ & & & r_1 & r_0 & r_5 \\ r_5 & & & & r_1 & r_0 \end{pmatrix}$$



<u>ALL</u> neighbor coupling

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

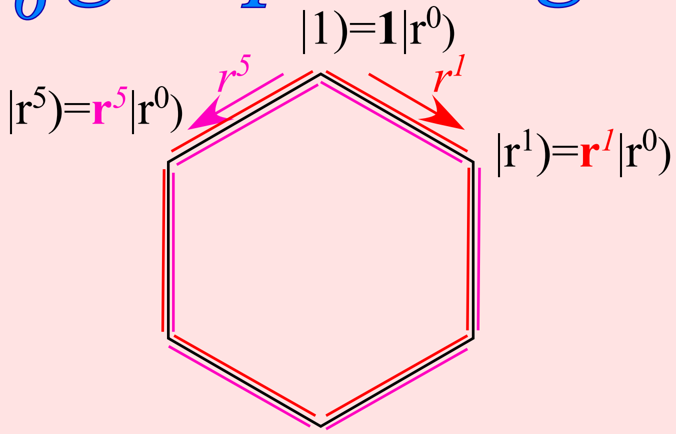
(a) 1st Neighbor C_6



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

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

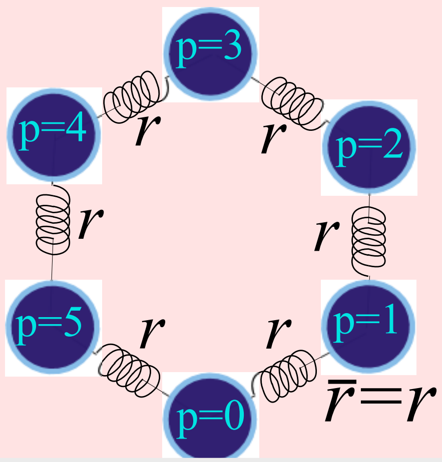
C_6 group table gives r-matrices,..



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



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

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

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

Conjugation symmetry

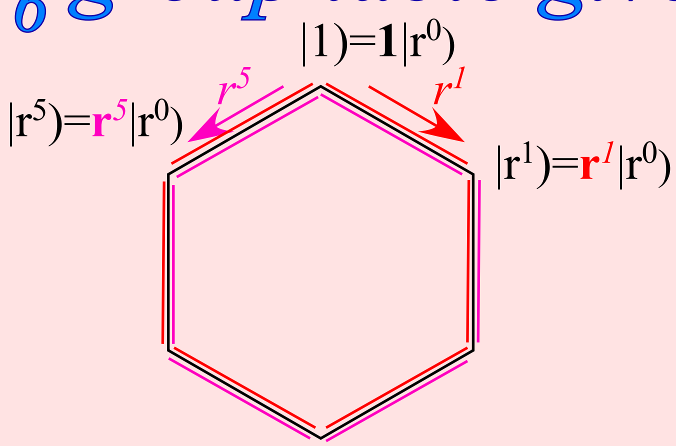
Hermitian Hamiltonian $(\mathbf{H}^*_{jk}=\mathbf{H}_{kj})$ requires $r_0^*=r_0$ and $r_1=r_5^*$.

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,..

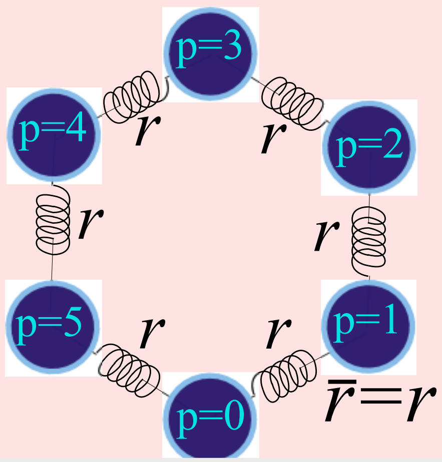


Elementary-Bloch-Model: Nearest neighbor coupling:

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

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

(a) 1^{st} Neighbor C_6

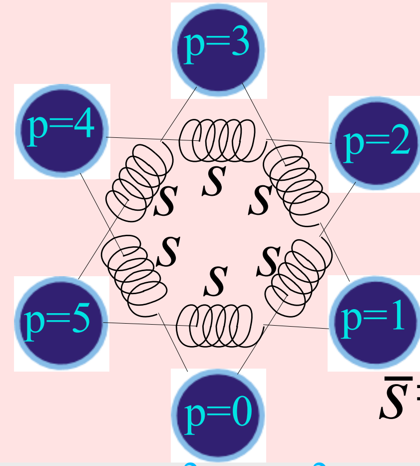


$\bar{r} = r^* = r$

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

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

(b) 2^{nd} Neighbor C_6



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

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

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

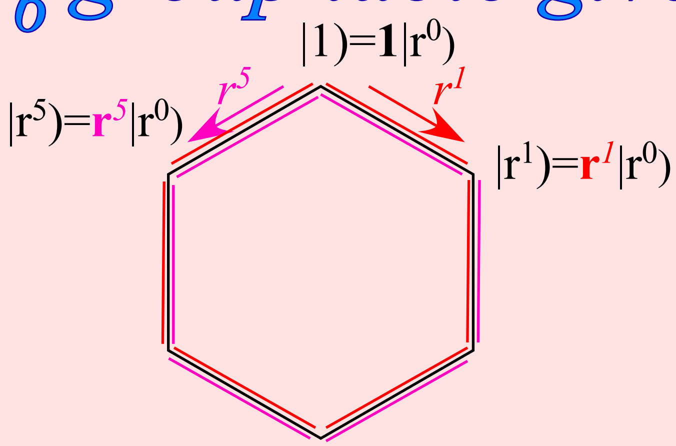
Conjugation symmetry

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

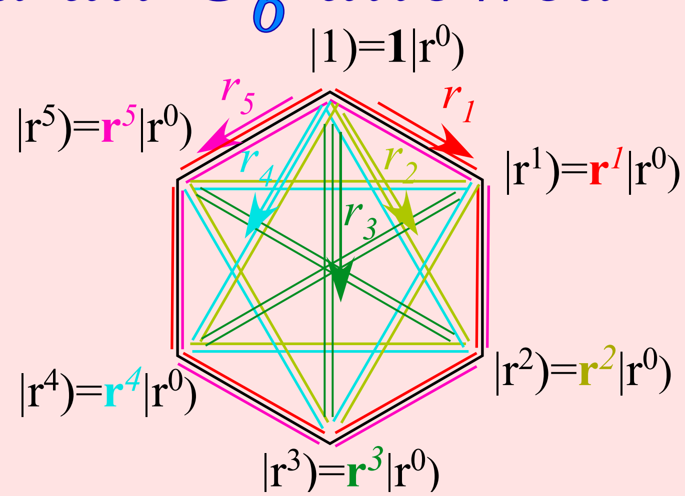
C_6 group table gives $\mathbf{r}$-matrices,..., and all C_6-allowed $\mathbb{H}$-matrices...



2^{nd} Nearest neighbor coupling:

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

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

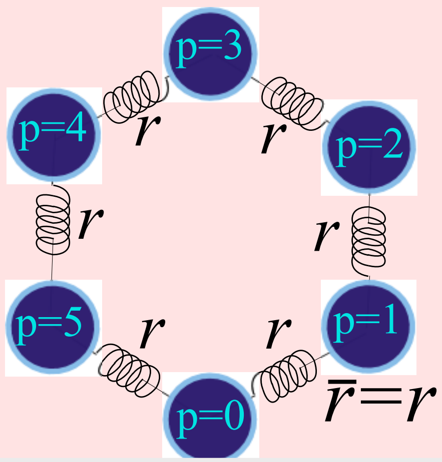


All – neighbor coupling:

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

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

(a) 1^{st} Neighbor C_6

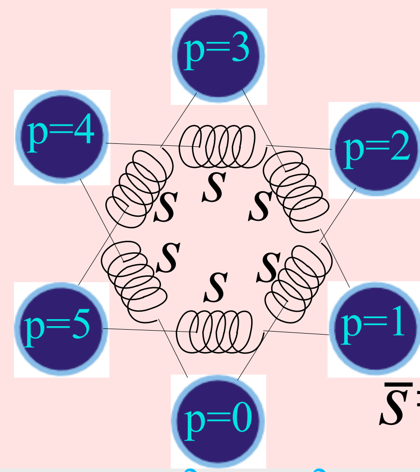


$\bar{r}=r^*=r$

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

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

Neighbor C_6

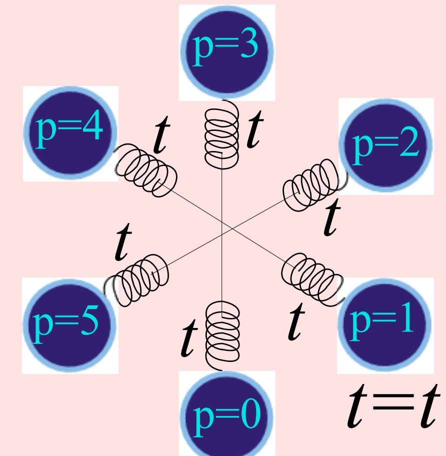


$\bar{s}=s^*=s$

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

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

(c) 3^{rd} Neighbor C_6



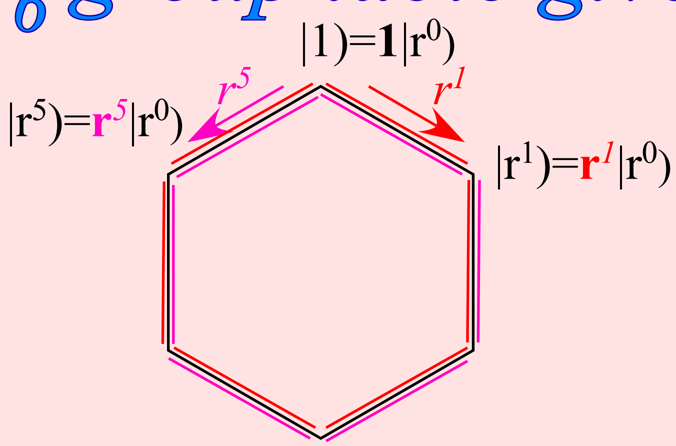
$t=t^*$

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

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

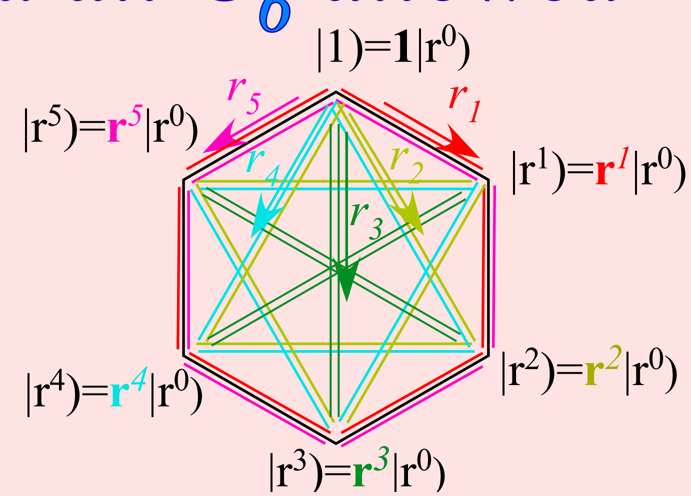
r_1 equals conjugate of r_5: ($r_1=r_5^*=-r$) $\quad (r_2=r_4^*=-s) \quad (r_3=r_3^*=t)$ *must* be real

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



Nearest neighbor coupling

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



<u>ALL</u> neighbor coupling

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

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*

$\psi_1^0 = 1$

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

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

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

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

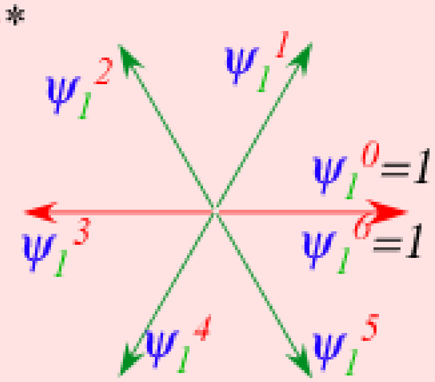
$\psi_1^5 = \psi_5^1 = \psi_1^{-1} = e^{-2\pi i/6}$

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

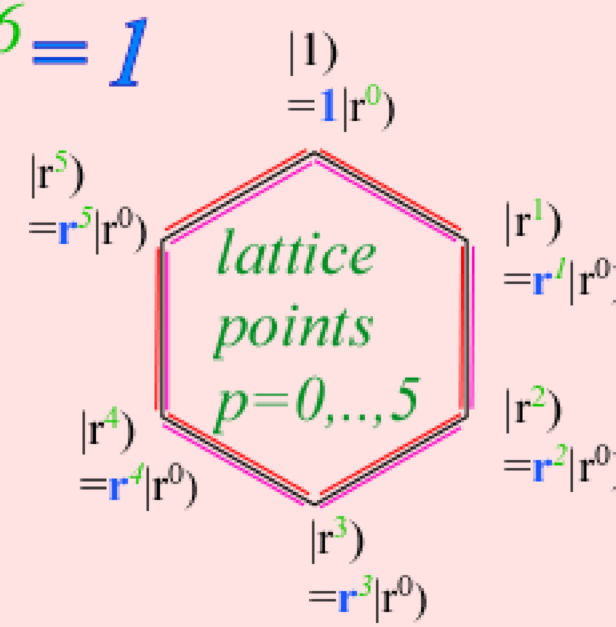
$$D^m(\mathbf{r}^p) = e^{-2\pi i m \cdot p/6} = \chi_p^m = \psi_p^{m*}$$

p = power (exponent)
or position point

m = momentum
or wave-number



6^{th}-roots of 1
$m = 0, \ldots, 5$



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*

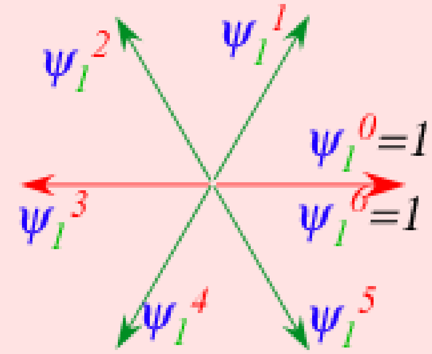
$$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1^{\ m} = \psi_1^{\ m*}$$

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

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

p = power (exponent) or position point

m = momentum or wave-number



6 ring	$\mathbf{P}^{(0)}$	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$	$\mathbf{P}^{(4)}$	$\mathbf{P}^{(5)}$
$\mathbf{P}^{(0)}$	$\mathbf{P}^{(0)}$	.	.	.	.	.
$\mathbf{P}^{(1)}$	.	$\mathbf{P}^{(1)}$	.	.	.	.
$\mathbf{P}^{(2)}$	.	.	$\mathbf{P}^{(2)}$	.	.	.
$\mathbf{P}^{(3)}$	.	.	.	$\mathbf{P}^{(3)}$	.	.
$\mathbf{P}^{(4)}$	.	.	.	.	$\mathbf{P}^{(4)}$	.
$\mathbf{P}^{(5)}$	.	.	.	.	.	$\mathbf{P}^{(5)}$

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

$$\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 $\boxed{\text{6th-roots-of-1}}$ *for eigenvalues*

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

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

p = power (exponent) or position point

m = momentum or wave-number

$\psi_1^{\,0} = 1$

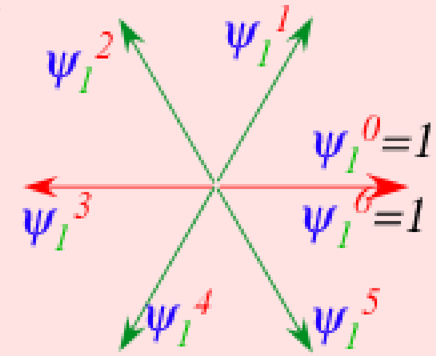
$\psi_1^{\,1} = e^{2\pi i/6}$

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

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

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

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



6 ring	$\mathbf{P}^{(0)}$	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$	$\mathbf{P}^{(4)}$	$\mathbf{P}^{(5)}$
$\mathbf{P}^{(0)}$	$\mathbf{P}^{(0)}$	·	·	·	·	·
$\mathbf{P}^{(1)}$	·	$\mathbf{P}^{(1)}$	·	·	·	·
$\mathbf{P}^{(2)}$	·	·	$\mathbf{P}^{(2)}$	·	·	·
$\mathbf{P}^{(3)}$	·	·	·	$\mathbf{P}^{(3)}$	·	·
$\mathbf{P}^{(4)}$	·	·	·	·	$\mathbf{P}^{(4)}$	·
$\mathbf{P}^{(5)}$	·	·	·	·	·	$\mathbf{P}^{(5)}$

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

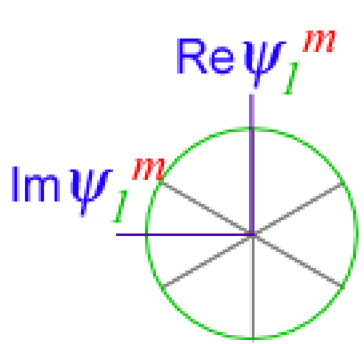
$$\begin{pmatrix} \chi_p^{\,0} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \chi_p^{\,1} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \chi_p^{\,2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \chi_p^{\,3} & \cdot & \cdot \end{pmatrix} = \chi_p^{\,0}\begin{pmatrix} 1 & \cdot & \cdot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

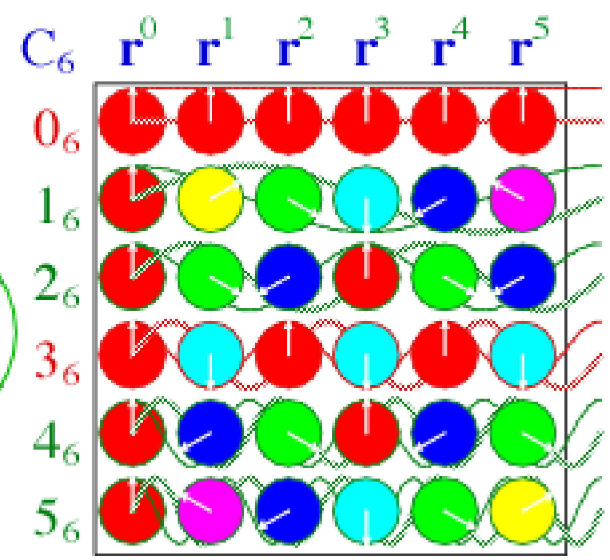
Inverse C_6 spectral resolution m-wave $\psi_p^{\,m} = D^{m*}(\mathbf{r}^p) = e^{+2\pi i m\cdot p/6}$:

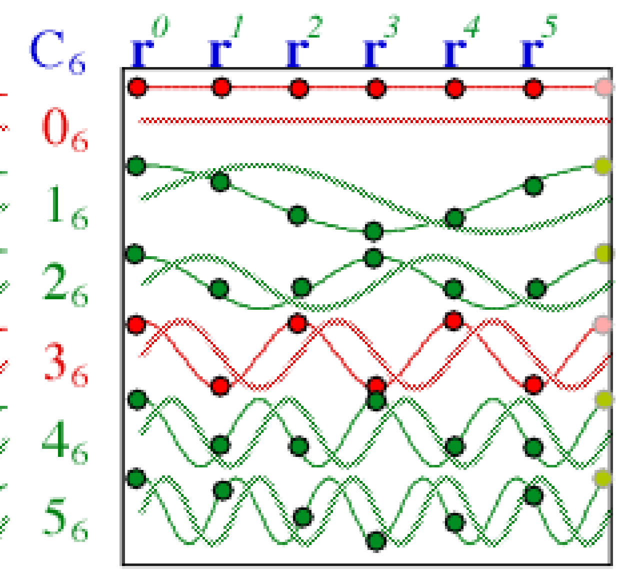
$$6\cdot\mathbf{P}^{(m)} = \psi_0^{\,m}\,\mathbf{r}^0 + \psi_1^{\,m}\,\mathbf{r}^1 + \psi_2^{\,m}\,\mathbf{r}^2 + \psi_3^{\,m}\,\mathbf{r}^3 + \psi_4^{\,m}\,\mathbf{r}^4 + \psi_5^{\,m}\,\mathbf{r}^5$$

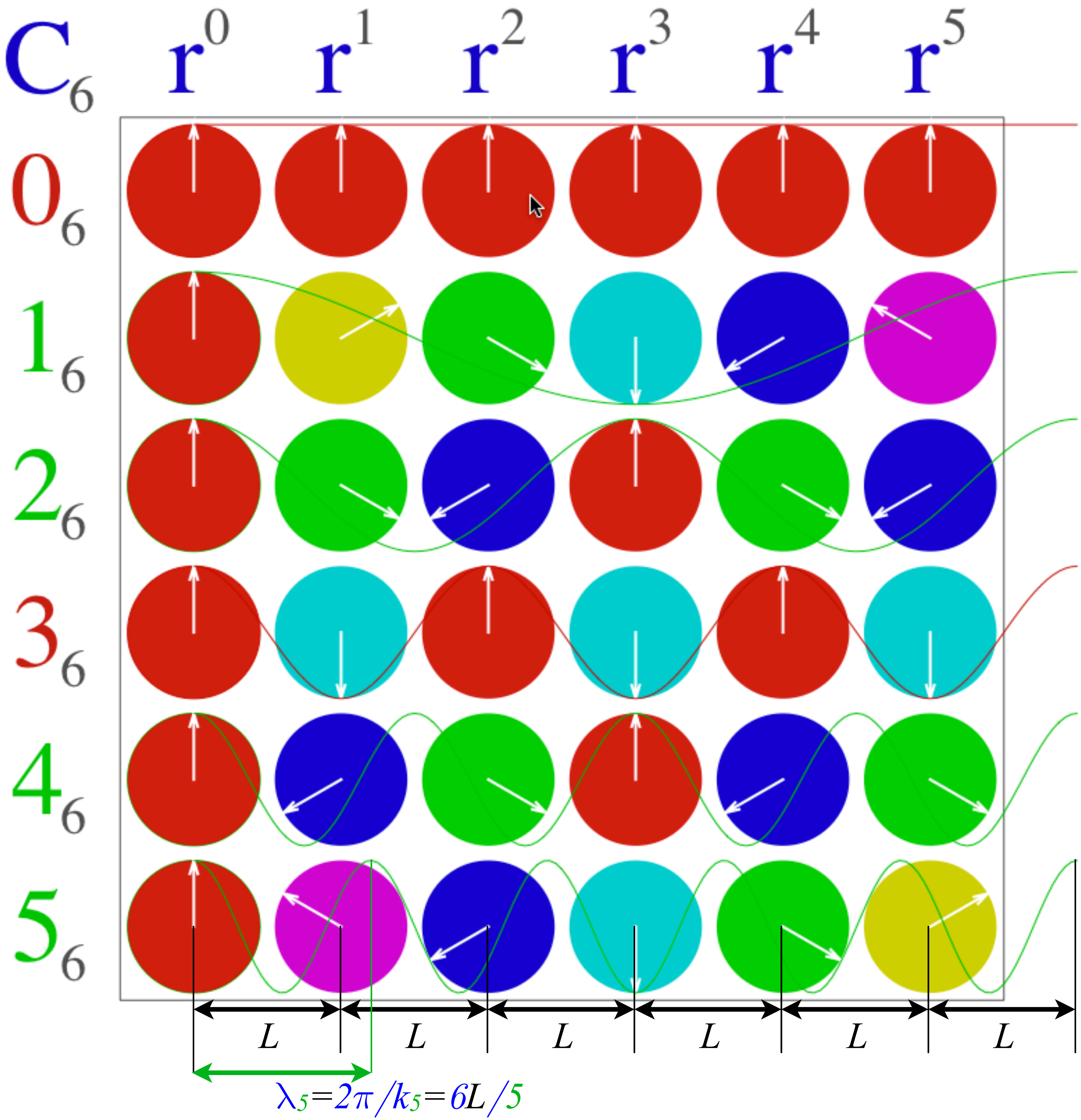
position p (or power of $\mathbf{r}^p$)

momentum m	p=0	1	2	3	4	5
m=0	$\psi_0^{\,0}$	$\psi_1^{\,0}$	$\psi_2^{\,0}$	$\psi_3^{\,0}$	$\psi_4^{\,0}$	$\psi_5^{\,0}$
m=1	$\psi_0^{\,1}$	$\psi_1^{\,1}$	$\psi_2^{\,1}$	$\psi_3^{\,1}$	$\psi_4^{\,1}$	$\psi_5^{\,1}$
m=2	$\psi_0^{\,2}$	$\psi_1^{\,2}$	$\psi_2^{\,2}$	$\psi_3^{\,2}$	$\psi_4^{\,2}$	$\psi_5^{\,2}$
m=3	$\psi_0^{\,3}$	$\psi_1^{\,3}$	$\psi_2^{\,3}$	$\psi_3^{\,3}$	$\psi_4^{\,3}$	$\psi_5^{\,3}$
m=4	$\psi_0^{\,4}$	$\psi_1^{\,4}$	$\psi_2^{\,4}$	$\psi_3^{\,4}$	$\psi_4^{\,4}$	$\psi_5^{\,4}$
m=5	$\psi_0^{\,5}$	$\psi_1^{\,5}$	$\psi_2^{\,5}$	$\psi_3^{\,5}$	$\psi_4^{\,5}$	$\psi_5^{\,5}$









C_6 character

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

is wave function conjugate

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

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

$$r_p = L \cdot p$$

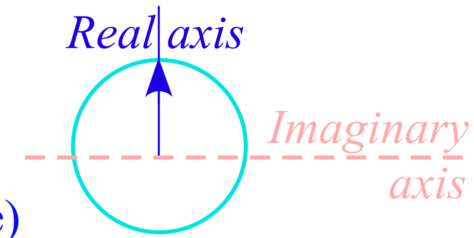
Wavevector

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

Wavelength

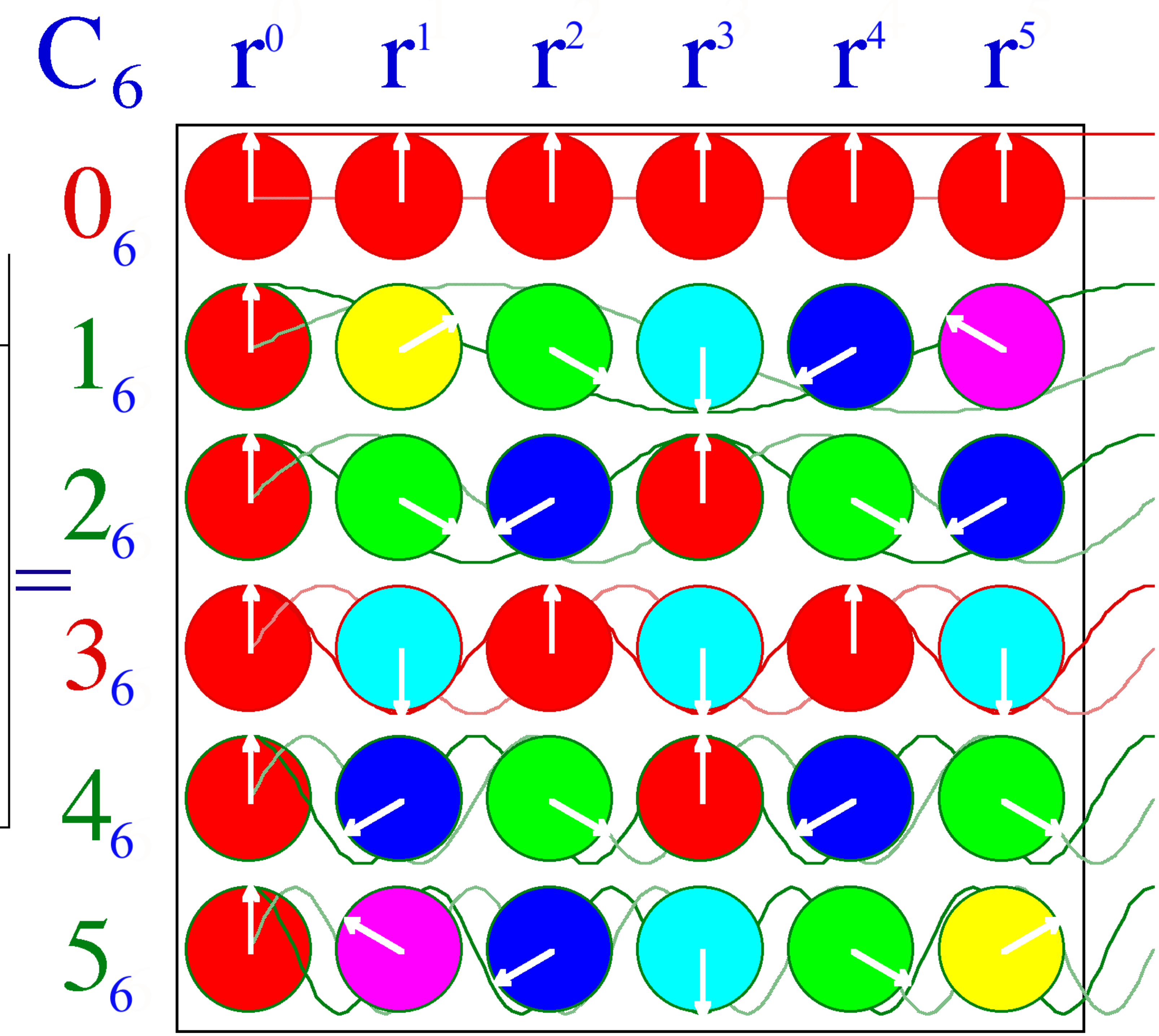
$$\lambda_m = 2\pi/k_m = 6L/m$$

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

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



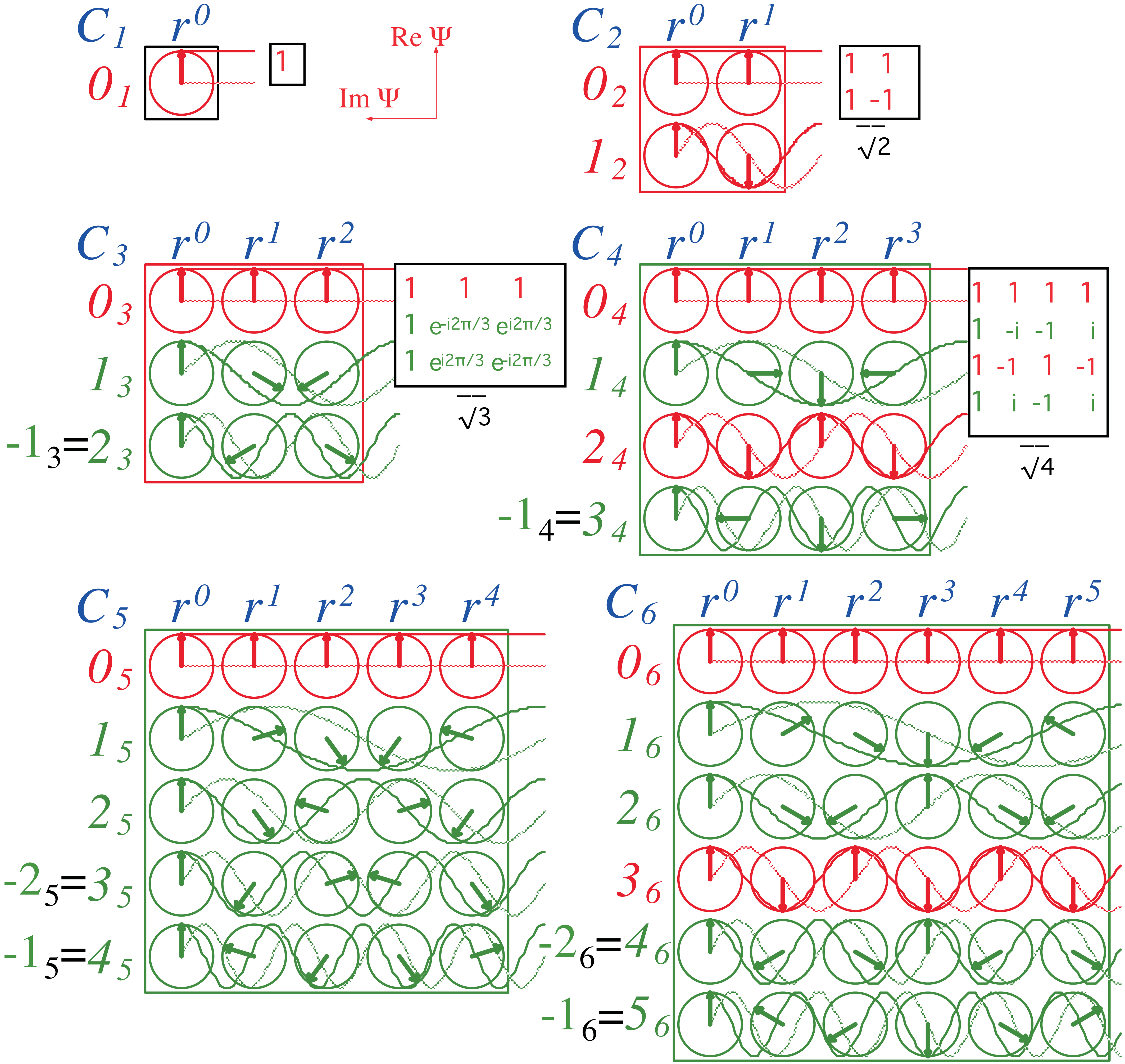
	0°	60°	120°	180°	-120°	-60°
α	1	1	1	1	1	1
β	1	ε^*	ε^{2*}	-1	ε^2	ε
γ	1	ε^{2*}	ε^2	1	ε^{2*}	ε^2
δ	1	-1	1	-1	1	-1
γ^*	1	ε^2	ε^{2*}	1	ε^2	ε^{2*}
β^*	1	ε	ε^2	-1	ε^{2*}	ε

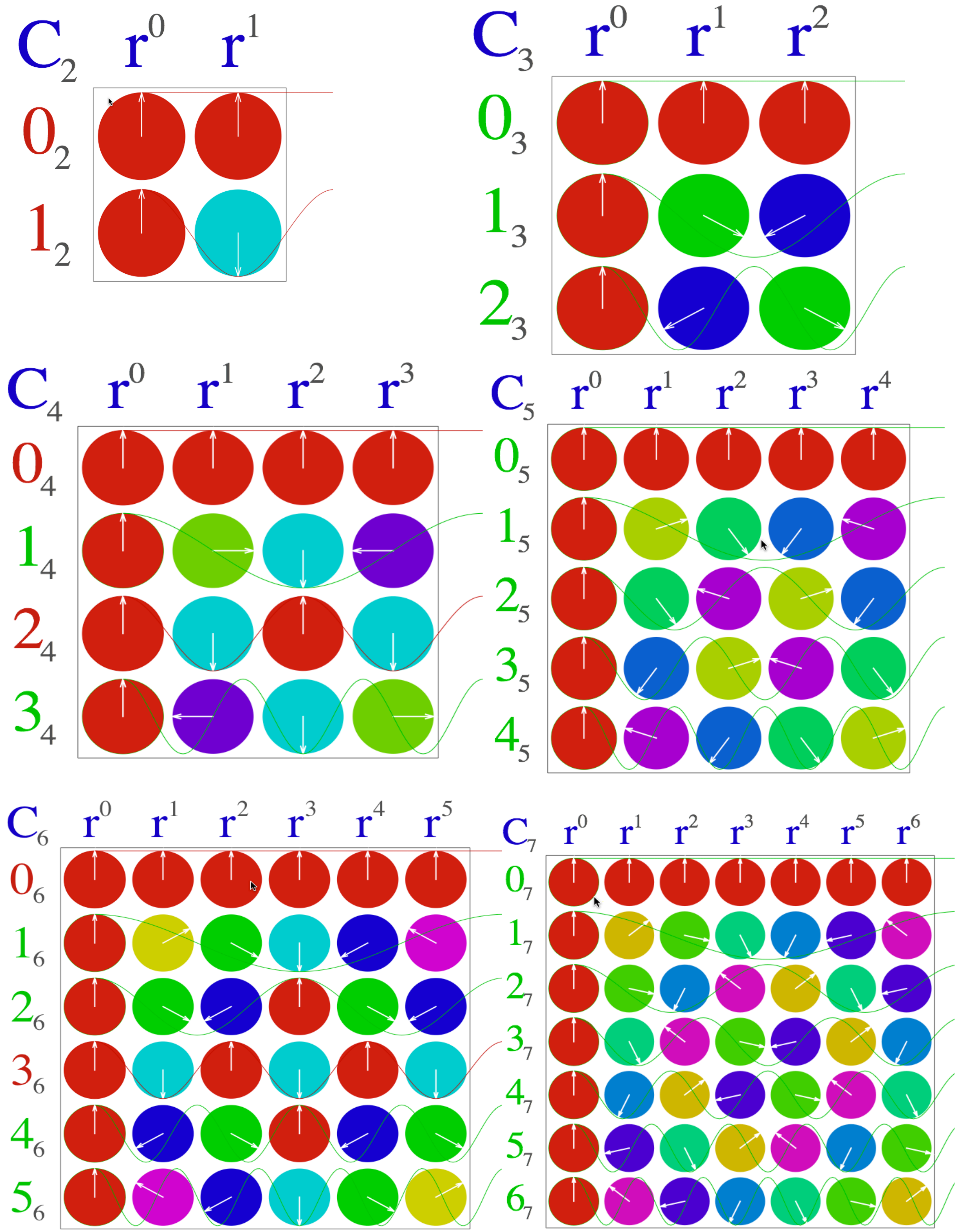
$\varepsilon = e^{i2\pi/6}$

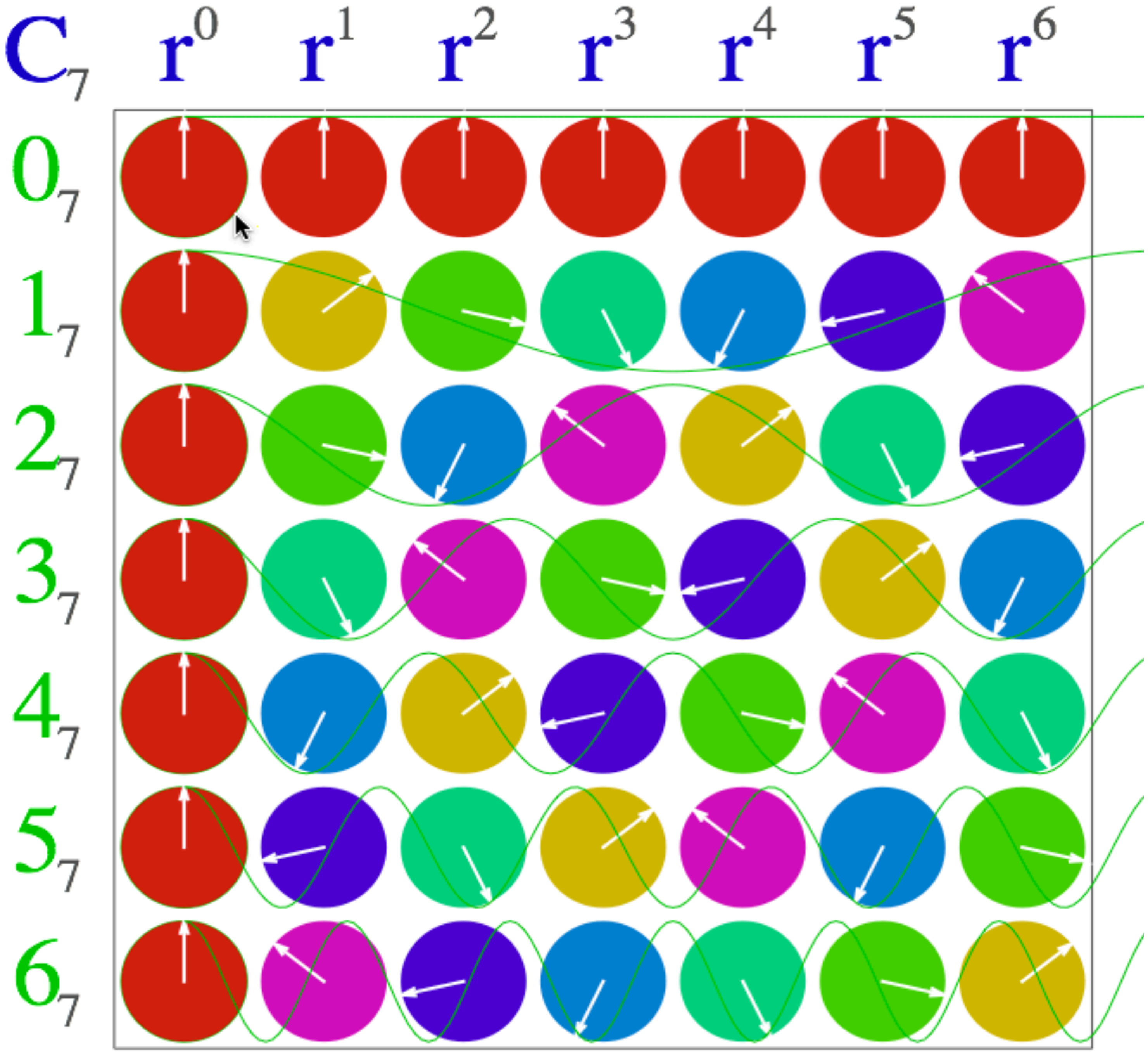
What you'll get if you look up C_6 characters in library

=

Wave phasor stuff? FUGggedd-aboudit!


C1 r0
01
1
Re Ψ
Im Ψ
C2 r0 r1
02
12
1 1
1 -1
√2
C3 r0 r1 r2
03
13
-13=23
1 1 1
1 e-i2π/3 ei2π/3
1 ei2π/3 e-i2π/3
√3
C4 r0 r1 r2 r3
04
14
24
-14=34
1 1 1 1
1 -i -1 i
1 -1 1 -1
1 i -1 i
√4
C5 r0 r1 r2 r3 r4
05
15
25
-25=35
-15=45
C6 r0 r1 r2 r3 r4 r5
06
16
26
36
-26=46
-16=56


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



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

C_N *Lattice position vector*

$r_p = L \cdot p$

Wavevector

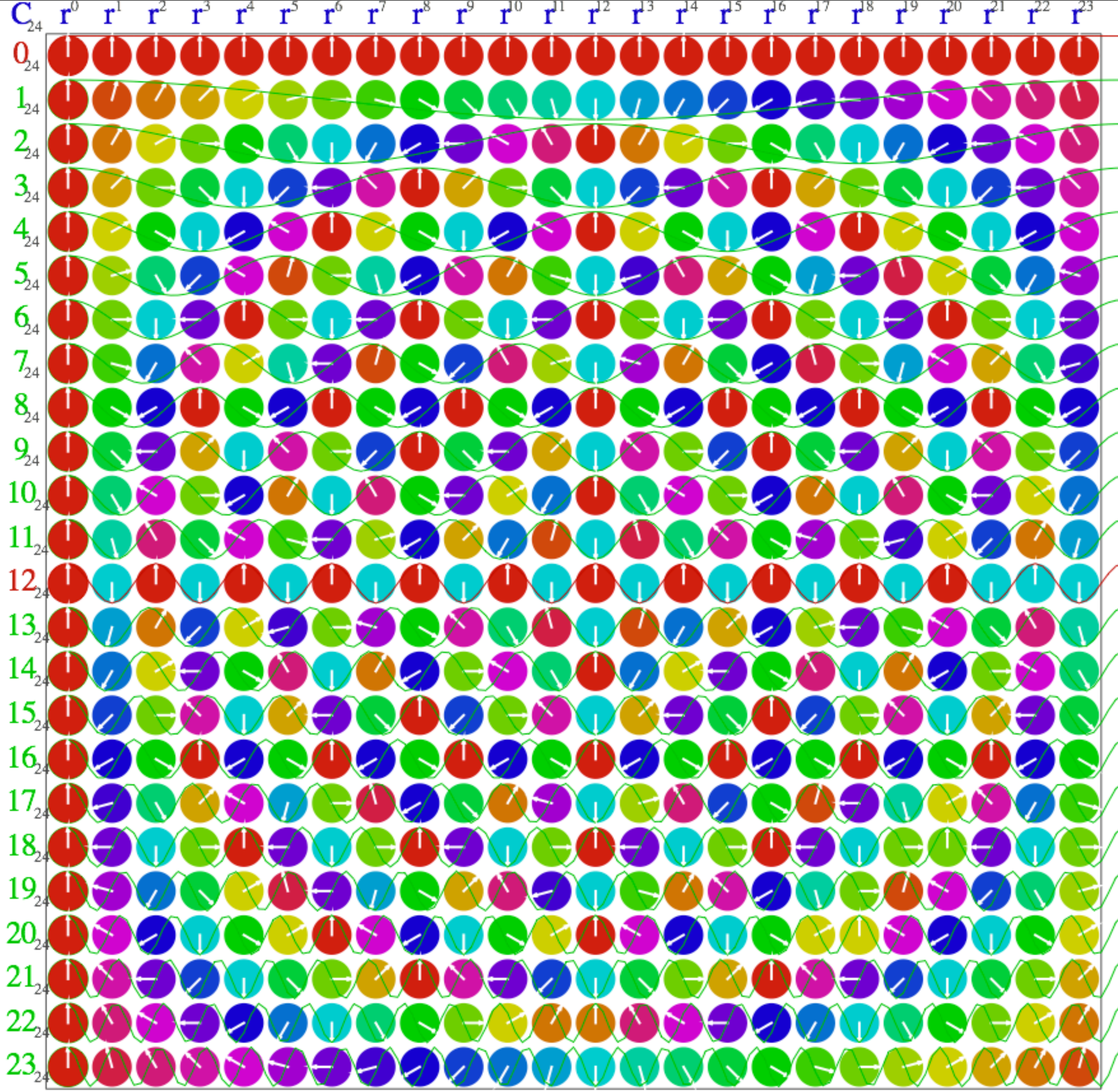
$k_m = 2\pi / \lambda_m$

$= 2\pi m / NL$

Wavelength

$\lambda_m = 2\pi / k_m$

$= NL / m$



C_N *Plane wave function*

$$\psi_m(x_p) = \frac{e^{i k_m \cdot x_p}}{\sqrt{N}} = \frac{e^{i m p 2\pi / N}}{\sqrt{N}}$$

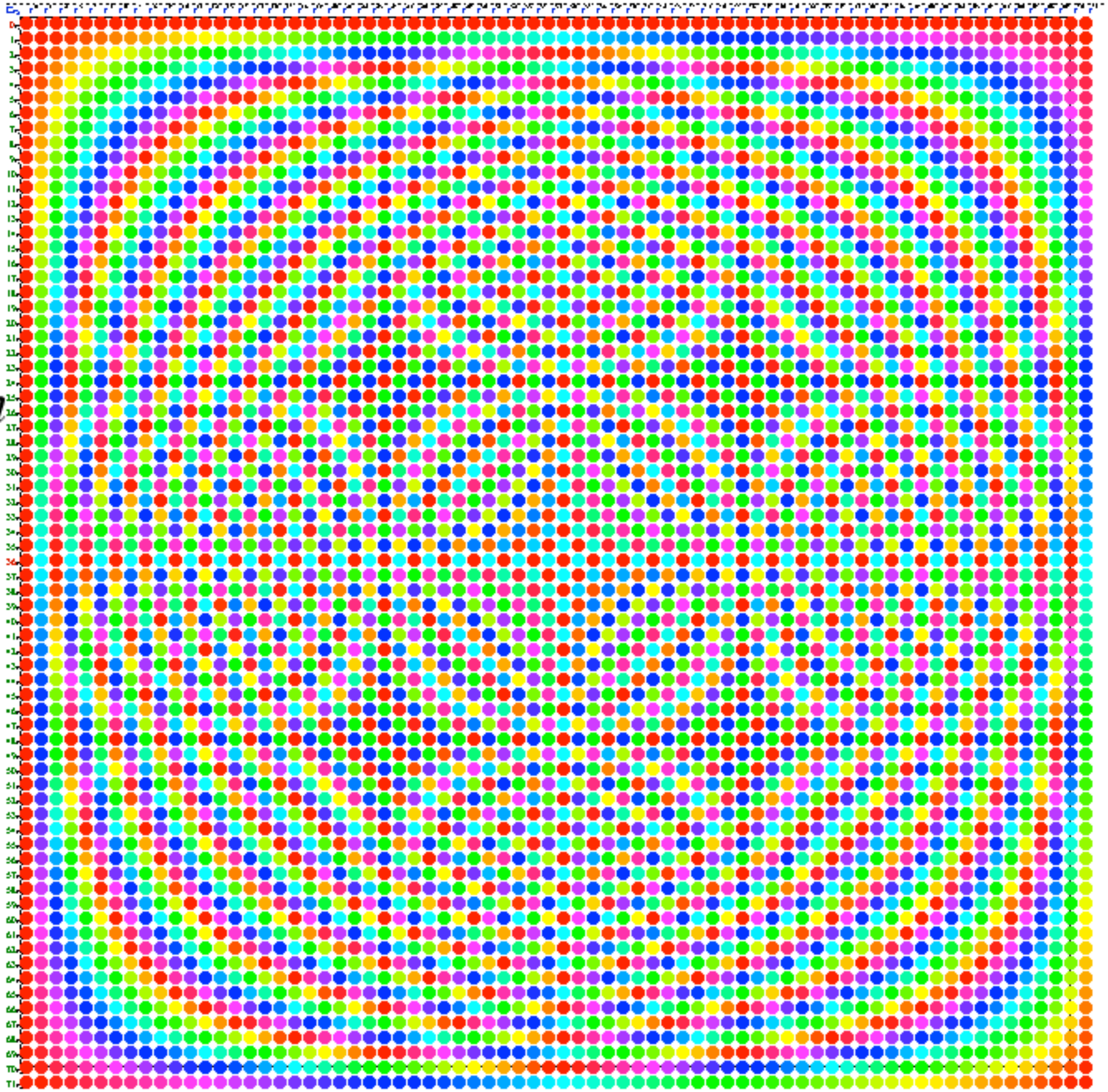
C_N *Lattice position vector*
$r_p = L \cdot p$

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

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

$N=72$

C_{72} Fourier transformation matrix



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$_3$ **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

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

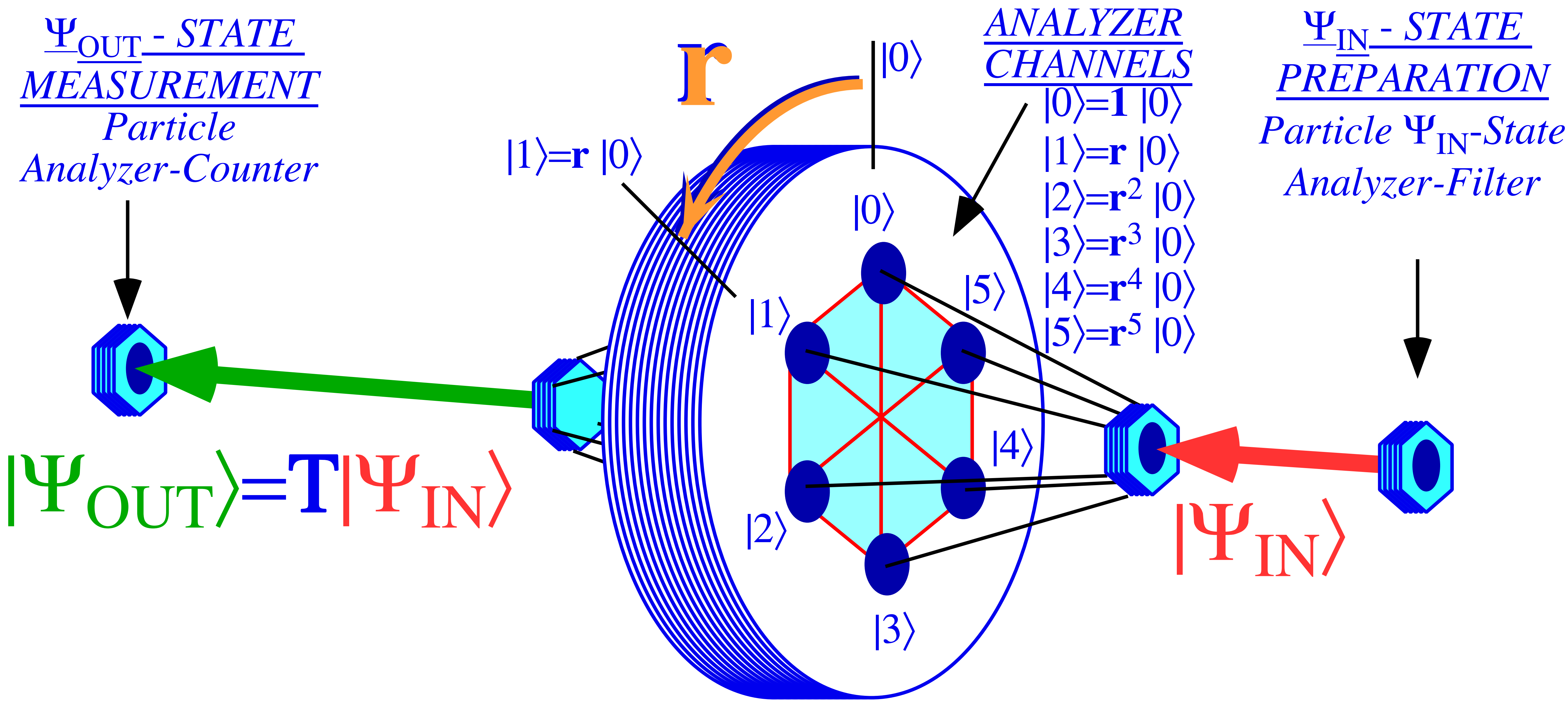


Fig. 8.1.1

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

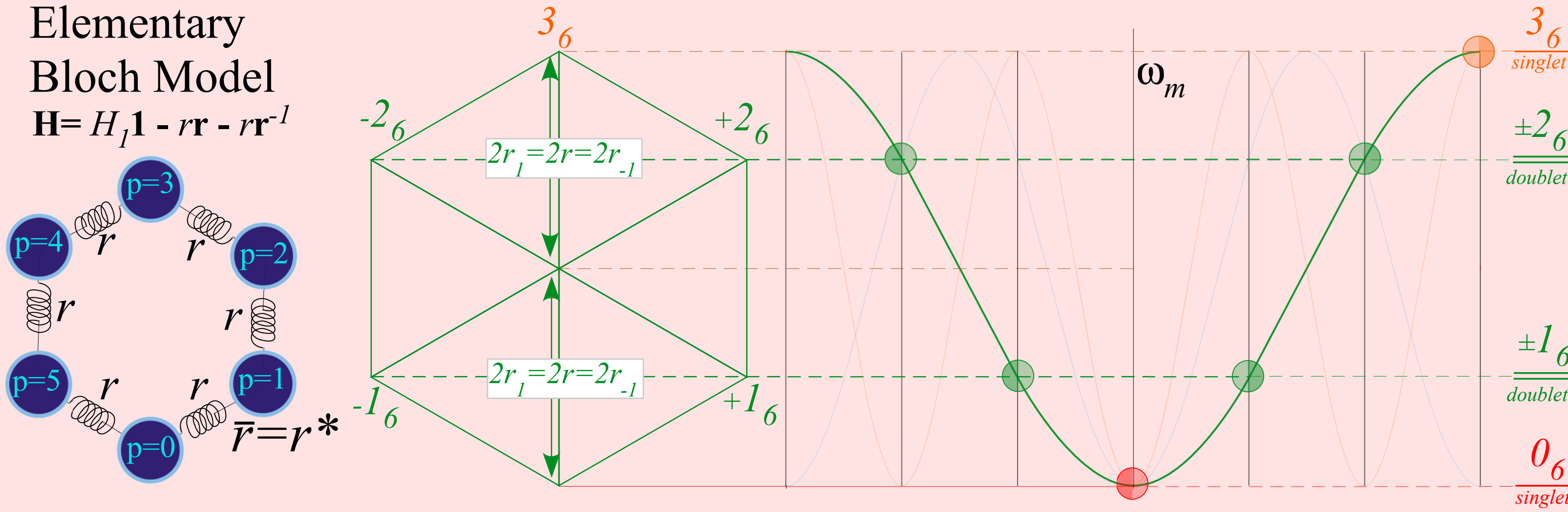
$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$ *(Dispersion functions)*

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

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



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

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

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

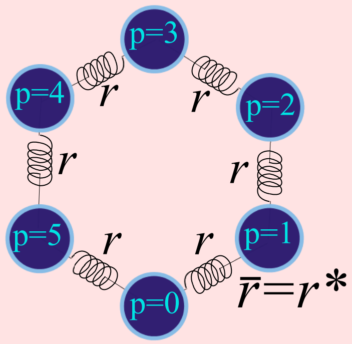
r_1 equals conjugate of r_5: ($r_1 = r_5^* = -r$)

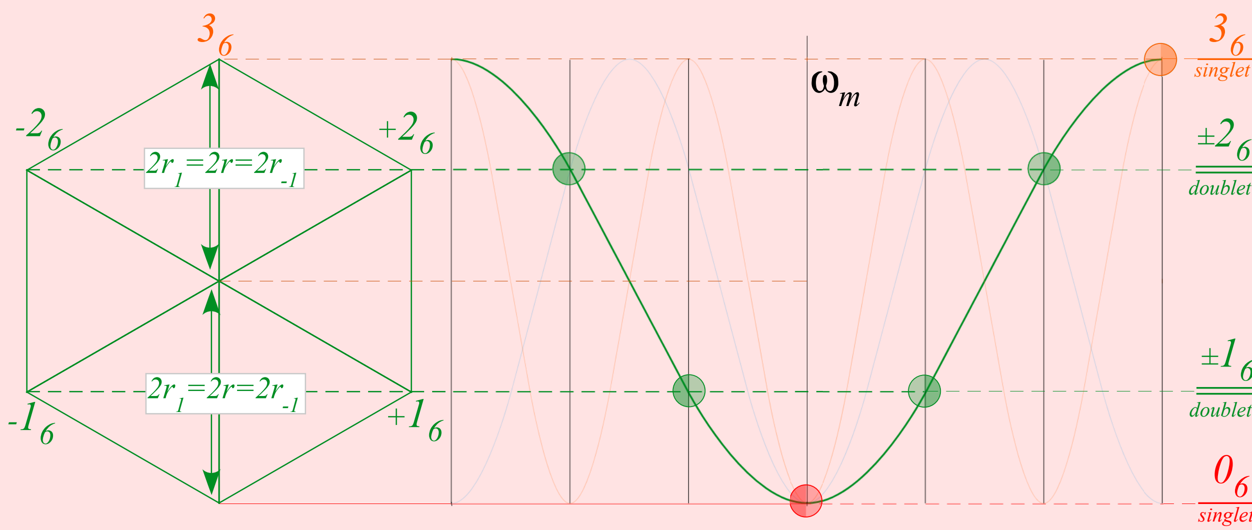
3^{rd} Step *Display all eigensolutions of all possible C_6 symmetric real H*

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

Elementary Bloch Model

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





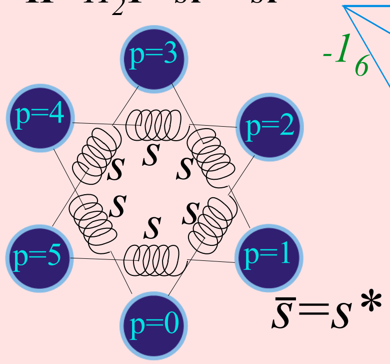
eigenvalues of $\mathbf{H}^{B1(6)}$

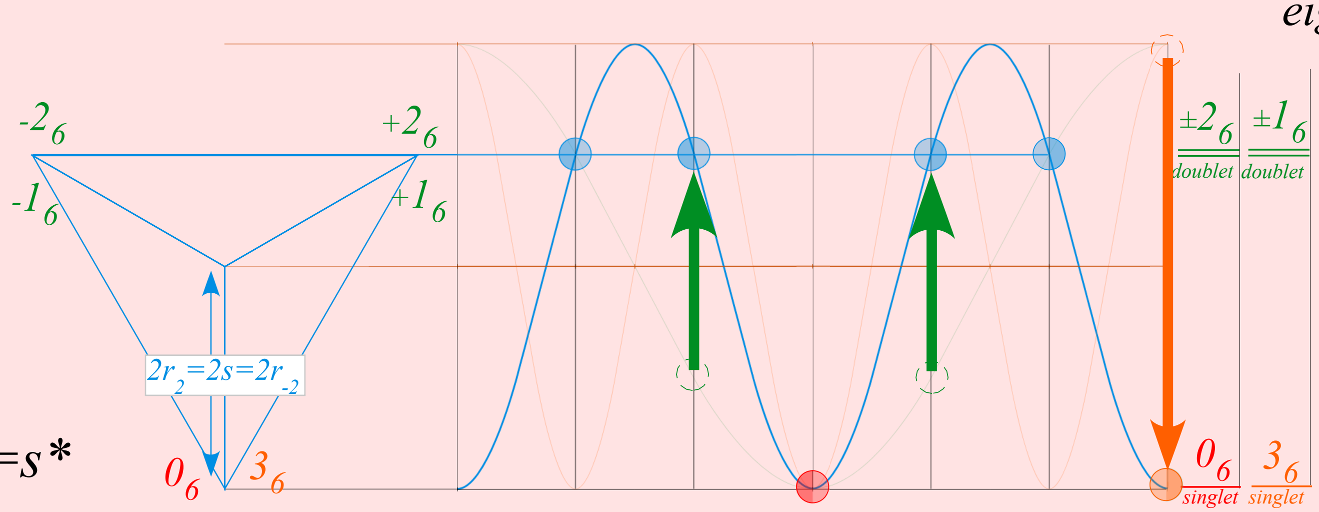
$$\begin{array}{c|c} \begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array} & \\ \begin{pmatrix} H_1 & -r & \cdot & \cdot & \cdot & -r \\ -r & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -r & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -r & H_1 & -r & \cdot \\ \cdot & \cdot & \cdot & -r & H_1 & -r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

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

2^{nd} Neighbor coupling

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





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

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

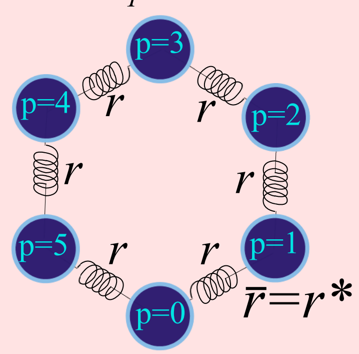
$$\omega^{B2(n)}(k_m) = r_0\chi_0^m + r_2\chi_2^m + r_{-2}\chi_{-2}^m = H_2 - 2s\,cos(4\pi m/6)$$

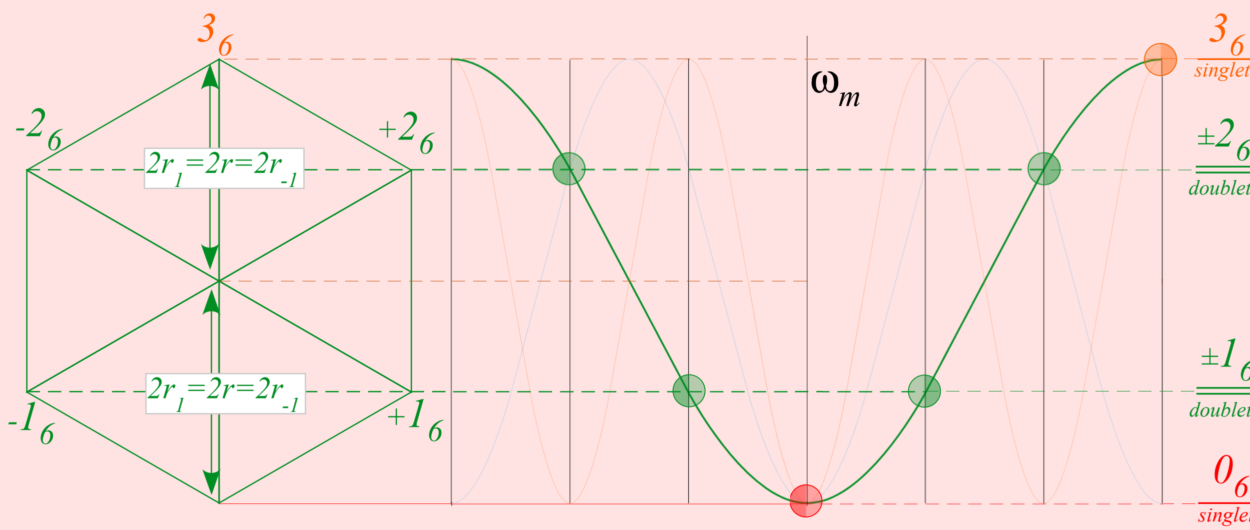
3rd Step *Display all eigensolutions of all possible C_6 symmetric real H*

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

Elementary Bloch Model

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





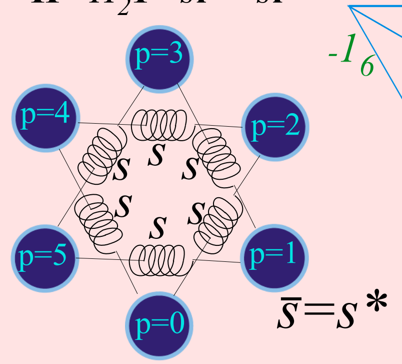
eigenvalues of $\mathbf{H}^{B1(6)}$

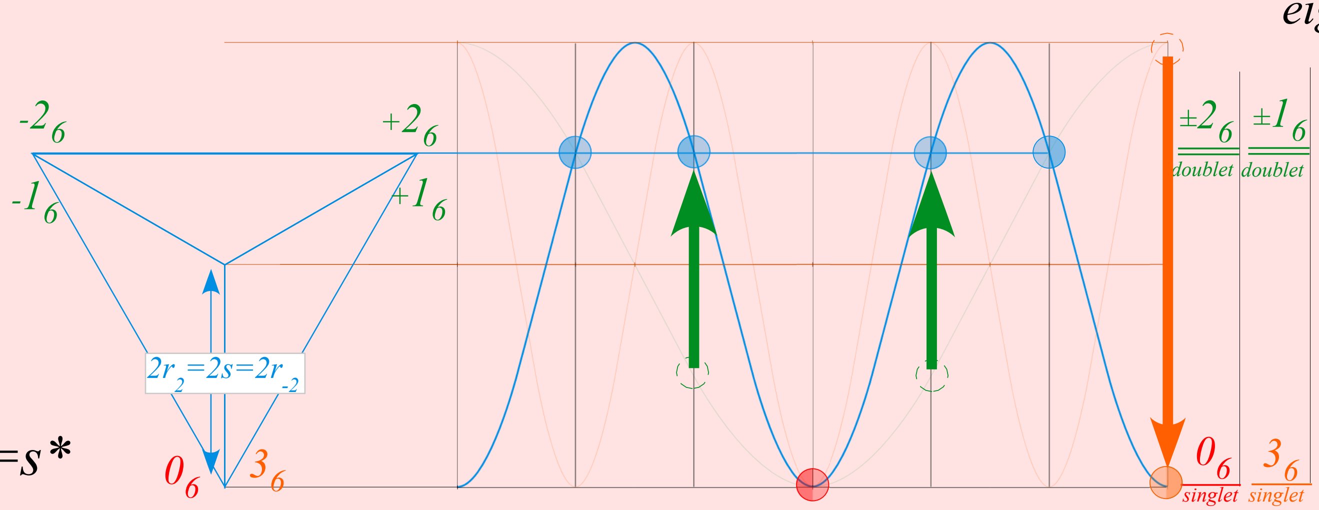
$$\begin{array}{c|c} & p=0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \\ \hline \begin{array}{c}0\\1\\2\\3\\4\\5\end{array} & \begin{pmatrix} H_1 & -r & \cdot & \cdot & \cdot & -r \\ -r & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -r & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -r & H_1 & -r & \cdot \\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

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

2nd Neighbor coupling

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





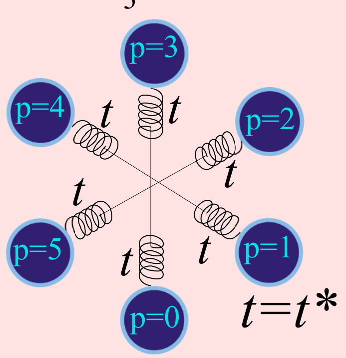
eigenvalues of $\mathbf{H}^{B2(6)}$

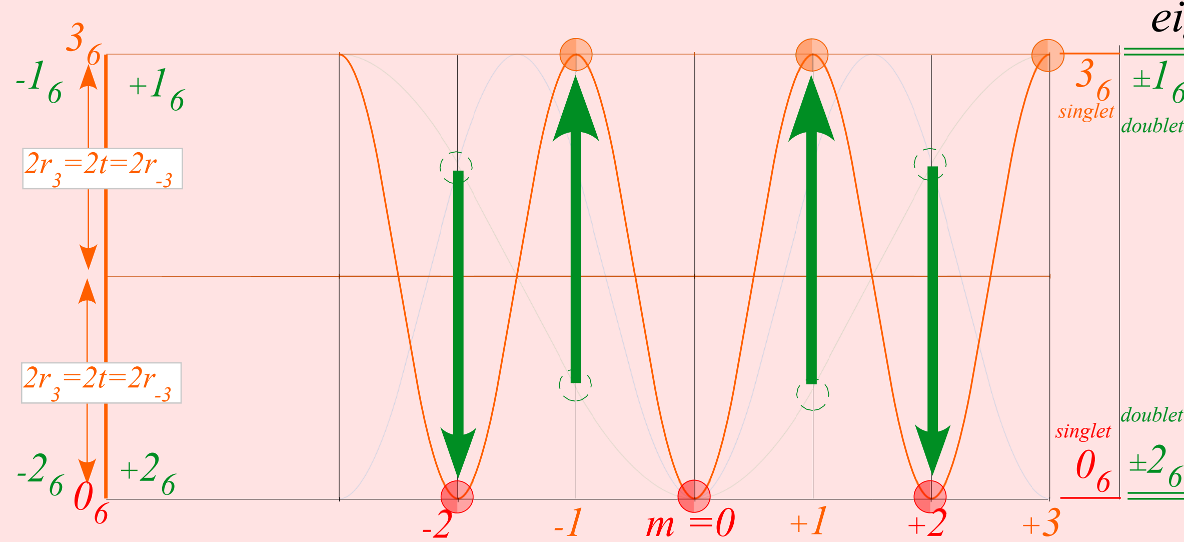
$$\begin{array}{c|c} & p=0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \\ \hline \begin{array}{c}0\\1\\2\\3\\4\\5\end{array} & \begin{pmatrix} H_2 & \cdot & -s & \cdot & -s & \cdot \\ \cdot & H_2 & \cdot & -s & \cdot & -s \\ -s & \cdot & H_2 & \cdot & -s & \cdot \\ \cdot & -s & \cdot & H_2 & \cdot & -s \\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

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

3rd Neighbor coupling

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





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

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

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

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 $\mathbf{H}^{GB(N)}$ eigenvalues are Fourier series with 4 (for $N=6$) Fourier parameters

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

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

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

giving 4 ω_m-levels:

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

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

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

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

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

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

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

Complex sets of C_6 coupling parameters and gauge shifts

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

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

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

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

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...

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

3rd Step (contd.)

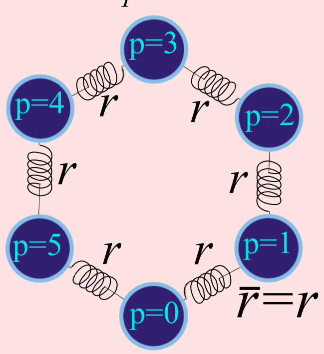
...eigensolutions for all possible C_6 symmetric complex H

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

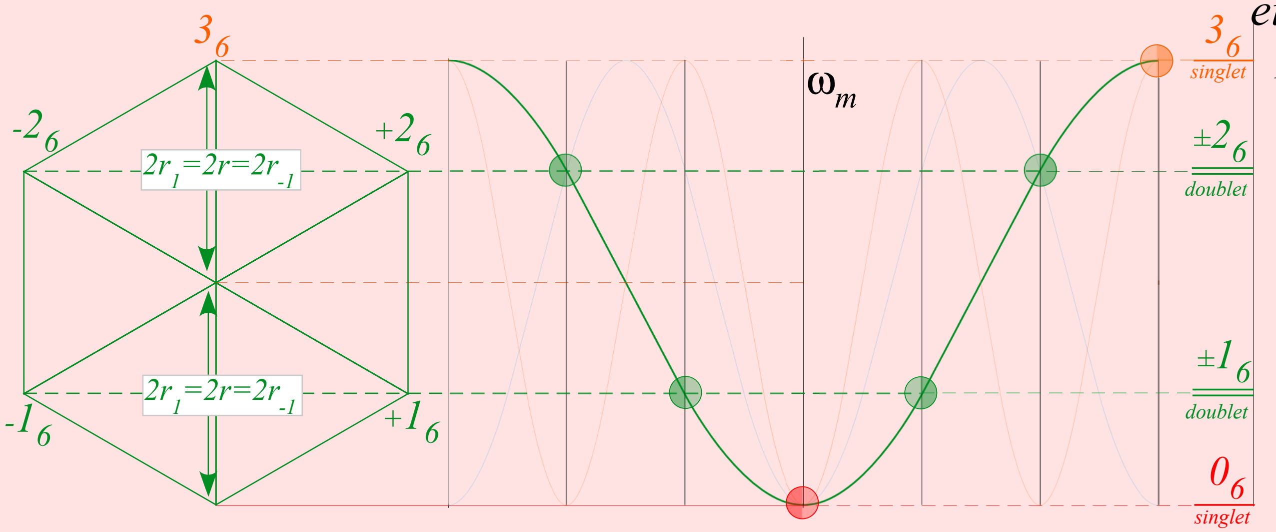
(Dispersion function)

Elementary Bloch Model

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



$\bar{r} = r^*$



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

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

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

Nearest neighbor coupling

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

3^{rd} Step (contd.)

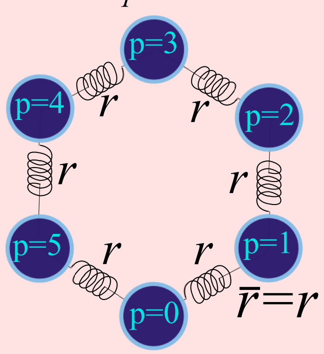
...eigensolutions for all possible C_6 symmetric complex H

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

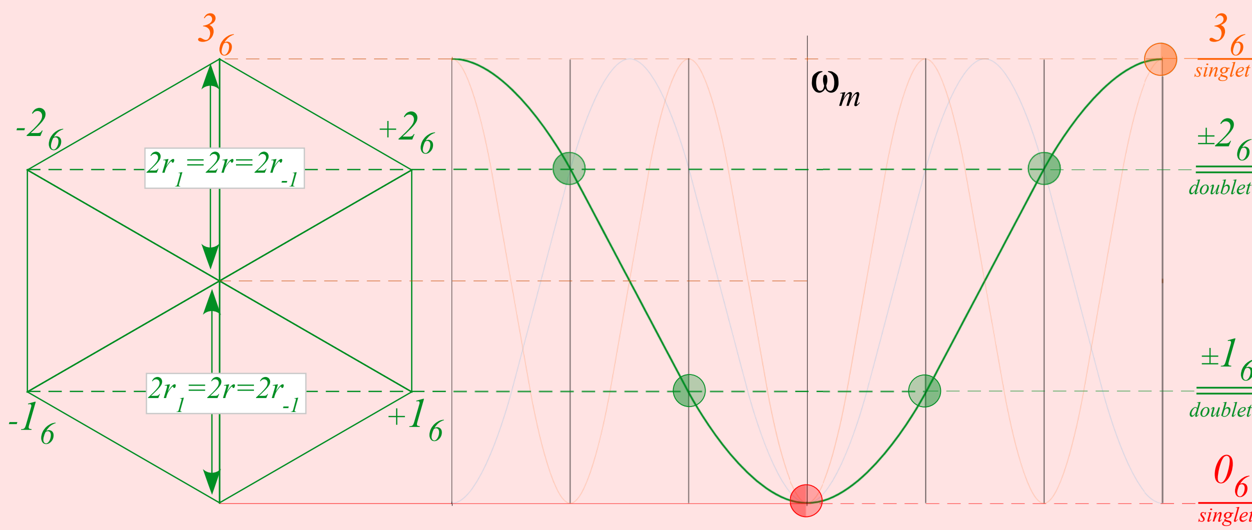
(Dispersion function)

Elementary Bloch Model

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



$\bar{r}=r^*$



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

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

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

Nearest neighbor coupling

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

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.)

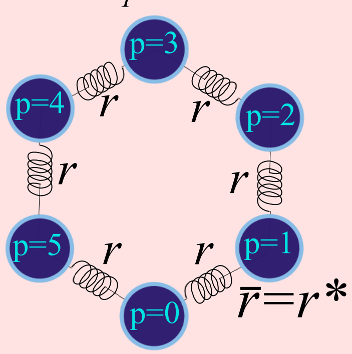
...eigensolutions for all possible C_6 symmetric complex H

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

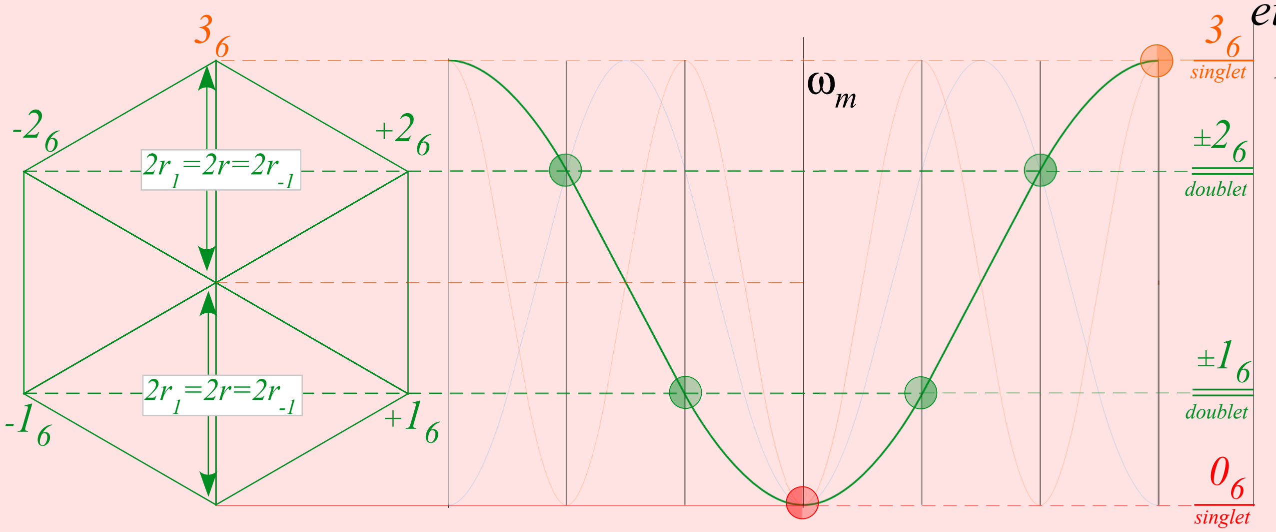
(Dispersion function)

Elementary Bloch Model

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



$\bar{r} = r^*$



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

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

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

Nearest neighbor coupling

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

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

complex components

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

conjugate components

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

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

3rd Step (contd.)

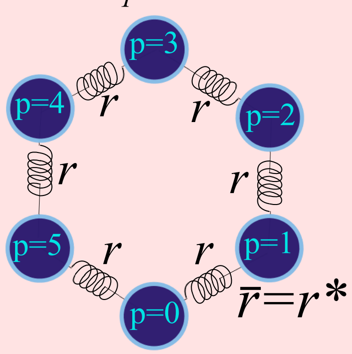
...*eigensolutions for all possible C_6 symmetric complex H*

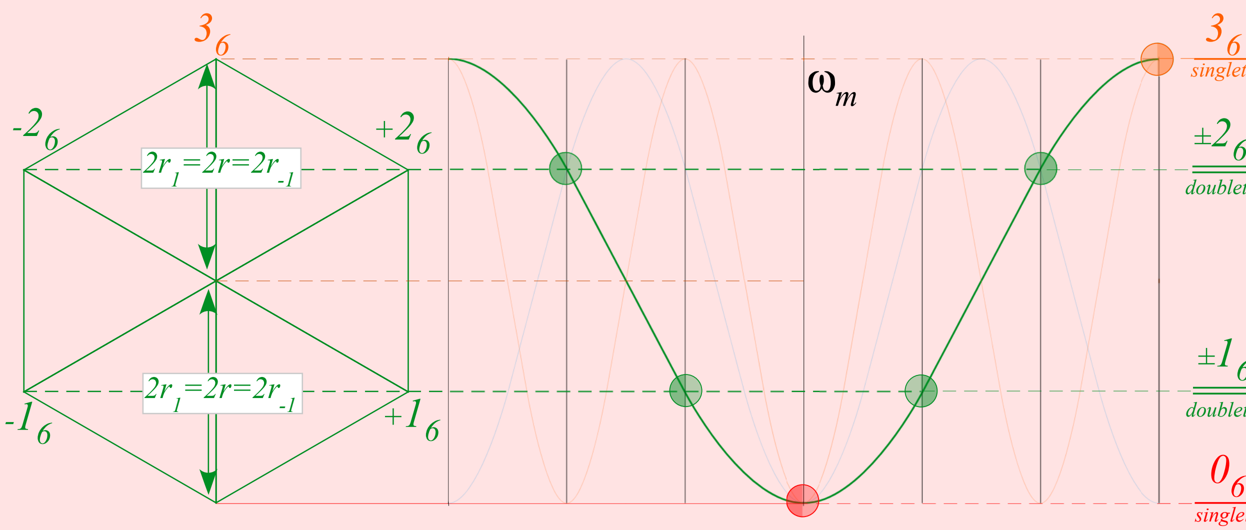
$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p=\sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)}=\sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)}=\sum_{p=0}^{n-1} r_p \chi_p^m=\omega(k_m)$$

(Dispersion function)

Elementary Bloch Model

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





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

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

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

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

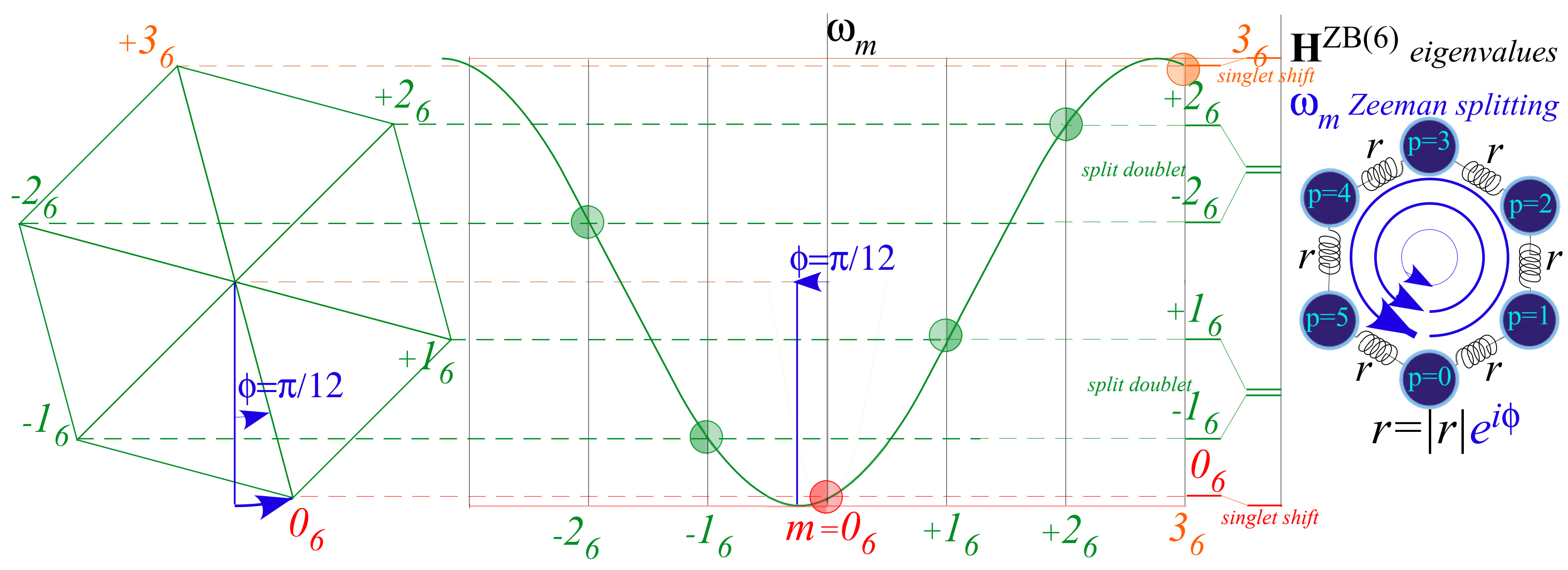
complex components

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

conjugate components

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

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



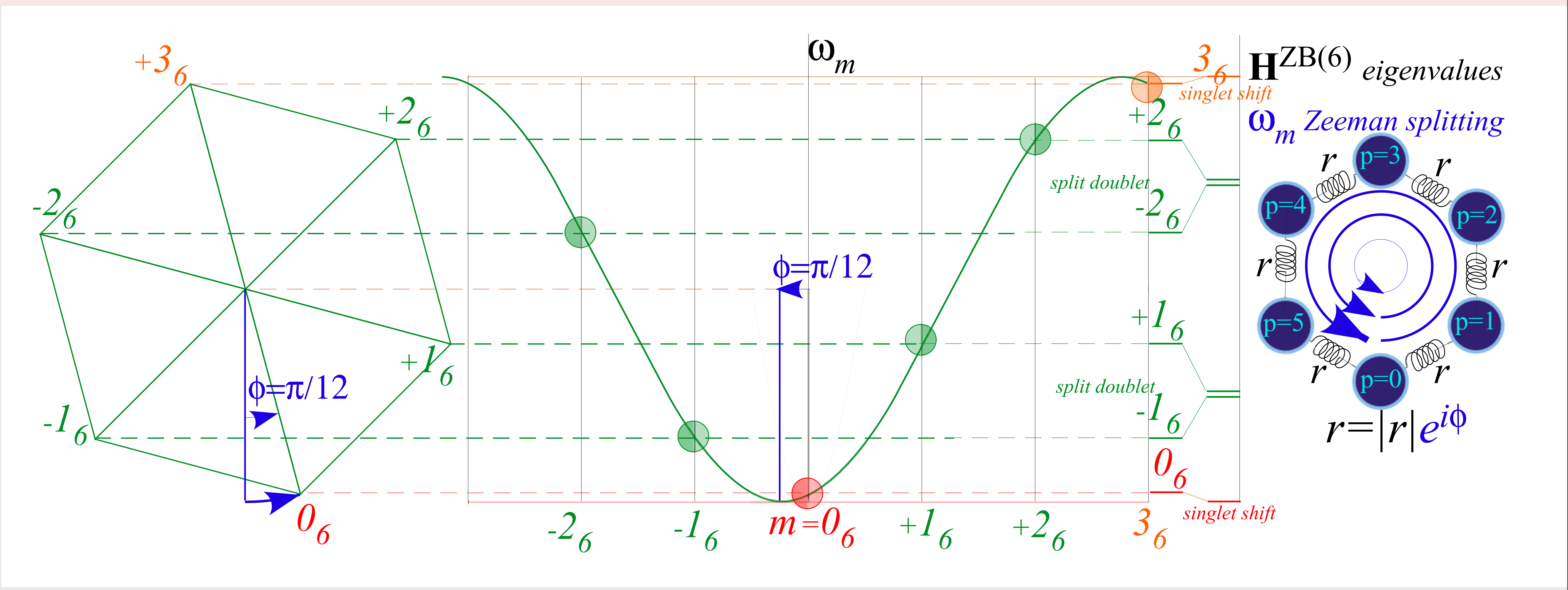
3^{rd} Step (contd.)

...eigensolutions for all possible C_6 symmetric complex H

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

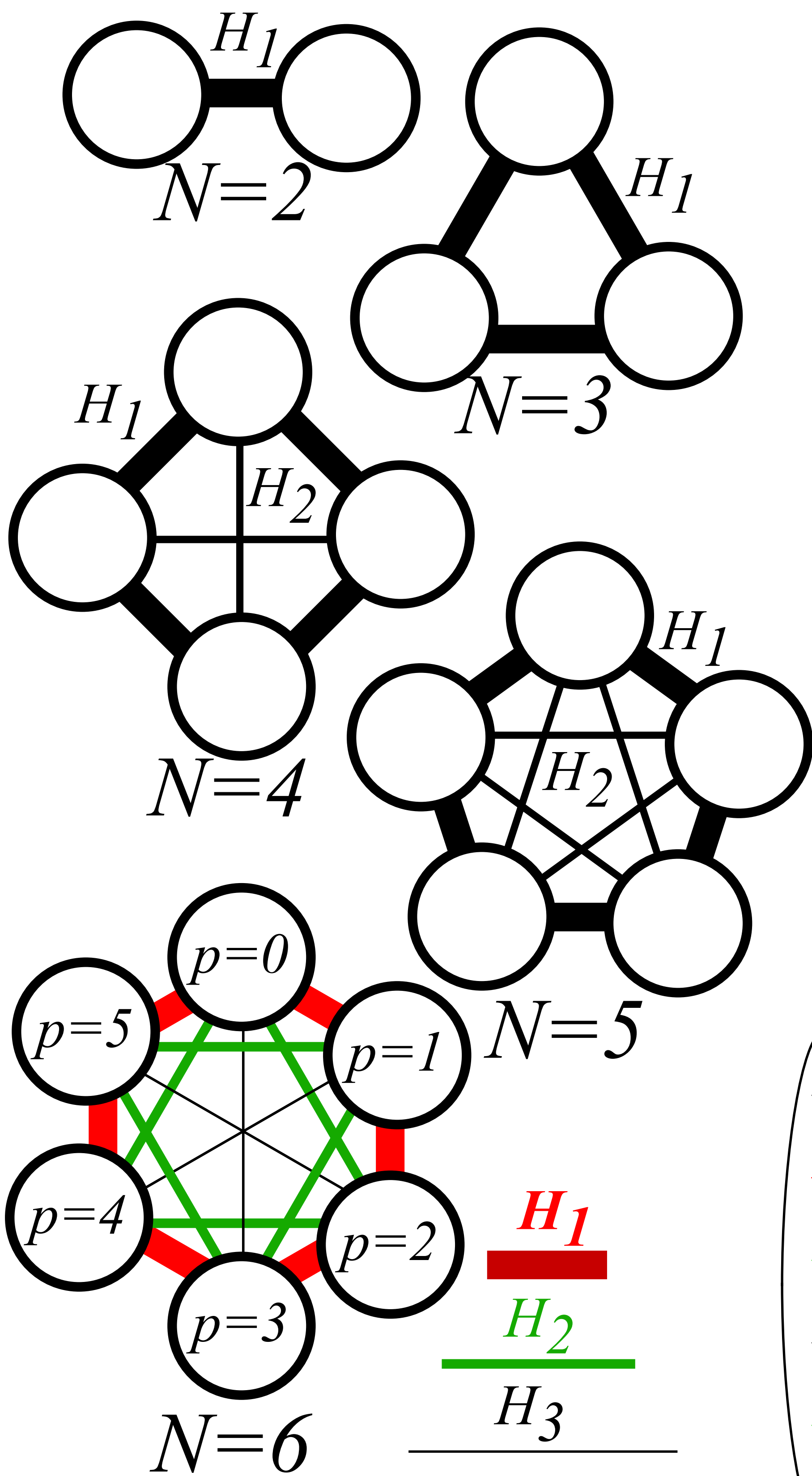
(Dispersion function)

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



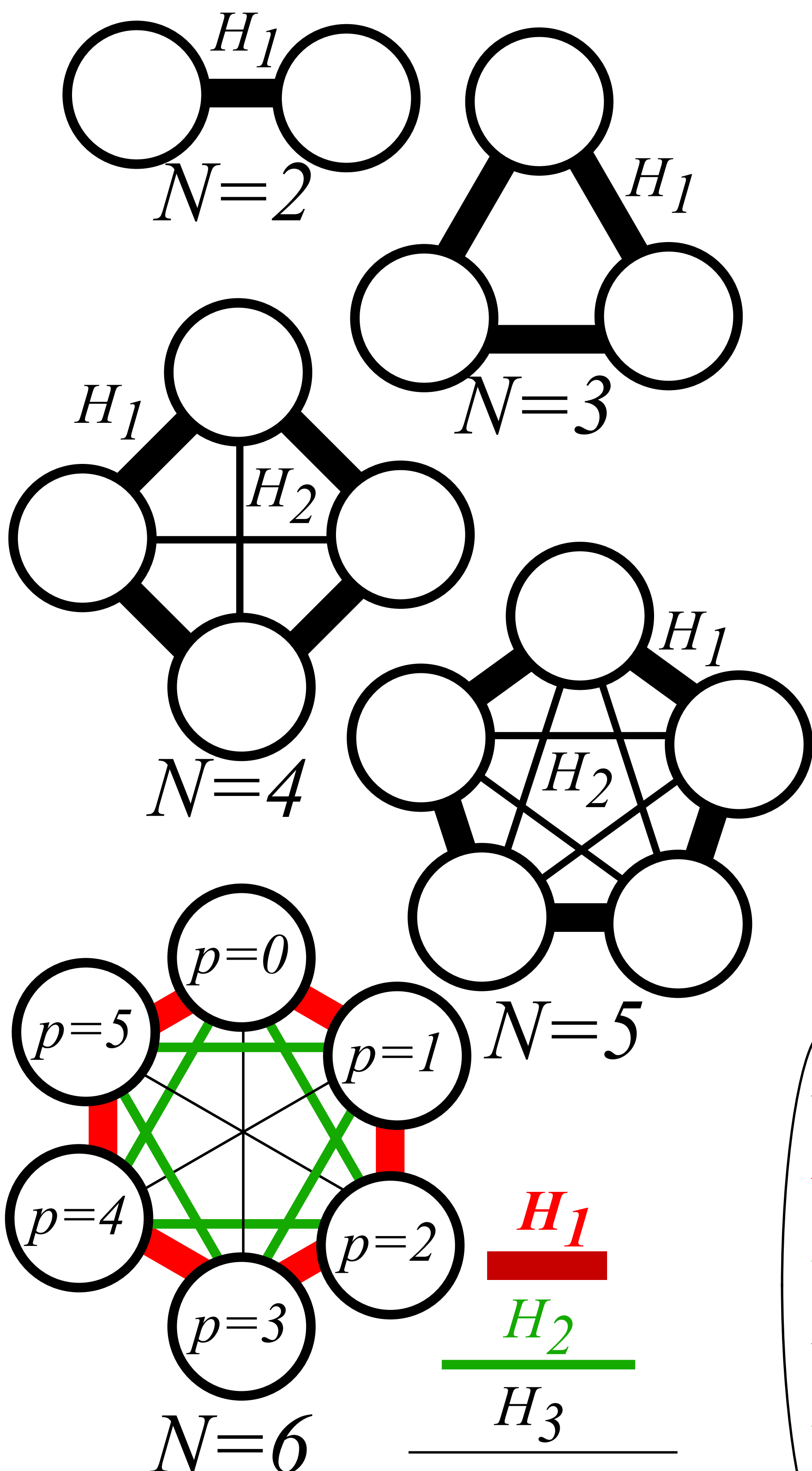
Simulating Complex Systems With Simpler Ones

Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots

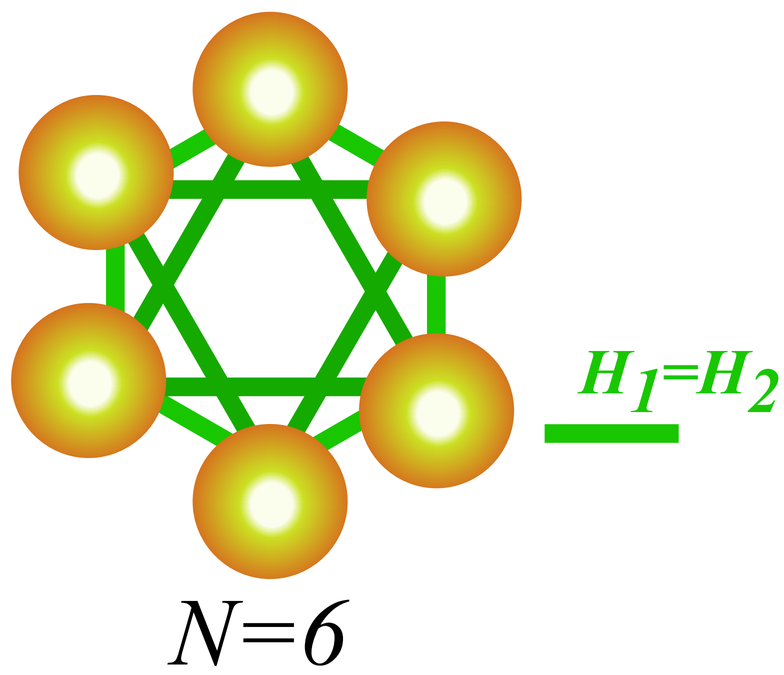


$$\begin{pmatrix} H_0 & \mathbf{H_1} & H_2 & H_3 & H_2 & \mathbf{H_1} \\ \mathbf{H1} & H_0 & \mathbf{H_1} & H_2 & H_3 & H_2 \\ H_2 & \mathbf{H_1} & H_0 & \mathbf{H_1} & H_2 & H_3 \\ H_3 & H_2 & \mathbf{H_1} & H_0 & \mathbf{H_1} & H_2 \\ H_2 & H_3 & H_2 & \mathbf{H_1} & H_0 & \mathbf{H_1} \\ \mathbf{H_1}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

Simulating Complex Systems With Simpler Ones



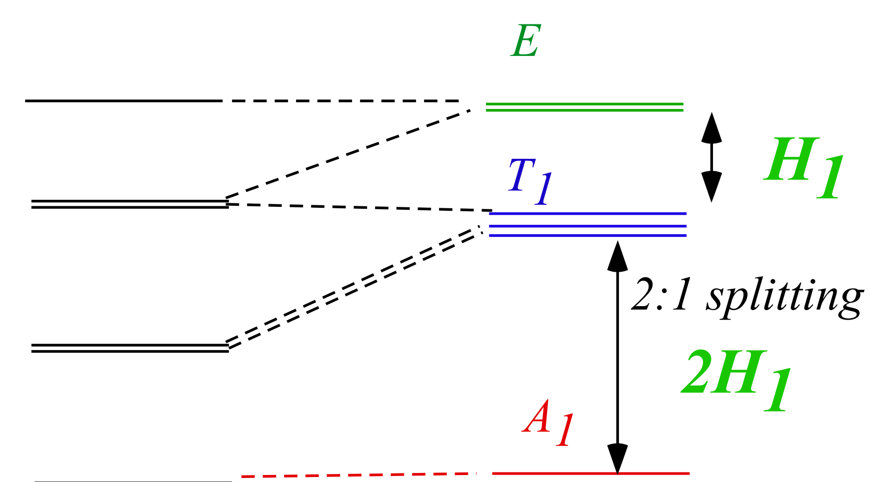
Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots



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

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