AMOP reference links on following page

1.22.18 class 3.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

Basic Projection operators GThLect.4 p.31-46 *1st page*

C_2 *spectral resolution for group* C_2 *GThLect.6 p.17* *1st page*

C_2 *spectral resolution for 2D oscillator GThLect.6 p.33*

C_2 *beat dynamics for 2D oscillator GThLect.6 p.35-46*

U(2) *beat phase dynamics for 2D oscillator GThLect.6 p.52-56*

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

C_3 *Basic group representation theory. GThLect.11 p6-12.* *1st page*

C_3 *group spectral resolution. GThLect.11 p14-27* *1st page*

C_3*Operator/State-Ortho-completeness GThLect.11 p29-38* *1st page*

C_3*Wavefunction bra-kets GThLect.11 p40-45.* *1st page*

C_3 *quantum number Mod-3 formulae GThLect.11 p47-52.* *1st page*

C_3 *character or irrep tables GThLect.11 p54-58.* *1st page*

C_3 *wave dispersion functions GThLect.11 p60-68.* *1st page* *Moving vs standing waves p71-73.*

Radial vs transverse waves p71-73.

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order *6*

1st Step: *Find* C_6 *symmetric* **H** *by* C_6 *product table of regular reps and coupling params* $\{r_0, r_1 \ldots r_5\}$ *GThLect12 p3-9* *1st page*

2nd Step: *Find* **H** *eigenfunctions by spectral resolution of* $C_6 = \{\mathbf{1}=\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2, \mathbf{r}^3, \mathbf{r}^4, \mathbf{r}^5\}$ *GThLect12 p11-16* *1st page*

Character tables of C_2, C_3, C_4, C_5, ... C_{144} *GThLect12 p18-24* *1st page*

3rd Step: *Dispersion functions and eigenvalues for various coupling parameter sets GThLect12 p27-30* *1st page*

Ortho-complete eigenvalue/parameters p32-38 *1st page* *Gauge shifting complex coupling p40-48* *1st page*

Bohr-Schrodinger dispersion p49-51

AMOP reference links (Updated list given on 2nd page of each class presentation)

Web Resources - front page

UAF Physics UTube channel

2014 AMOP

2017 Group Theory for QM

2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978 (Alt Scanned version)
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - ajp-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Rotation–vibration spectra of icosahedral molecules.

I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989
II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989
III) Half-integral angular momentum - harter-reimer-jcp-1991

QTCA Unit 10 Ch 30 - 2013
AMOP Ch 32 Molecular Symmetry and Dynamics - 2019
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS

I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) https://kb.osu.edu/dspace/handle/1811/52324
II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)
Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996
Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013
Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001

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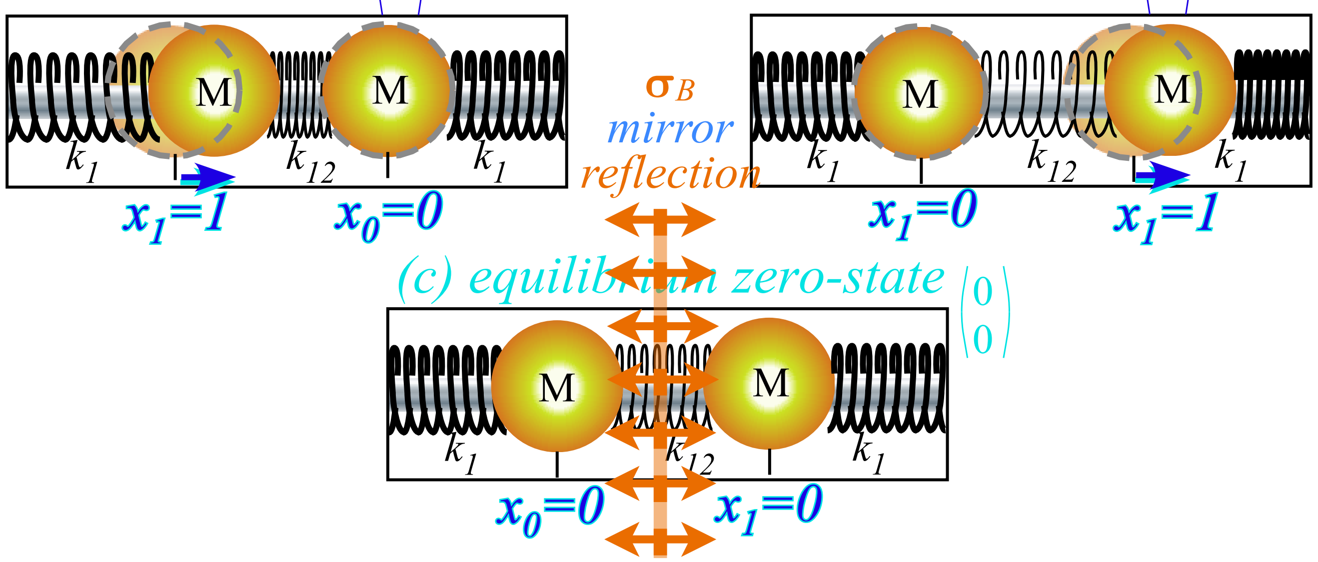
Bohr-Schrodinger dispersion p49-51

C_2 Symmetric two-dimensional harmonic oscillators (2DHO)

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

(a) unit base state $|0\rangle=|x\rangle=|2\rangle=\begin{pmatrix}1\\0\end{pmatrix}$

(b) unit base state $|1\rangle=|y\rangle=|-1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$



2D HO Matrix operator equations

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

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

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

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

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: $M=1$)

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

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

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* $\{|0\rangle=\mathbf{1}|0\rangle\equiv|\mathbf{1}\rangle\ ,\ |1\rangle=\boldsymbol{\sigma}_B|0\rangle\equiv|\sigma_B\rangle\}$

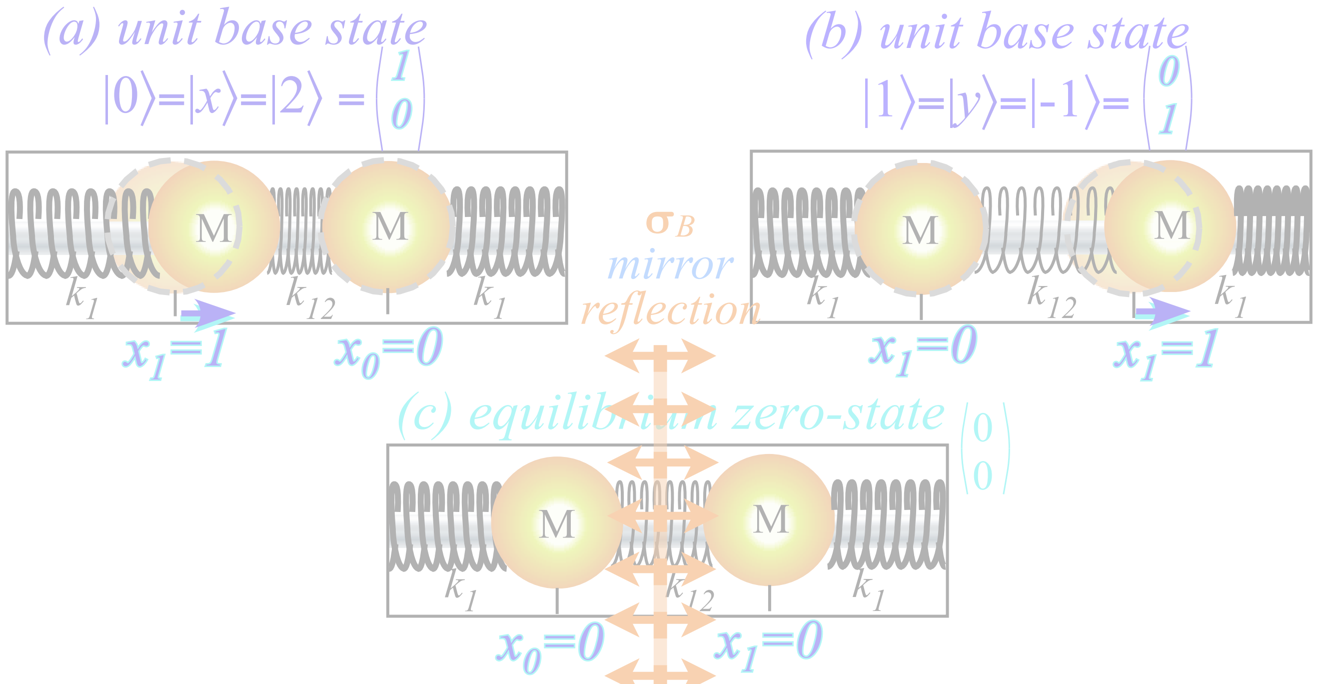
$$\begin{pmatrix}\langle\mathbf{1}|\mathbf{1}|\mathbf{1}\rangle & \langle\mathbf{1}|\mathbf{1}|\sigma_B\rangle\\ \langle\sigma_B|\mathbf{1}|\mathbf{1}\rangle & \langle\sigma_B|\mathbf{1}|\sigma_B\rangle\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\qquad \begin{pmatrix}\langle\mathbf{1}|\boldsymbol{\sigma}_B|\mathbf{1}\rangle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

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

1st page p. 6

C_2 Symmetric two-dimensional harmonic oscillators (2DHO)

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



2D HO Matrix operator equations

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

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

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

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

C_2 spectral resolution for group C_2 GThLect.6 p.17 1st page

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	$\mathbf{1}$

Basic Projection operators GThLect.4 p.31-46

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:

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

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

factored projectors

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

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

Eigenvalues of σ_B :

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

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

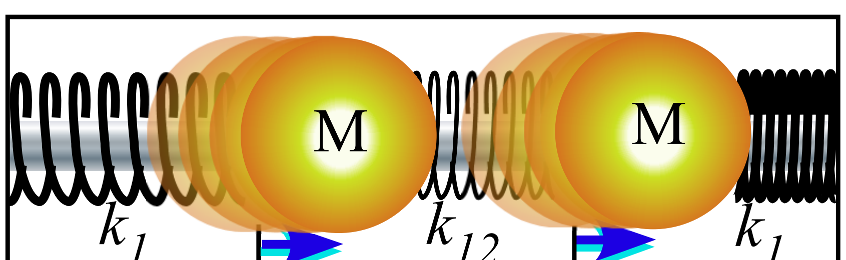
$$\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}k_1+k_{12}&-k_{12}\\-k_{12}&k_1+k_{12}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}\end{pmatrix}=\begin{pmatrix}k_1&0\\0&k_1+2k_{12}\end{pmatrix}$$

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

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

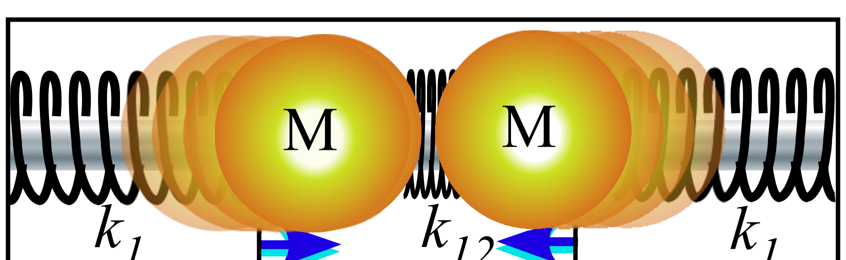
$\quad=k_1 \qquad\qquad\qquad\quad =k_1+2k_{12}$

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



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

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

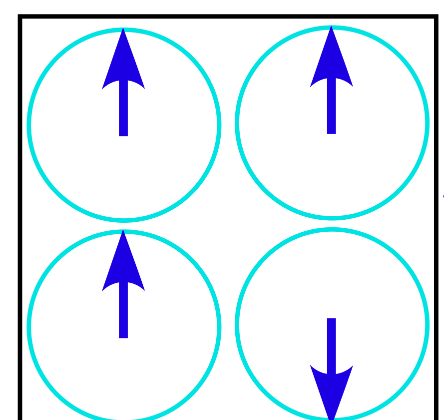


$x_0=1/\sqrt{2} \qquad x_1=-1/\sqrt{2}$

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!)

C2 spectral resolution for 2D oscillator Lecture 6 p.33

WaveIt Web Simulation - C2 Characters as Phasors

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C_2 Symmetric 2DHO uncoupling

2D HO Matrix operator equations are coupled in $\{x_1,x_2\}$-basis *...but are* ***un****coupled in* $\{+,-\}$-basis

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

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

$$\begin{pmatrix}\langle x_1|\ddot{\mathbf{x}}\rangle\\ \langle x_2|\ddot{\mathbf{x}}\rangle\end{pmatrix} = -\begin{pmatrix}\langle x_1|\mathbf{K}|x_1\rangle & \langle x_1|\mathbf{K}|x_2\rangle\\ \langle x_2|\mathbf{K}|x_1\rangle & \langle x_2|\mathbf{K}|x_2\rangle\end{pmatrix}\begin{pmatrix}\langle x_1|\mathbf{x}\rangle\\ \langle x_2|\mathbf{x}\rangle\end{pmatrix}$$

$$\begin{pmatrix}\ddot{x}_+\\ \ddot{x}_-\end{pmatrix} = -\begin{pmatrix}k_1 & 0\\ 0 & k_1+2k_{12}\end{pmatrix}\begin{pmatrix}x_+\\ x_-\end{pmatrix}$$

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

$$\begin{pmatrix}\langle +|\ddot{\mathbf{x}}\rangle\\ \langle -|\ddot{\mathbf{x}}\rangle\end{pmatrix} = -\begin{pmatrix}\langle +|\mathbf{K}|+\rangle & \cancel{\langle +|\mathbf{K}|-\rangle}\\ \cancel{\langle -|\mathbf{K}|+\rangle} & \langle -|\mathbf{K}|-\rangle\end{pmatrix}\begin{pmatrix}\langle +|\mathbf{x}\rangle\\ \langle -|\mathbf{x}\rangle\end{pmatrix}$$

Eigenbra vectors: $\langle +| = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}$, $\langle -| = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}$

Eigenket vectors: $|+\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}$, $|-\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{pmatrix}$

C_2 Symmetric 2DHO ***un****coupled dynamics*

$$\begin{pmatrix}M\ddot{x}_+ + (k_1)x_+\\ M\ddot{x}_- + (k_1+2k_{12})x_-\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix}$$

Each mode runs independently

$(+)$*-mode at frequency* $\omega_+=\sqrt{(k_1/M)}$

$(-)$*-mode at frequency* $\omega_-=\sqrt{(k_1+2k_{12})/M}$

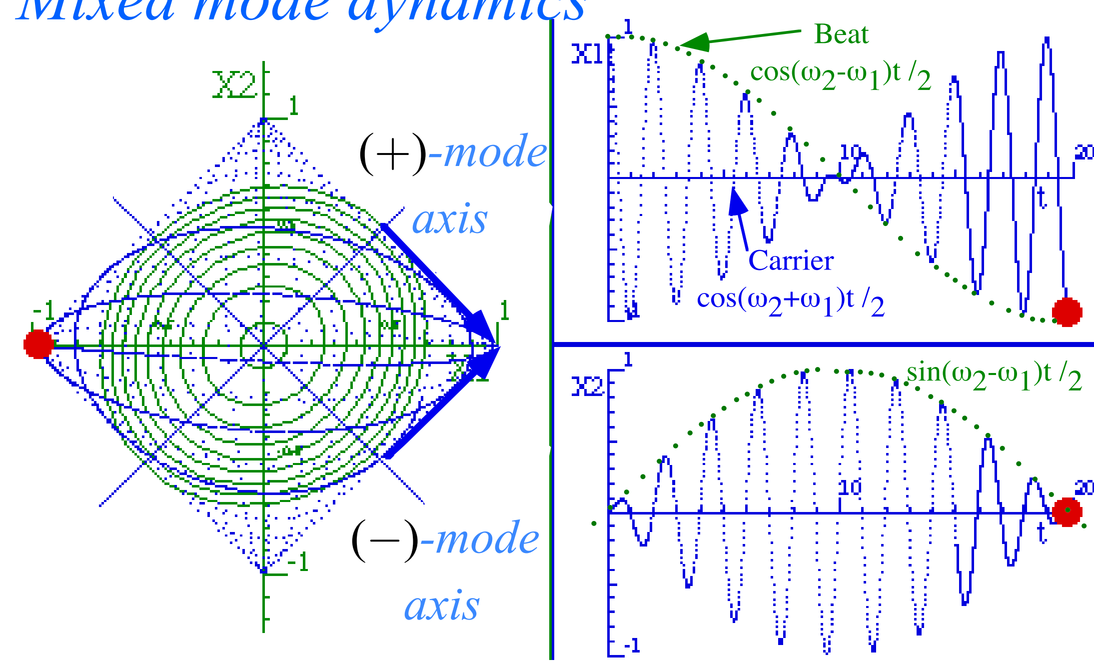
Spectral decomposition of initial state $\mathbf{x}(0)=(x_1\ \ x_2)=(1,0)$:

$$\mathbf{1}\cdot\mathbf{x}(0) = (\mathbf{P}_+ + \mathbf{P}_-)\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\otimes\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} + \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{pmatrix}\otimes\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix}$$

$$\mathbf{x}(0) = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\left(\frac{1}{\sqrt{2}}\right) + \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{pmatrix}\left(\frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle = \begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\end{pmatrix} + \begin{pmatrix}\frac{1}{2}\\ \frac{-1}{2}\end{pmatrix}$$

$$\text{so: } \mathbf{x}(t) = e^{-i\omega_+ t}\begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\end{pmatrix} + e^{-i\omega_- t}\begin{pmatrix}\frac{1}{2}\\ \frac{-1}{2}\end{pmatrix}$$

Mixed mode dynamics



C_2 *beats of 2D osc. GThLect.6 p.35-46*

100% AM modulation results

$$\frac{e^{ia}+e^{ib}}{2} = e^{i\frac{a+b}{2}}\frac{e^{i\frac{a-b}{2}}+e^{-i\frac{a-b}{2}}}{2} = e^{i\frac{a+b}{2}}\cos\left(\frac{a-b}{2}\right)$$

$$\begin{pmatrix}x_1(t)\\ x_2(t)\end{pmatrix} = \begin{pmatrix}\dfrac{e^{-i\omega_+ t}+e^{-i\omega_- t}}{2}\\ \dfrac{e^{-i\omega_+ t}-e^{-i\omega_- t}}{2}\end{pmatrix} = \frac{e^{-i\frac{(\omega_++\omega_-)}{2}t}}{2}\begin{pmatrix}e^{-i\frac{(\omega_+-\omega_-)}{2}t}+e^{i\frac{(\omega_+-\omega_-)}{2}t}\\ e^{-i\frac{(\omega_+-\omega_-)}{2}t}-e^{i\frac{(\omega_+-\omega_-)}{2}t}\end{pmatrix} = e^{-i\frac{(\omega_++\omega_-)}{2}t}\begin{pmatrix}\cos\frac{(\omega_- - \omega_+)t}{2}\\ i\sin\frac{(\omega_- - \omega_+)t}{2}\end{pmatrix}$$

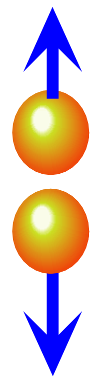
Note i phase

BoxIt Web Simulation
Coupled Oscillators $K_{11}=10$, $K_{12}=-1$

Three famous 2-state systems and two-complex-component coordinates

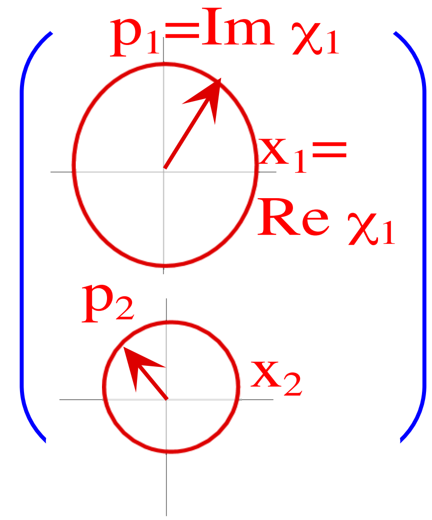
(a) Electron Spin-1/2-Polarization

Spin-up
$|1\rangle=|\uparrow\rangle$



Spin-dn
$|2\rangle=|\downarrow\rangle$

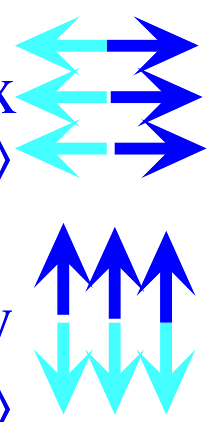
$$|\chi\rangle = \begin{pmatrix}\chi_\uparrow \\ \chi_\downarrow\end{pmatrix} = \begin{pmatrix}\langle\uparrow|\chi\rangle \\ \langle\downarrow|\chi\rangle\end{pmatrix} =$$



$$=|\uparrow\rangle\langle\uparrow|\Psi\rangle+|\downarrow\rangle\langle\downarrow|\Psi\rangle$$

Rabi, Ramsey, and Schwinger 1954
Rev. Mod. Phys. **26** *167 (1954)*

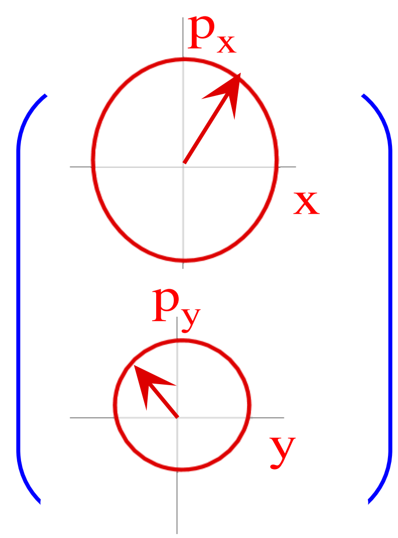
(b) Photon Spin-1-Polarization



Plane-x
$|1\rangle=|x\rangle$

Plane-y
$|2\rangle=|y\rangle$

$$|\psi\rangle = \begin{pmatrix}\psi_x \\ \psi_y\end{pmatrix} = \begin{pmatrix}\langle x|\psi\rangle \\ \langle y|\psi\rangle\end{pmatrix} =$$



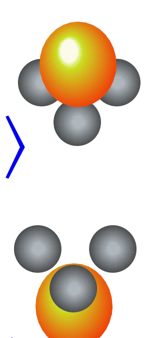
$$=|x\rangle\langle x|\psi\rangle+|y\rangle\langle y|\psi\rangle$$

John Stokes 1862
Proc. Soc. London **11** *547 (1862)*

Harter and Dos Santos
Am. J. Phys. **46** *251 (1986)*
J. Chem. Phys. **85** *5560 (1986)*

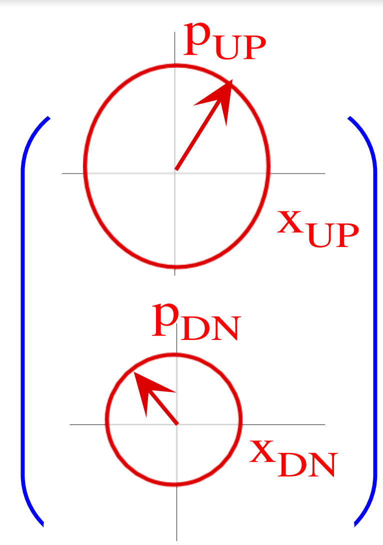
(c) Ammonia (NH_3) Inversion States

N-UP
$|1\rangle=|UP\rangle$



N-DN
$|2\rangle=|DN\rangle$

$$|\nu\rangle = \begin{pmatrix}\nu_{UP} \\ \nu_{DN}\end{pmatrix} = \begin{pmatrix}\langle UP|\nu\rangle \\ \langle DN|\nu\rangle\end{pmatrix} =$$



$$=|UP\rangle\langle UP|\nu\rangle+|DN\rangle\langle DN|\nu\rangle$$

Feynman, Vernon, and Hellwarth 1957
J. Appl. Phys. **28** *49 (1957)*

Fig. 10.5.1
QTCA Unit 3 Chapter 10

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$
=>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order *6*

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 **g†=g**$^{-1}$ in the 1st column
so all *unit* **1=g**$^{-1}$**g** *elements* lie on diagonal.

C_3 *Basic group representation theory. GThLect.11 p6-12.* *1st page*

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

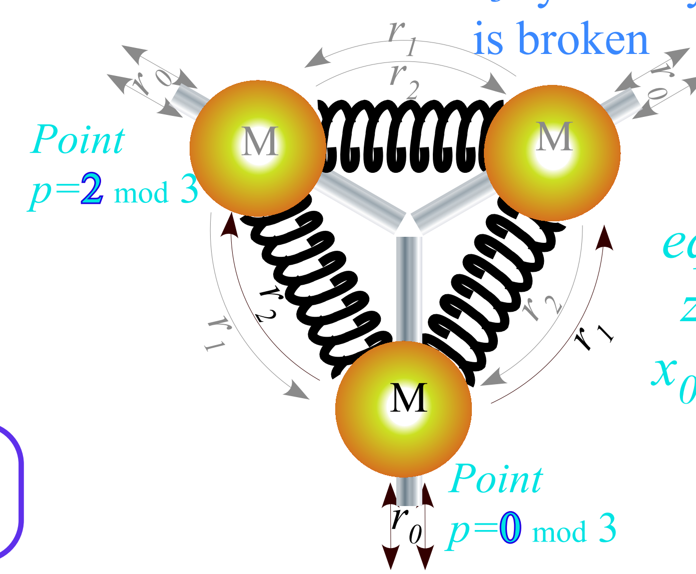
$$\mathbf{H}=\begin{pmatrix} r_0 & r_1 & r_2 \\ r_2 & r_0 & r_1 \\ r_1 & r_2 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + r_1\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} + r_2\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

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

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 C_3 symmetry is broken

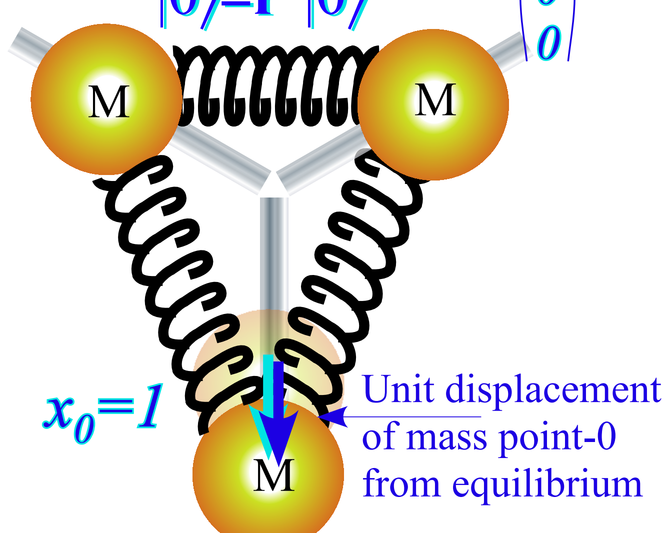


equilibrium zero-state
$x_0=x_1=x_2=0$

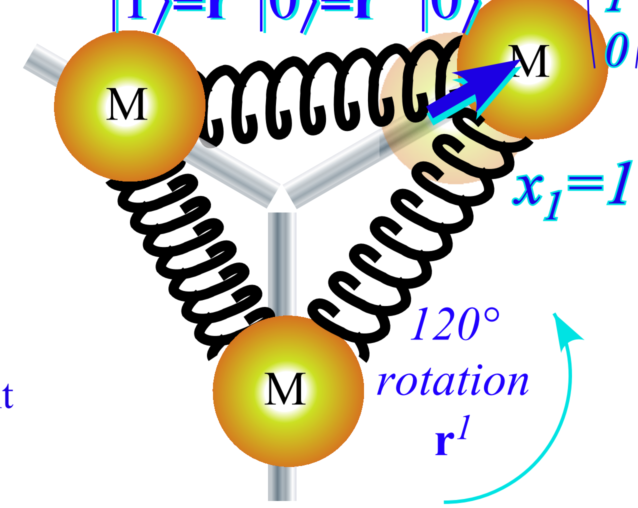
$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

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

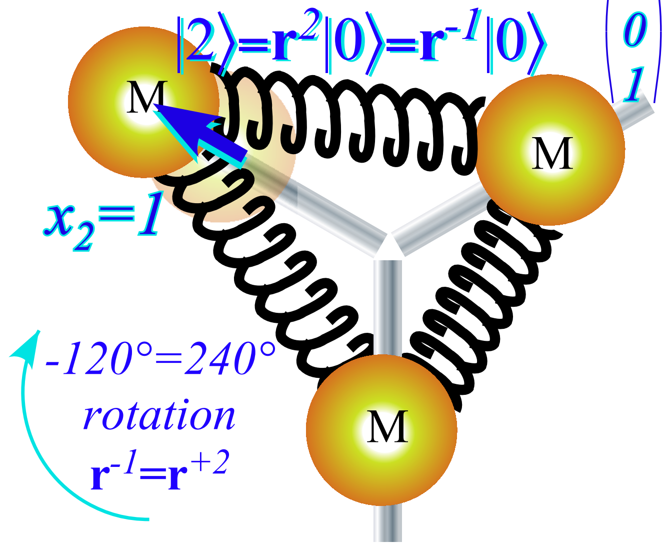
(p=0) unit base state
$|0\rangle=\mathbf{r}^0|0\rangle$ $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$



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

“Chi”(χ) refers to <u>characters</u> or characteristic roots

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

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

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

$$\mathbf{1}=\mathbf{r}^3 \text{ implies: } \mathbf{0}=\mathbf{r}^3-\mathbf{1}=(\mathbf{r}-\chi_0\mathbf{1})(\mathbf{r}-\chi_1\mathbf{1})(\mathbf{r}-\chi_2\mathbf{1}) \text{ where: } \chi_m=e^{-im\frac{2\pi}{3}}=\psi^*_m \begin{cases}\chi_0=e^{-i0\frac{2\pi}{3}}=1\\ \chi_1=e^{-i1\frac{2\pi}{3}}=\psi^*_1\\ \chi_2=e^{-i2\frac{2\pi}{3}}=\psi^*_2\end{cases}$$

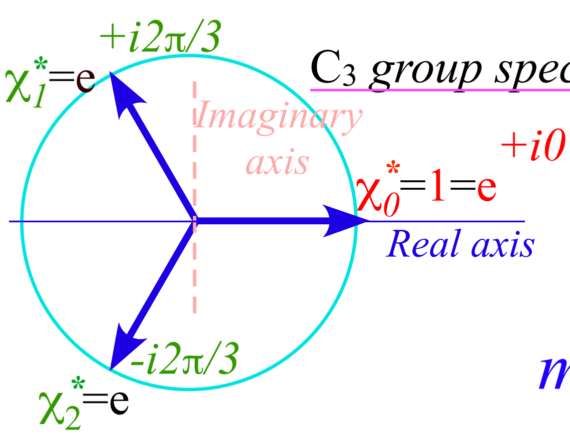
We know there is an idempotent projector $\mathbf{P}^{(m)}$ such that $\mathbf{r}\cdot\mathbf{P}^{(m)}=\chi_m\mathbf{P}^{(m)}$ for each eigenvalue χ_m of **r**,

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

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

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

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



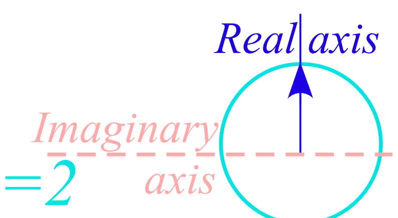
<u>C_3 group spectral resolution. GThLect.11 p14-27</u> <u>1st page</u>

C_3 mode phase character table

<u>wave-number</u> $m=$ “momentum”

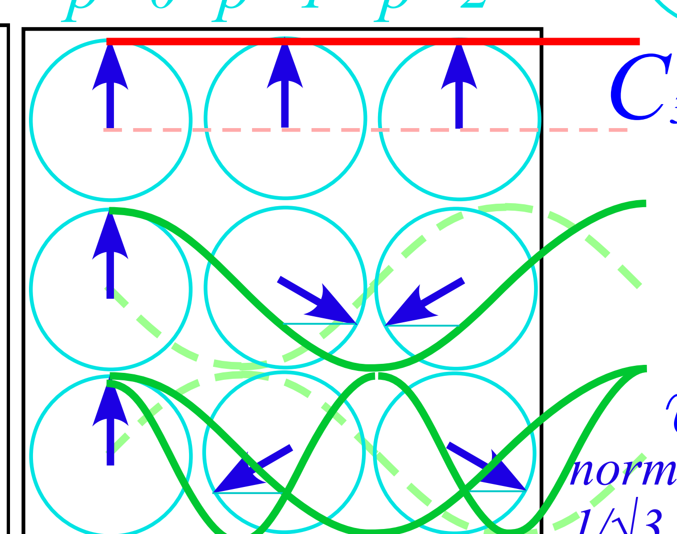
	p=0	p=1	p=2
$m=0_3$	$\chi_{00}=1$	$\chi_{01}=1$	$\chi_{02}=1$
$m=1_3$	$\chi_{10}=1$	$\chi_{11}=e^{-i2\pi/3}$	$\chi_{12}=e^{i2\pi/3}$
$m=2_3$	$\chi_{20}=1$	$\chi_{21}=e^{i2\pi/3}$	$\chi_{22}=e^{-i2\pi/3}$

<u>*p is position*</u>



<u>*MolVibes App C3v N3*</u>

<u>*WaveIt App - N3 Wave*</u>



C_3 character conjugate

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

is wave function

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

Given unitary *Ortho-Completeness operator* relations:

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

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

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

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

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

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

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

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

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

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

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

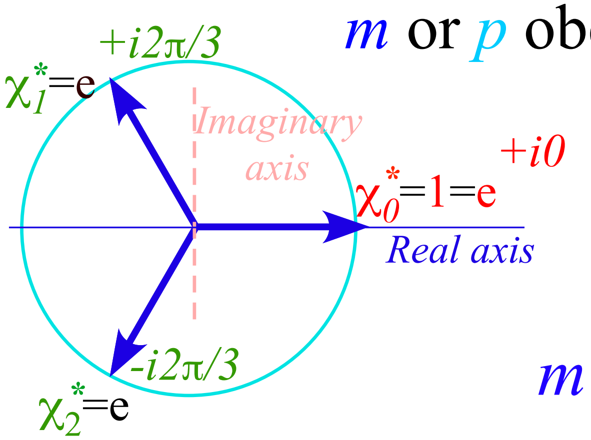
C3*Operator/State-Ortho-completeness GThLect.11 p29-38* *1st page*

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

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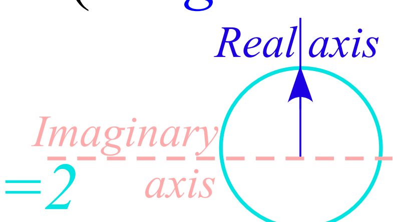
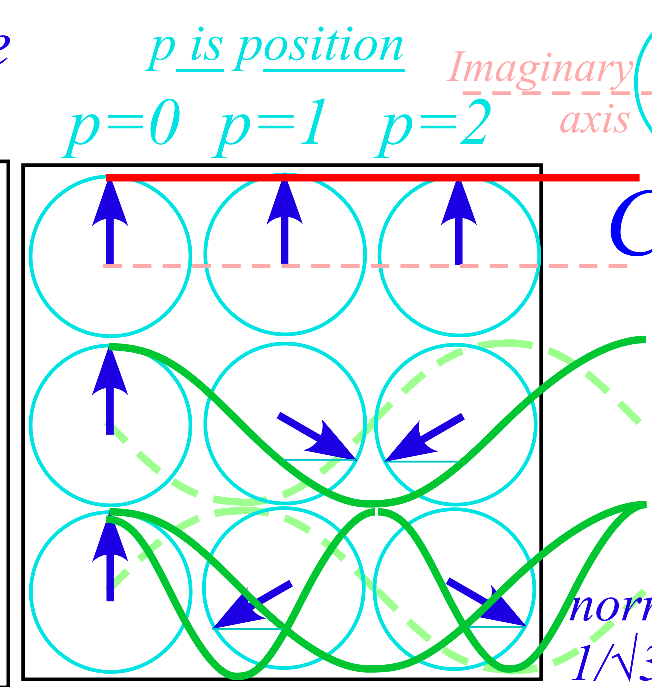
wave-number
m=
"momentum"



MolVibes App C3v N3

WaveIt App - N3 Wave



C_3 character conjugate

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

is wave function

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

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

⋮

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order *6*

$\mathscr{G}$ = C_n = Cyclic (or Circle) group of order n

Comparing wave function operator algebra to bra-ket algebra

C_3 Plane wave function

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

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

C_3 Lattice position point-p vector

$x_p=L\cdot p$

Wavevector for mode or momentum-m

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

Wavelength

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

position kets *position bras*

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

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

(Norm factors left out)

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

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

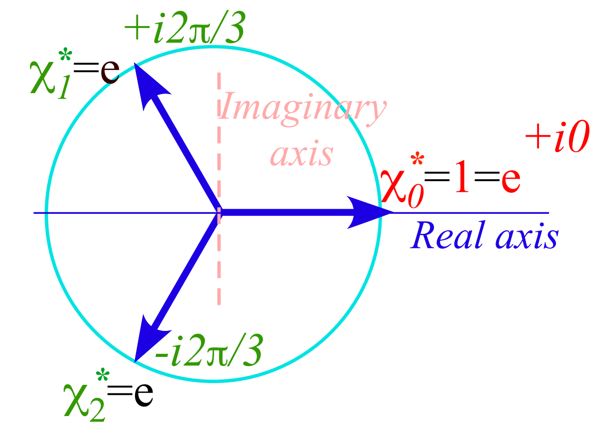
This implies:

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

mode or momentum (m) kets

Modular quantum number arithmetic

C_3 *quantum number Mod-3 formulae GThLect.11 p47-52.* *1st page*



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 $e^{imp\cdot 2\pi/3}= e^{i4\cdot 2\pi/3}= e^{i1\cdot 2\pi/3}\, e^{i3\cdot 2\pi/3}= e^{i2\pi/3}=\rho_1$.

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

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

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

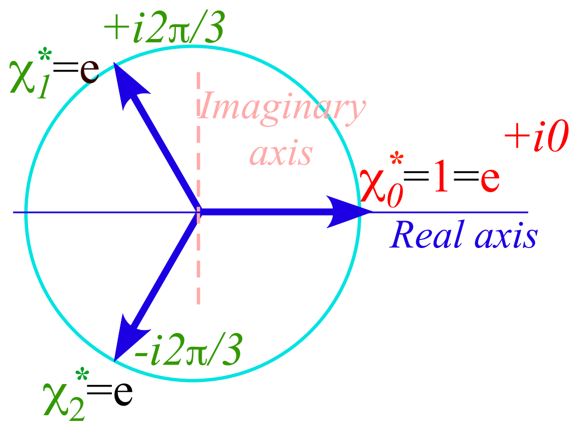
Imagine going around ring reading off address points $p=$... *0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2,....*

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

$e^{imp2\pi/3}$ 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-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 (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
$\chi_2=\chi_1^{-1}$	χ_2	χ_0	χ_1
$\chi_1=\chi_2^{-2}$	χ_1	χ_2	χ_0

C_3 *character or irrep tables GThLect.11 p54-58.*

1st page

*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	$e^{+\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$

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

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

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

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)

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

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:

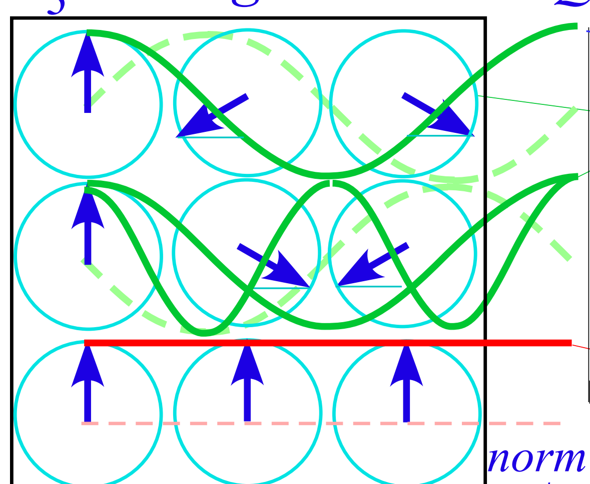
$$\begin{pmatrix} K & -k & -k \\ -k & K & -k \\ -k & -k & K \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}} \end{pmatrix} \underset{\text{K-eigenvalue...}}{=} \left(K - 2k\cos\left(\tfrac{2m\pi}{3}\right)\right)\begin{pmatrix} 1 \\ e^{i\frac{2m\pi}{3}} \\ e^{-i\frac{2m\pi}{3}}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

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

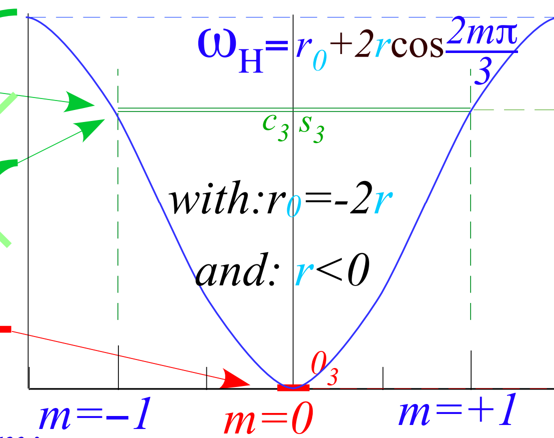
	p=0	p=1	p=2
$+1_3$	1	$e^{+2\pi i/3}$	$e^{-2\pi i/3}$
	right-hand moving wave		
-1_3	1	$e^{-2\pi i/3}$	$e^{+2\pi i/3}$
	left-hand moving wave		
0_3	1	1	1
	scalar standing wave		

p is position

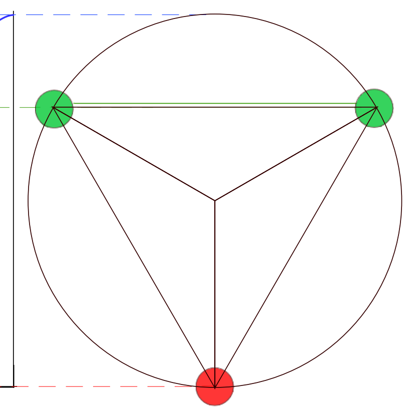
C_3 moving waves



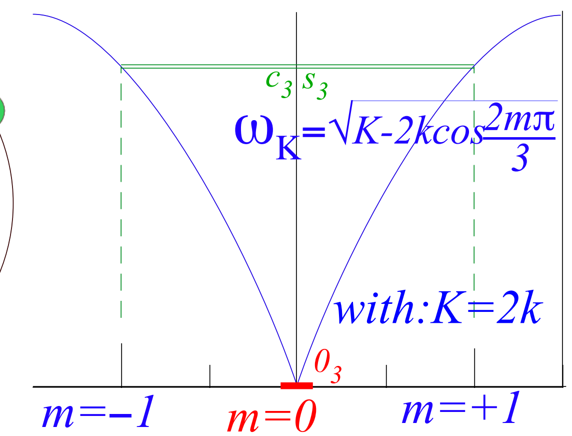
*Quantum **H**-dispersion*



geometry



*Classical **K**-dispersion*



This is an *exciton-like* dispersion function

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

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

$\omega_H(m)$ is *quadratic* for low m
(long wavelength λ)

This is a *phonon-like* dispersion function

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

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

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

$\omega_K(m)$ is *linear* for low m
(long wavelength λ)

C_3 *wave dispersion functions GThLect.11 p60-68. 1st page*

MolVibes App C3v N3

WaveIt App - N3 Wave

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)*

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

Quantum **H**-values:

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

Classical **K**-values:

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

Moving vs standing waves p71-73. *1st page*

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

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

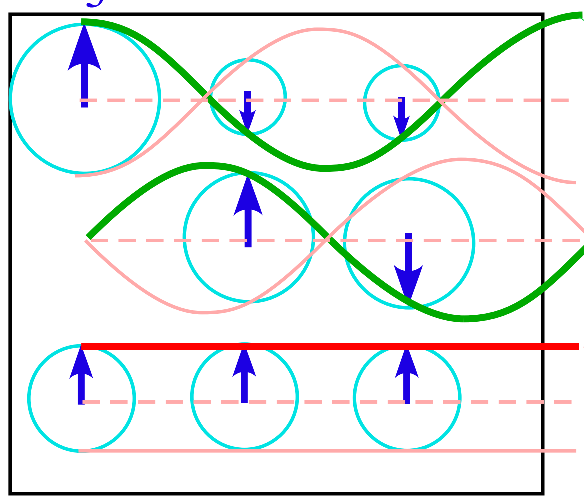
States $|(+)\rangle$ and $|(-)\rangle$ in *any mixtures* are still *stationary* due to $(\pm)$-*degeneracy* (cos(+x)=cos(-x))

Eigenvalues and wave dispersion functions - Standing waves

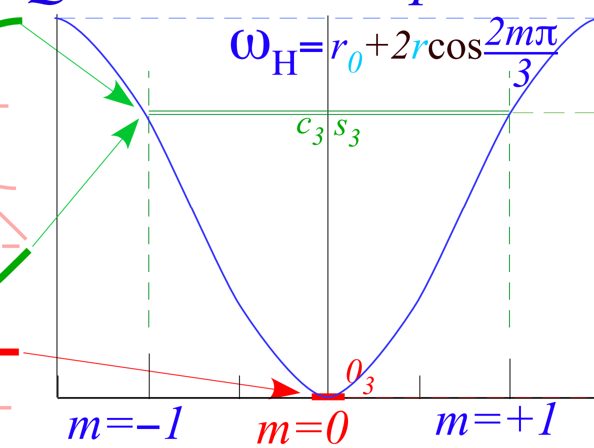
(Possible if **H** *is all-real)*

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

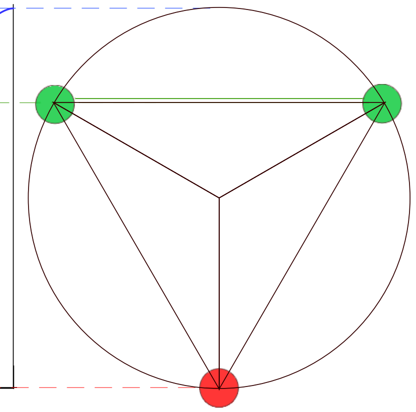
C_3 standing waves



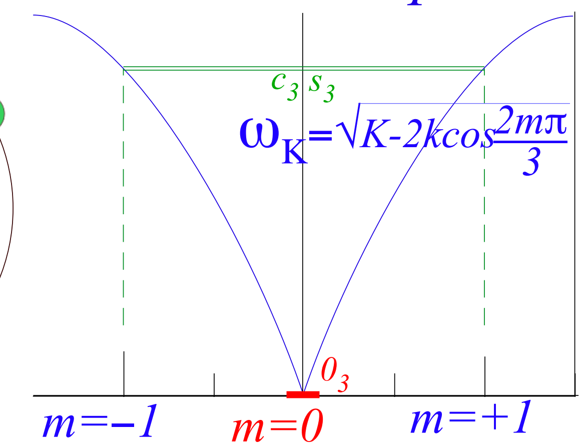
Quantum **H**-*dispersion*



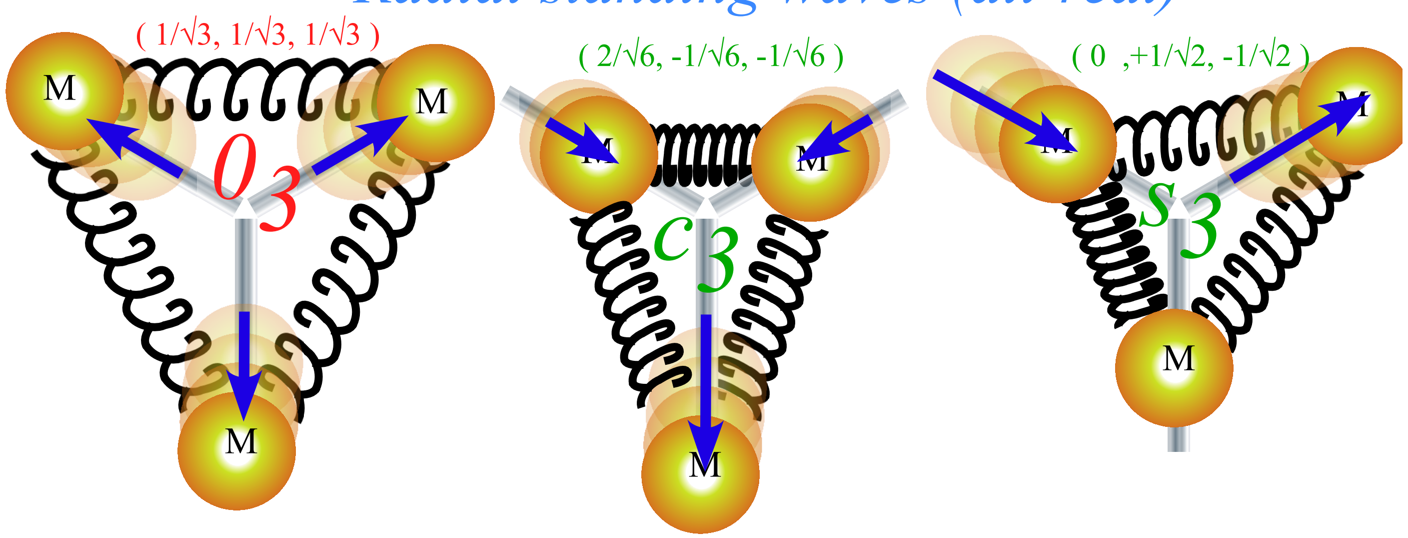
geometry



Classical **K**-*dispersion*



Radial standing waves (all-real)



Moving vs standing waves p71-73.

Radial vs transverse waves p71-73.

MolVibes App C3v N3

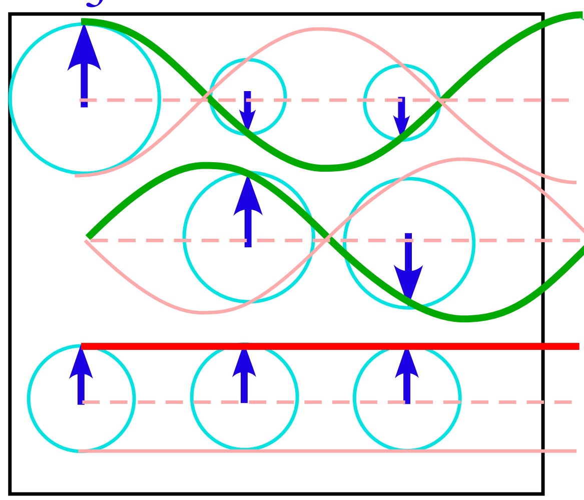
WaveIt App - N3 Wave

Eigenvalues and wave dispersion functions - Standing waves

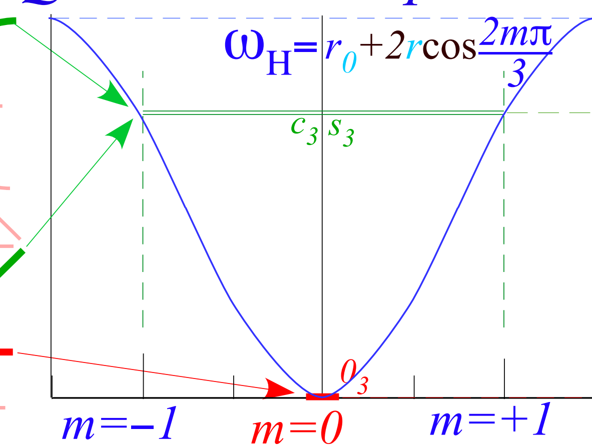
(Possible if **H** *is all-real)*

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

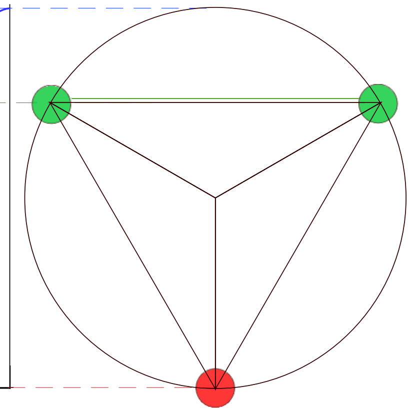
C_3 standing waves



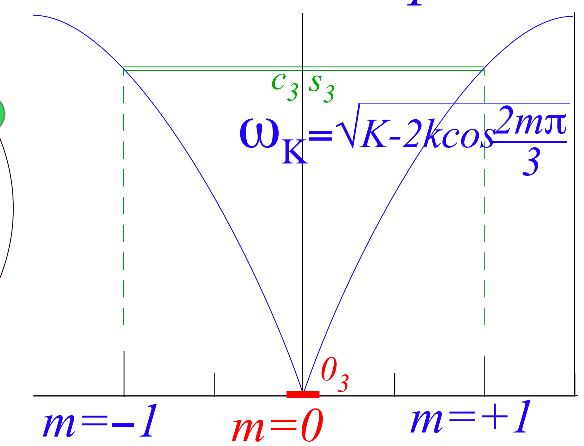
Quantum **H***-dispersion*



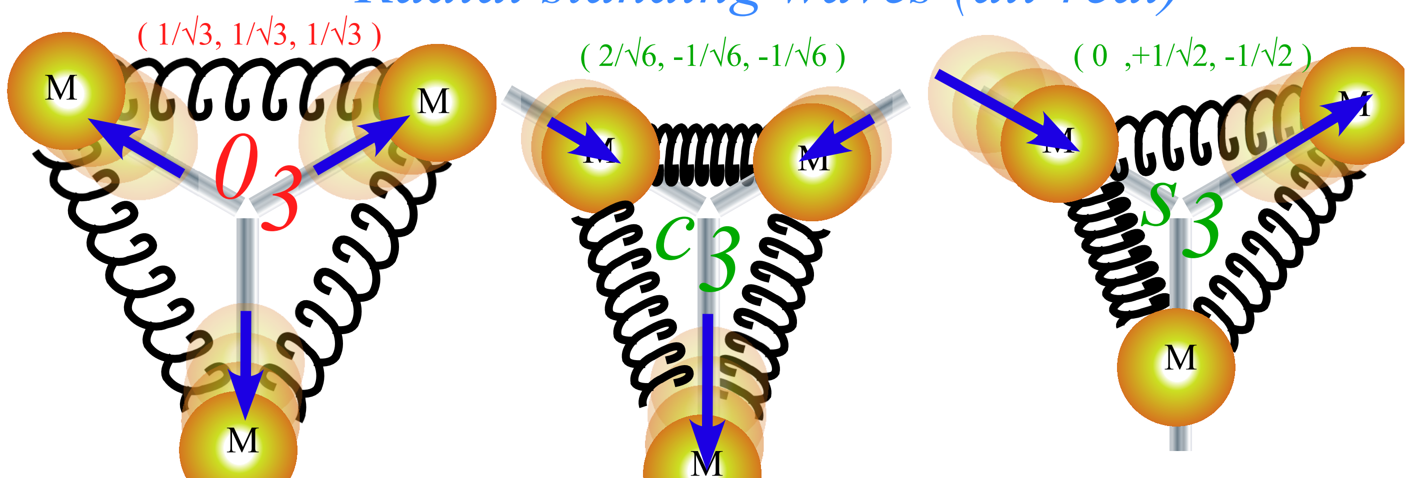
geometry



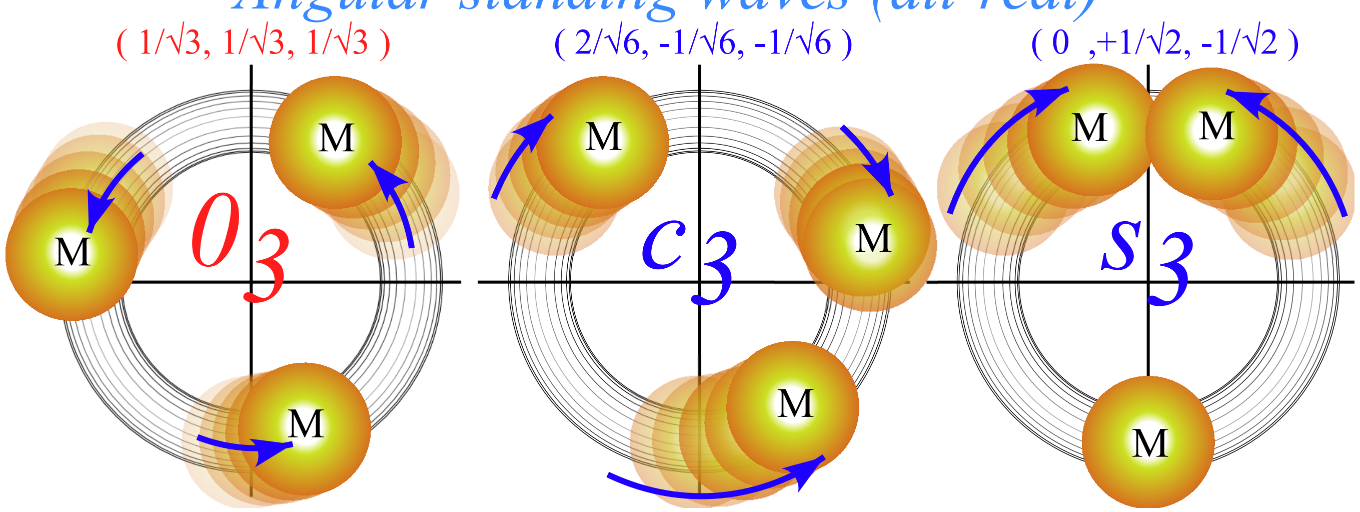
Classical **K***-dispersion*



Radial standing waves (all-real)



Angular standing waves (all-real)



Moving vs standing waves p71-73.

Radial vs transverse waves p71-73.

MolVibes App C3v N3

WaveIt App - N3 Wave

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

1^{st} Step in Abelian symmetry analysis

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

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

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 $\mathbf{r}$-matrices,...

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

1st Step in Abelian symmetry analysis

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

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

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,...*

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($\overset{gg^\dagger}{form}$)

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

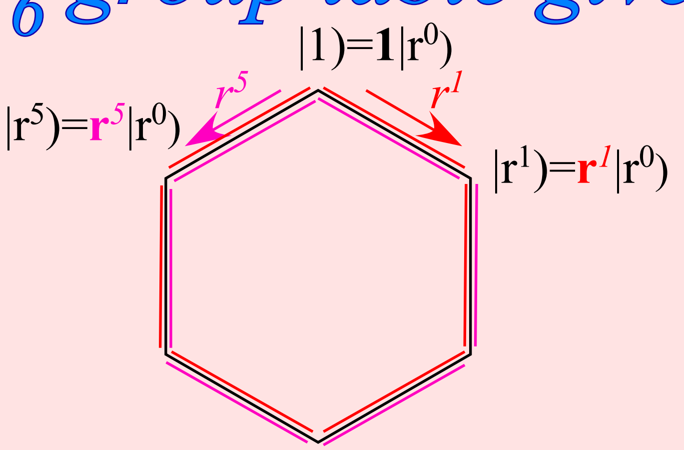
$g^\dagger$ (columns), g (rows):

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

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

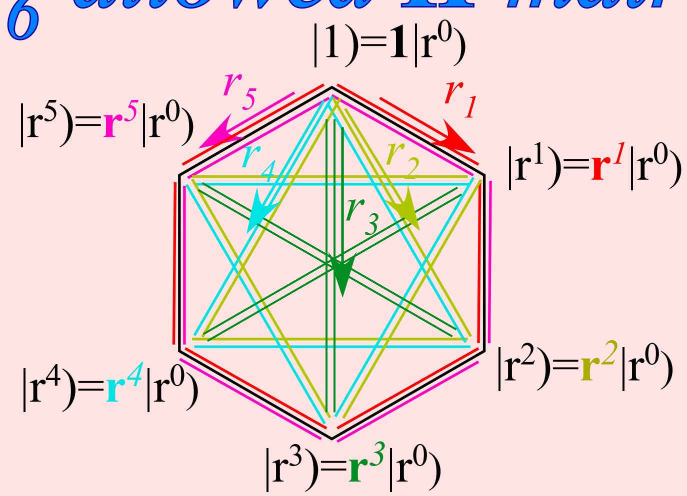
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot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

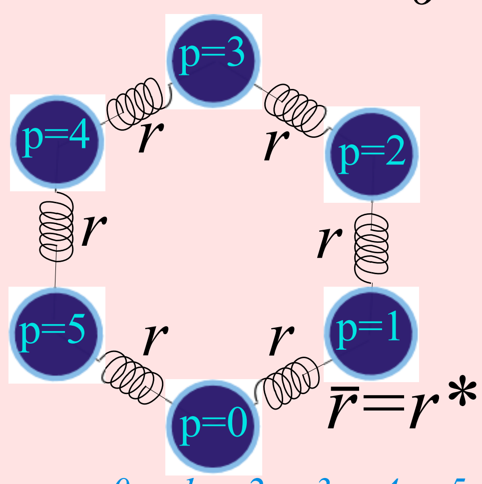
$$\begin{pmatrix} r_0 & r_5 & & & & r_1 \\ r_1 & r_0 & r_5 & & & \\ & r_1 & r_0 & r_5 & & \\ & & r_1 & r_0 & r_5 & \\ & & & r_1 & r_0 & r_5 \\ r_5 & & & & r_1 & r_0 \end{pmatrix}$$



ALL neighbor coupling

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

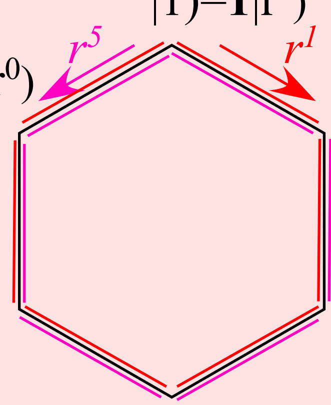
(a) 1^{st} Neighbor C_6



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

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

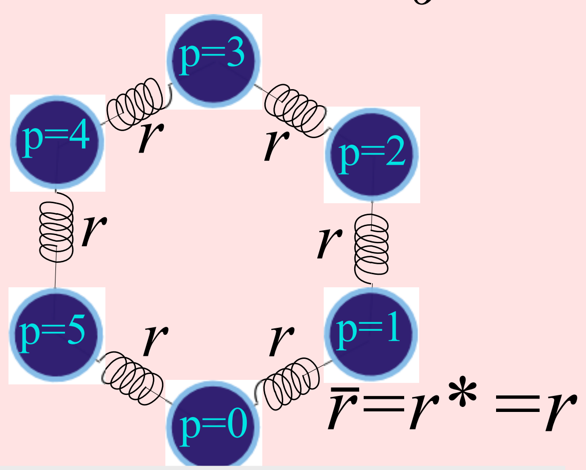
C_6 group table gives r-matrices,..



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



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

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

Conjugation symmetry

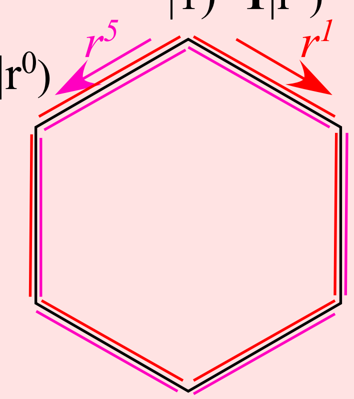
Hermitian Hamiltonian ($\mathbf{H}^*_{jk}=\mathbf{H}_{kj}$) requires $r_0^*=r_0$ and $r_1=r_5^*$.

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 r-matrices,..

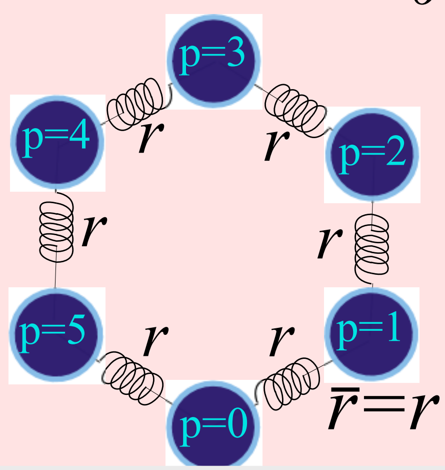


Elementary - Bloch - Model : Nearest neighbor coupling:

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

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

(a) 1^{st} Neighbor C_6

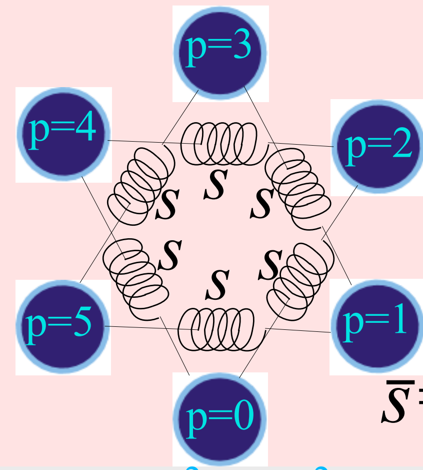


$\bar{r} = r^* = r$

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

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

(b) 2^{nd} Neighbor C_6



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

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

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

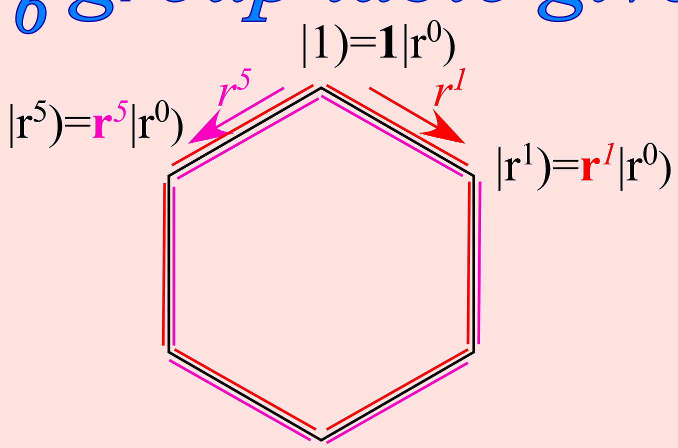
Conjugation symmetry

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

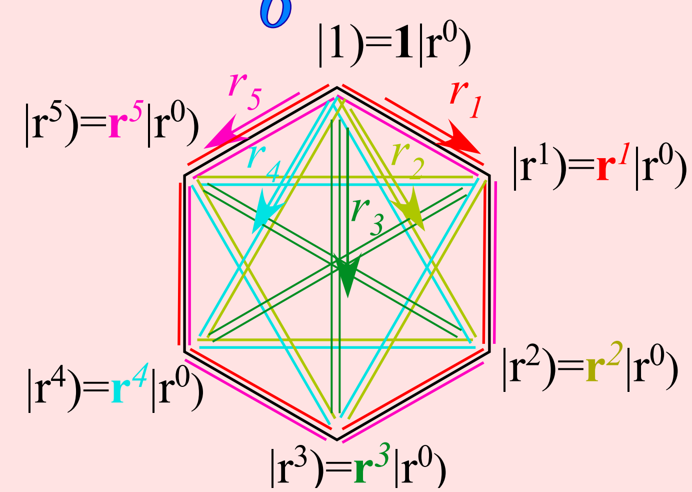
C_6 group table gives $\mathbf{r}$*-matrices,..., and all C_6-allowed* $\mathbf{H}$*-matrices...*



2^{nd} Nearest neighbor coupling:

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

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

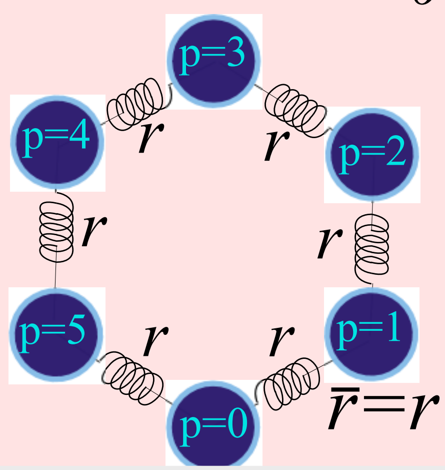


All – neighbor coupling:

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

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

(a) 1^{st} Neighbor C_6

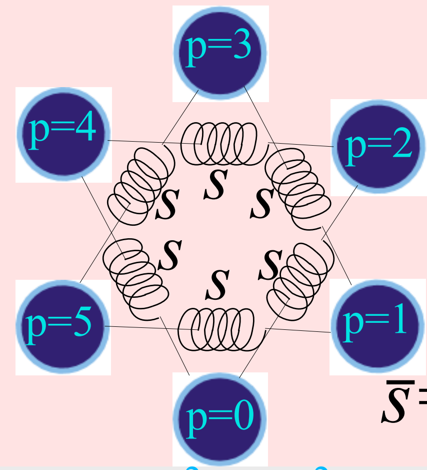


$\bar{r} = r^* = r$

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

0	1	2	3	4	5	p
$2r$	$-r$	·	·	·	$-r$	0
$-r$	$2r$	$-r$	·	·	·	1
·	$-r$	$2r$	$-r$	·	·	2
·	·	$-r$	$2r$	$-r$	·	3
·	·	·	$-r$	$2r$	$-r$	4
$-r$	·	·	·	$-r$	$2r$	5

Neighbor C_6

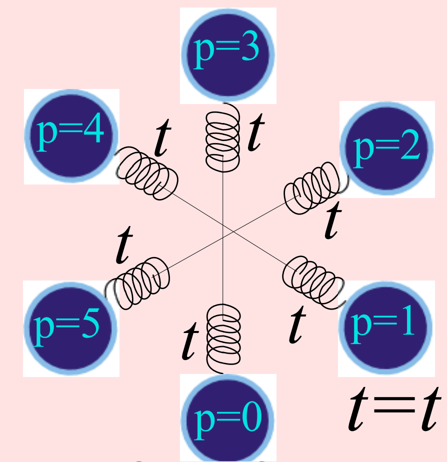


$\bar{s} = s^* = s$

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

0	1	2	3	4	5	p
H_2	·	$-s$	·	$-s$	·	0
·	H_2	·	$-s$	·	$-s$	1
$-s$	·	H_2	·	$-s$	·	2
·	$-s$	·	H_2	·	$-s$	3
$-s$	·	$-s$	·	H_2	·	4
·	$-s$	·	$-s$	·	H_2	5

(c) 3^{rd} Neighbor C_6



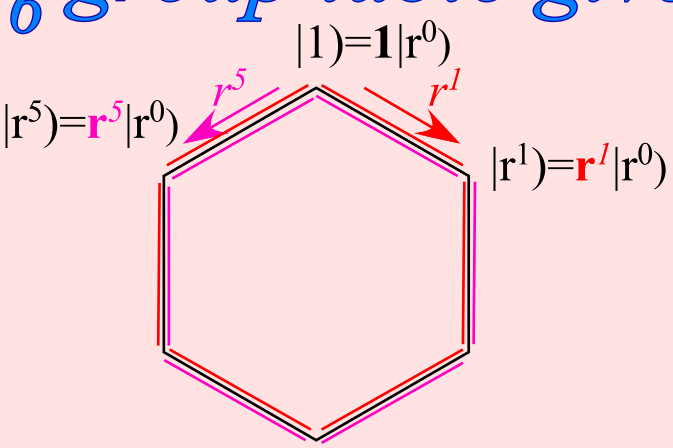
$t = t^*$

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

0	1	2	3	4	5	p
H_3	·	·	$-t$	·	·	0
·	H_3	·	·	$-t$	·	1
·	·	H_3	·	·	$-t$	2
$-t$	·	·	H_3	·	·	3
·	$-t$	·	·	H_3	·	4
·	·	$-t$	·	·	H_3	5

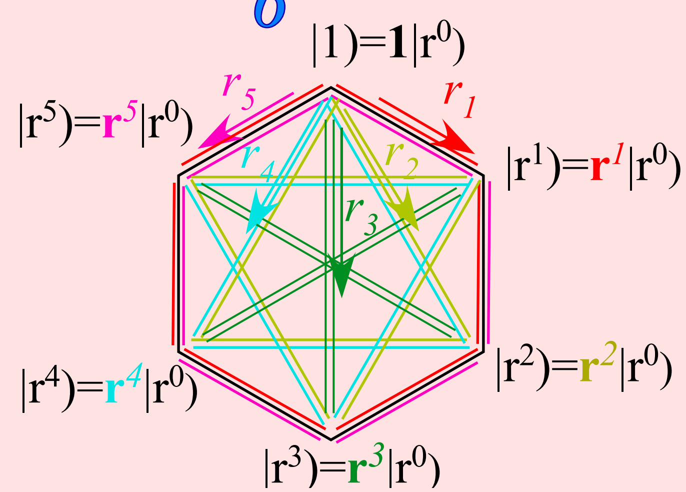
r_1 equals conjugate of r_5: ($r_1 = r_5^* = -r$) $(r_2 = r_4^* = -s)$ $(r_3 = r_3^* = t)$ *must* be real

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

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

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order *6*

2^{nd} Step

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

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

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

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

$\psi_1^0=1$

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

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

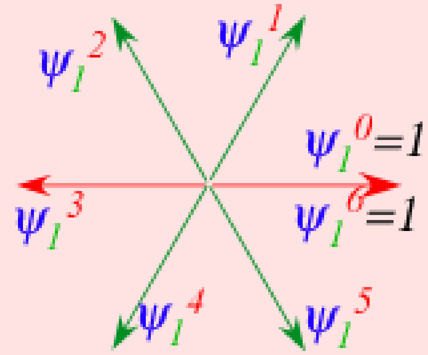
$\psi_1^3=\psi_3^1=-1$

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

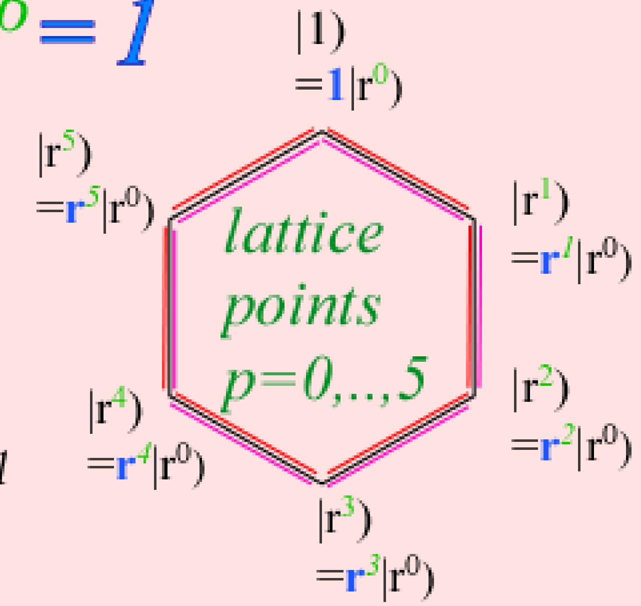
$\psi_1^5=\psi_5^1=\psi_1^{-1}=e^{-2\pi i/6}$

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*

2nd Step (contd.)

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

top-row flip not needed...

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

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

$$\boxed{\begin{array}{l} D^m(\mathbf{r}) = e^{-2\pi i m/6} \\ D^m(\mathbf{r}^p) = e^{-2\pi i m\cdot p/6} \end{array}} \begin{array}{l} = \chi_1^{\,m} = \psi_1^{\,m*} \\ = \chi_p^{\,m} = \psi_p^{\,m*} \end{array}$$

p = power (exponent) or position point

m = momentum or wave-number

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

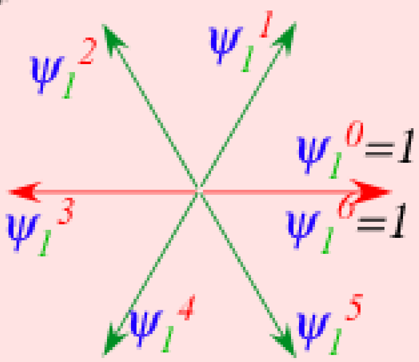
$\psi_1^{\,1} = e^{2\pi i/6}$

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

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

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

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



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

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

$$\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: $\mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \dots + \mathbf{P}^{(5)} = \mathbf{1}$

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

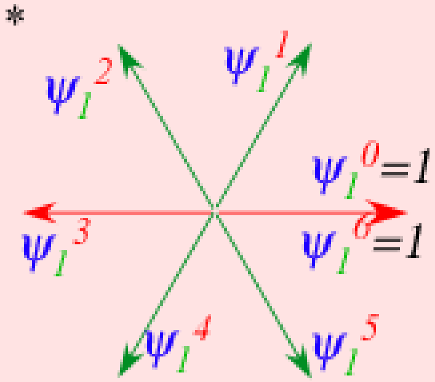
$$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1{}^m = \psi_1{}^{m*}$$

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

p = power (exponent) or position point

m = momentum or wave-number

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



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

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

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

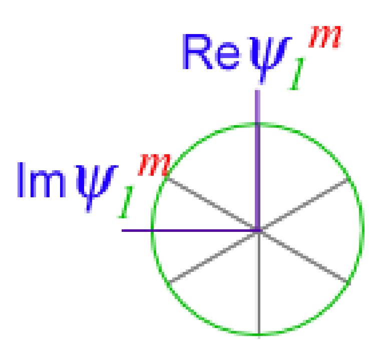
Inverse C_6 spectral resolution m-wave $\psi_p{}^m = D^{m*}(\mathbf{r}^p) = e^{+2\pi i m\cdot p/6}$:

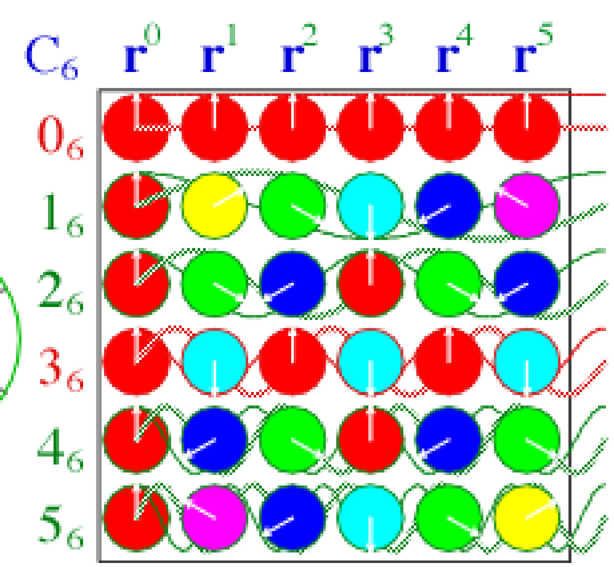
$$6\cdot\mathbf{P}^{(m)} = \psi_0{}^m\,\mathbf{r}^0 + \psi_1{}^m\,\mathbf{r}^1 + \psi_2{}^m\,\mathbf{r}^2 + \psi_3{}^m\,\mathbf{r}^3 + \psi_4{}^m\,\mathbf{r}^4 + \psi_5{}^m\,\mathbf{r}^5$$

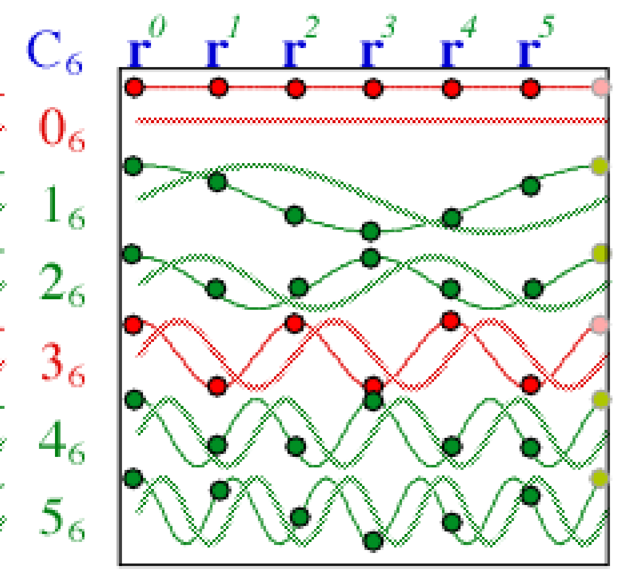
position p (or power of $\mathbf{r}^p$)

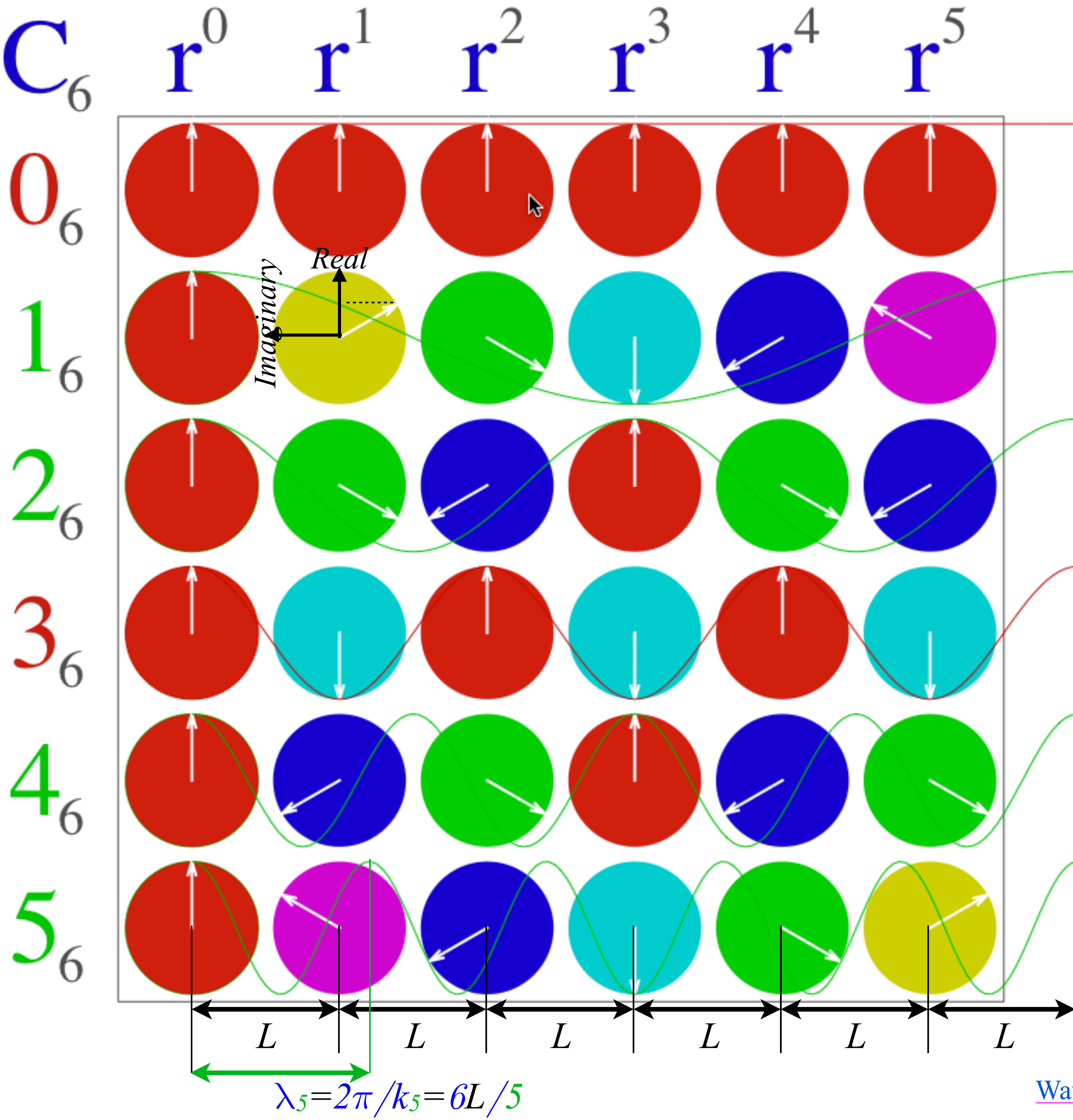
momentum m

	$p=0$	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

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

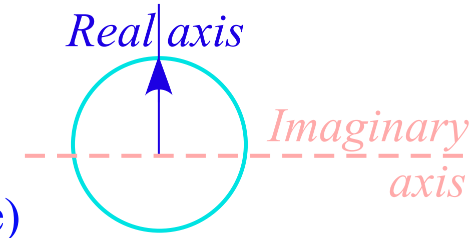
$$k_m=2\pi m/6L=2\pi/\lambda_m$$

Wavelength

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

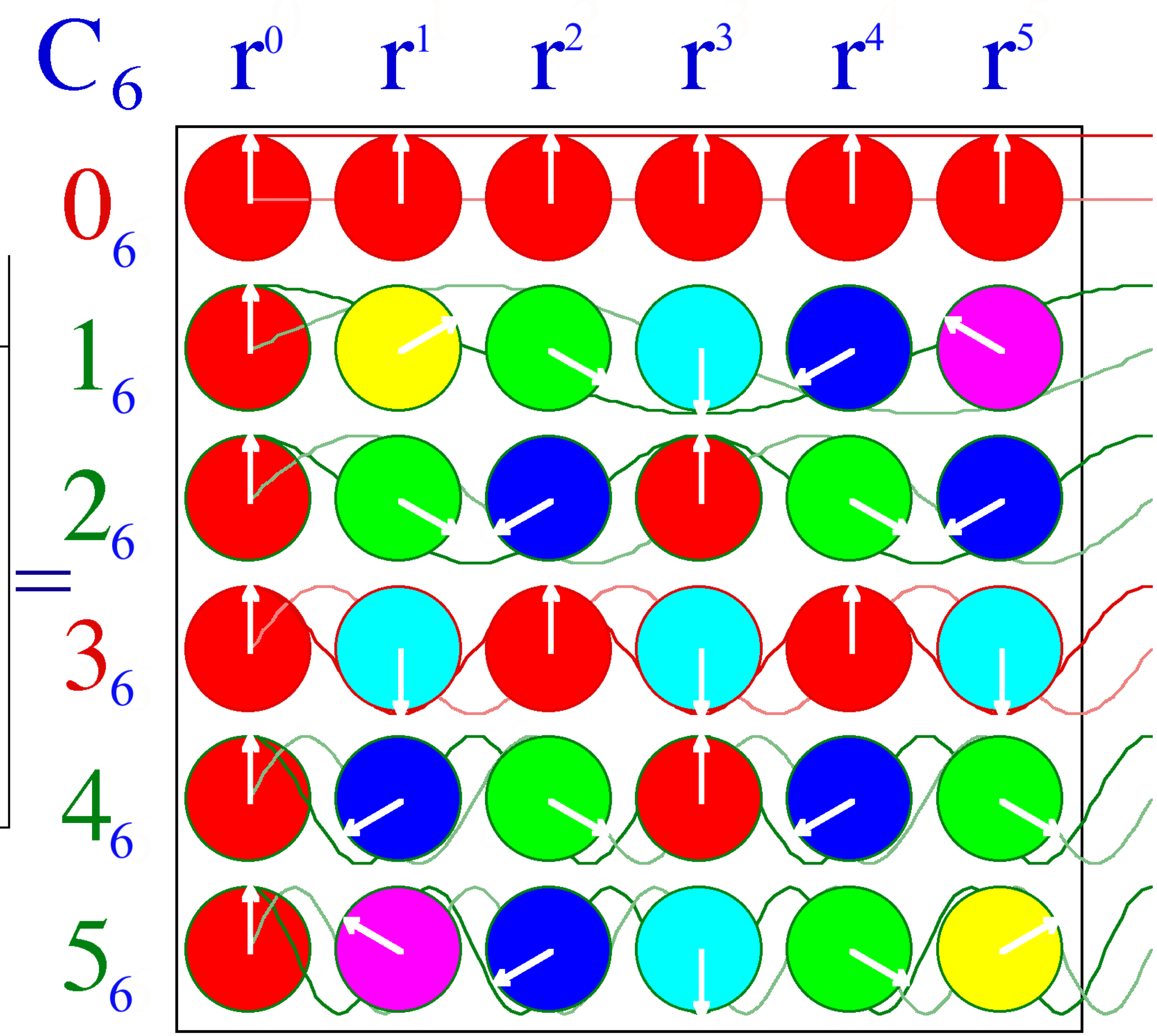
WaveIt *C_6 Character Phasors* Web Simulation

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 C_6 *Character Phasors* Web Simulation

	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 *C_6 Character Phasors* Web Simulation]

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

Basic Projection operators GThLect.4 p.31-46 *1st page*

C_2 *spectral resolution for group* C_2 *GThLect.6 p.17* *1st page*

C_2 *spectral resolution for 2D oscillator GThLect.6 p.33*

C_2 *beat dynamics for 2D oscillator GThLect.6 p.35-46*

U(2) *beat phase dynamics for 2D oscillator GThLect.6 p.52-56*

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

C_3 *Basic group representation theory. GThLect.11 p6-12.* *1st page*

C_3 *group spectral resolution. GThLect.11 p14-27* *1st page*

C_3 *Operator/State-Ortho-completeness GThLect.11 p29-38* *1st page*

C_3 *Wavefunction bra-kets GThLect.11 p40-45.* *1st page*

C_3 *quantum number Mod-3 formulae GThLect.11 p47-52.* *1st page*

C_3 *character or irrep tables GThLect.11 p54-58.* *1st page*

C_3 *wave dispersion functions GThLect.11 p60-68.* *1st page*

Moving vs standing waves p71-73.

Radial vs transverse waves p71-73.

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order 6

1st Step: Find C_6 symmetric **H** *by C_6 product table of regular reps and coupling params* $\{r_0, r_1 \ldots r_5\}$ *GThLect12 p3-9* *1st page*

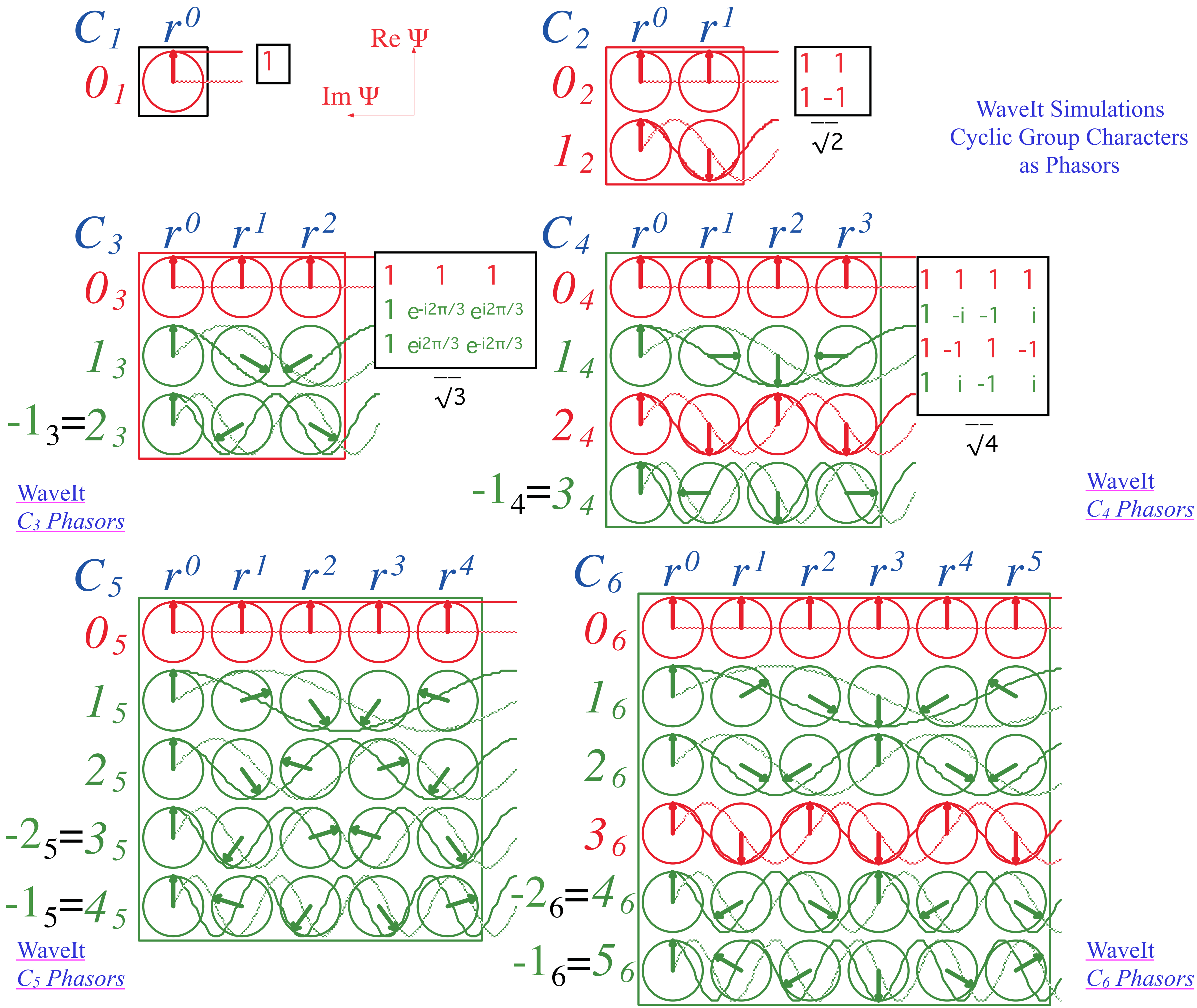
2nd Step: Find **H** *eigenfunctions by spectral resolution of* $C_6 = \{\mathbf{1}=\mathbf{r}^0, \mathbf{r}^1, \mathbf{r}^2, \mathbf{r}^3, \mathbf{r}^4, \mathbf{r}^5\}$ *GThLect12 p11-16* *1st page*

Character tables of C_2, C_3, C_4, C_5, ... C_{144} GThLect12 p18-24 *1st page*

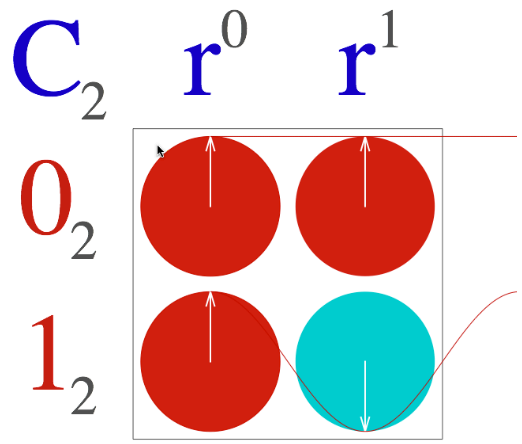
3rd Step: Dispersion functions and eigenvalues for various coupling parameter sets GThLect12 p27-30 *1st page*

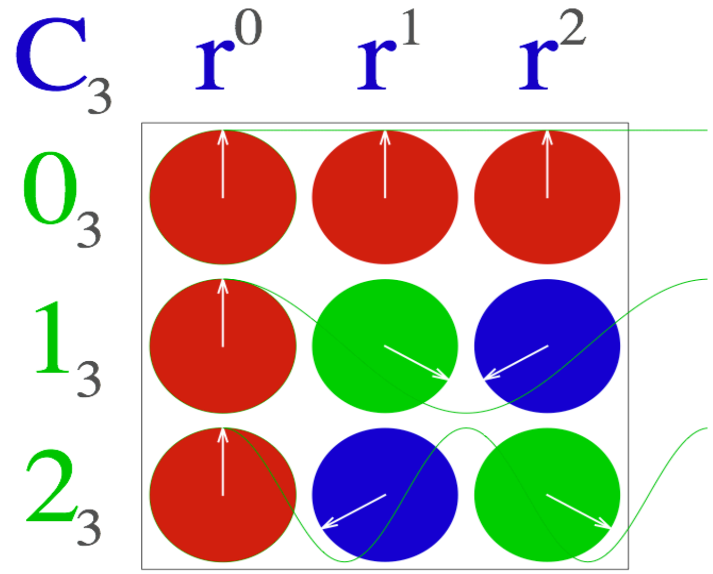
Ortho-complete eigenvalue/parameters p32-38 *1st page*

Gauge shifting complex coupling p40-48 *1st page*

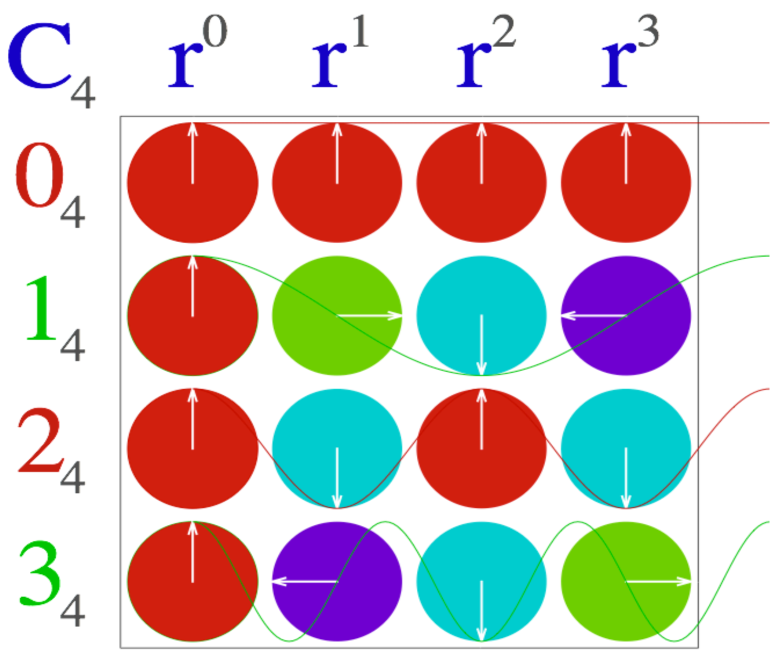


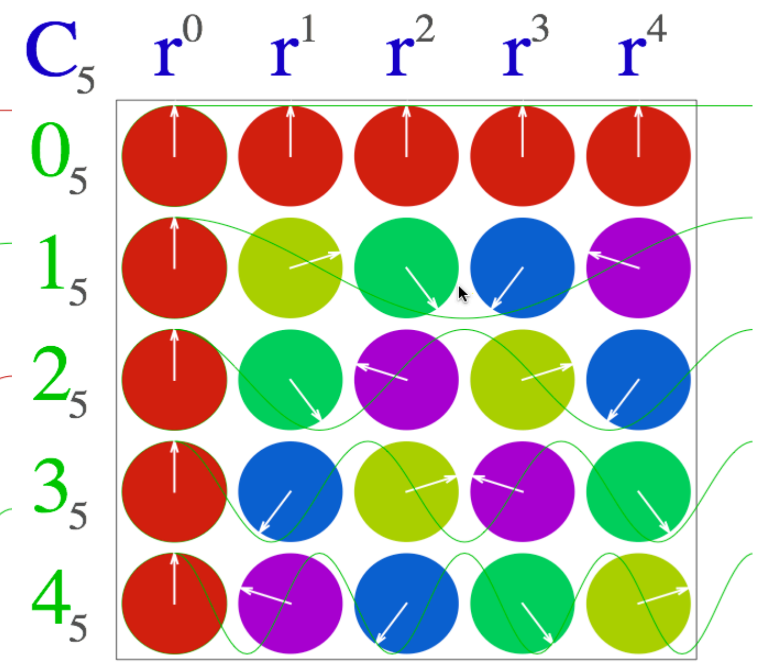
WaveIt Simulations
Cyclic Group Characters
as Phasors
C1 r0
01
1
Re Ψ
Im Ψ
C2 r0 r1
02
12
1 1
1 -1
√2
C3 r0 r1 r2
03
13
-13=23
1 1 1
1 e-i2π/3 ei2π/3
1 ei2π/3 e-i2π/3
√3
C4 r0 r1 r2 r3
04
14
24
-14=34
1 1 1 1
1 -i -1 i
1 -1 1 -1
1 i -1 i
√4
WaveIt
C3 Phasors
WaveIt
C4 Phasors
C5 r0 r1 r2 r3 r4
05
15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



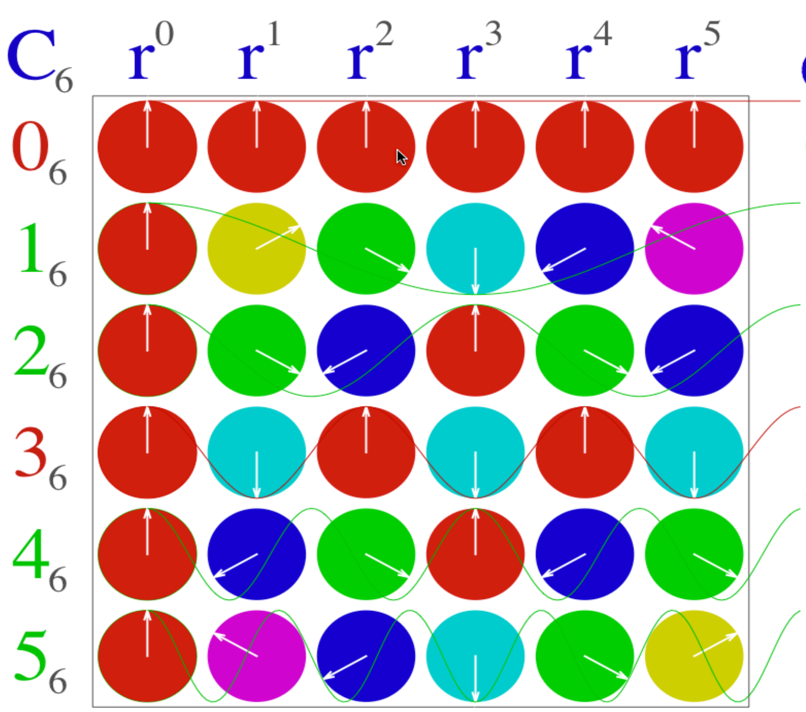


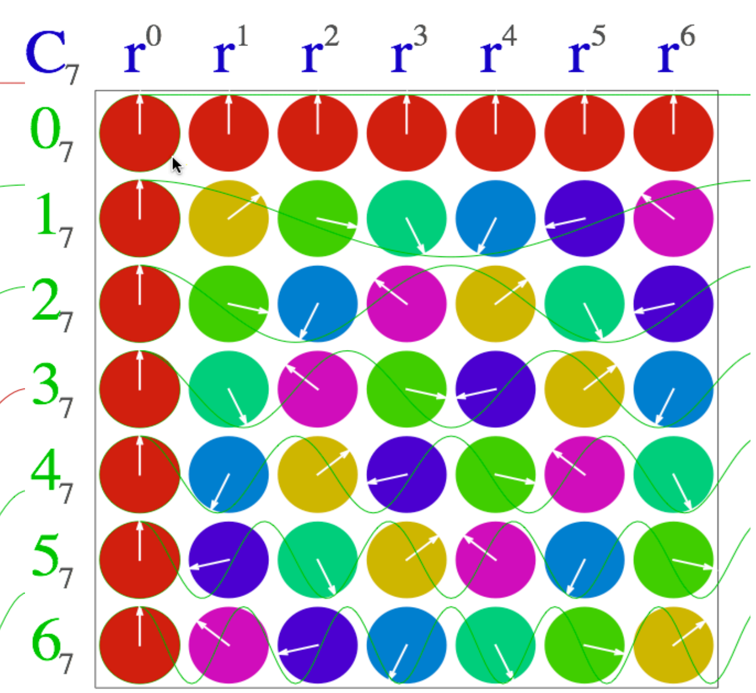
WaveIt
C2 Phasors



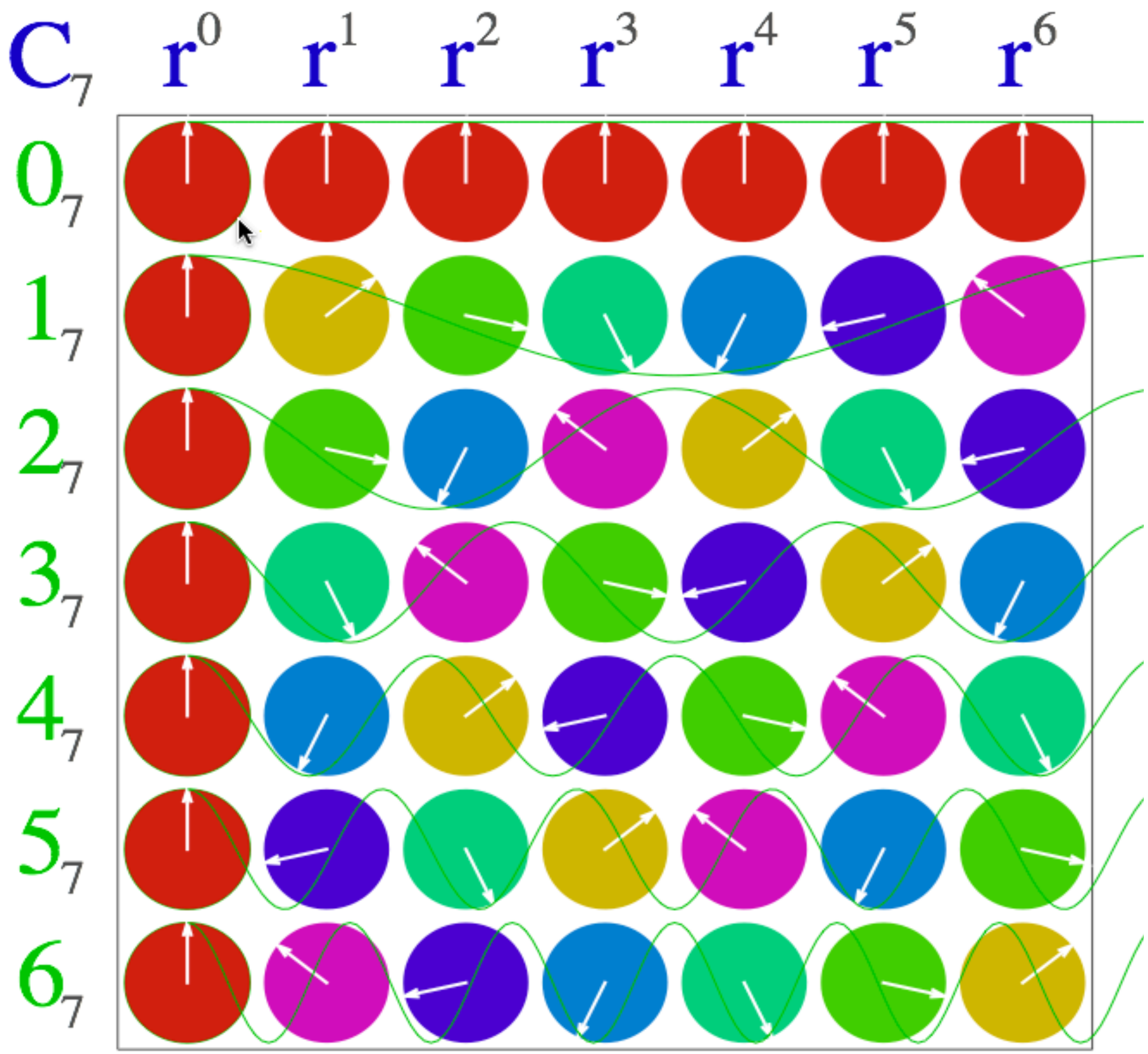


WaveIt
C4 Phasors





WaveIt
C6 Phasors



WaveIt
C_7 Phasors

C_N Lattice position vector

$r_p = L \cdot p$

Wavevector

$k_m = 2\pi/\lambda_m$

$= 2\pi m/NL$

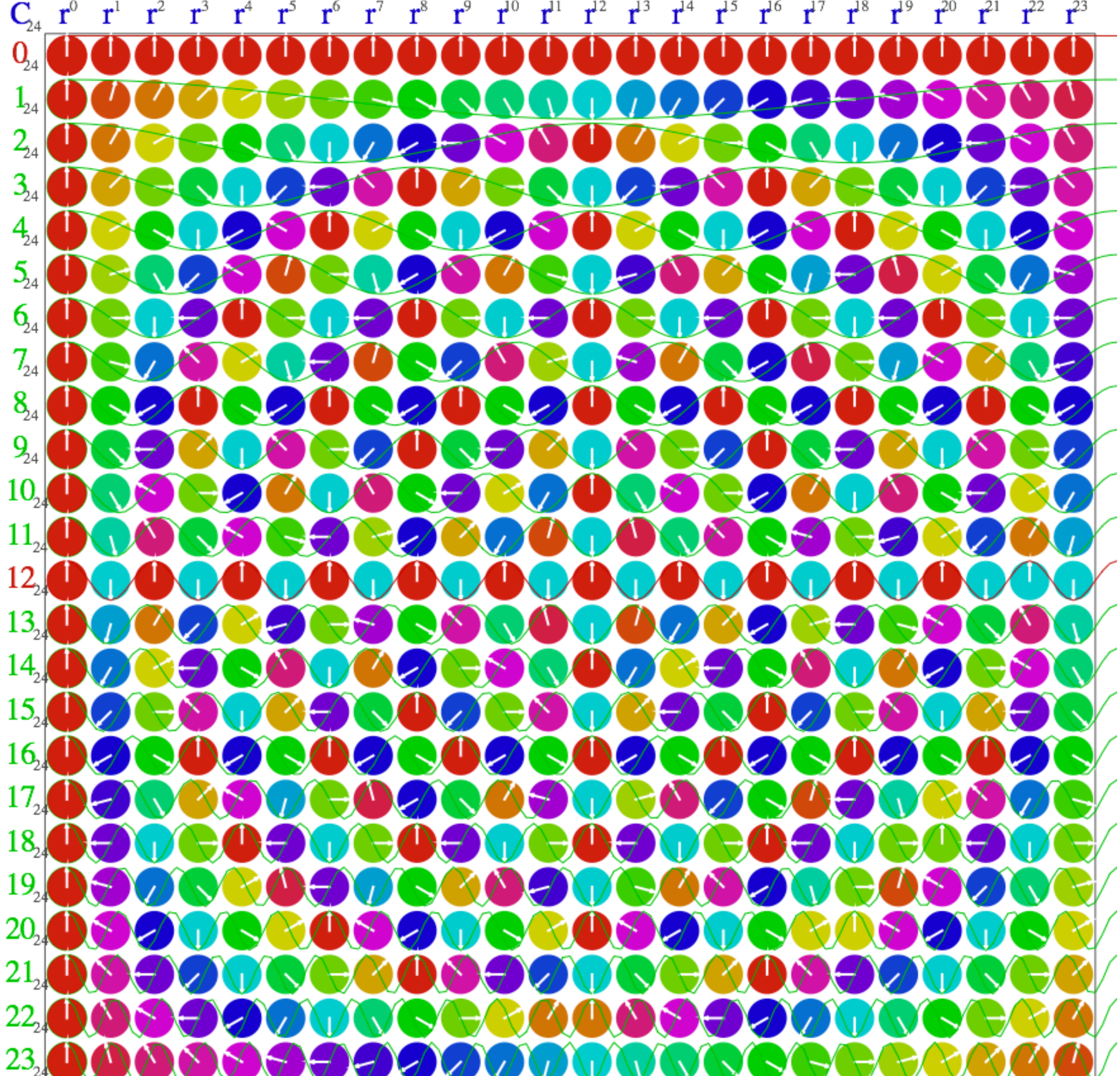
Wavelength

$\lambda_m = 2\pi/k_m$

$= NL/m$

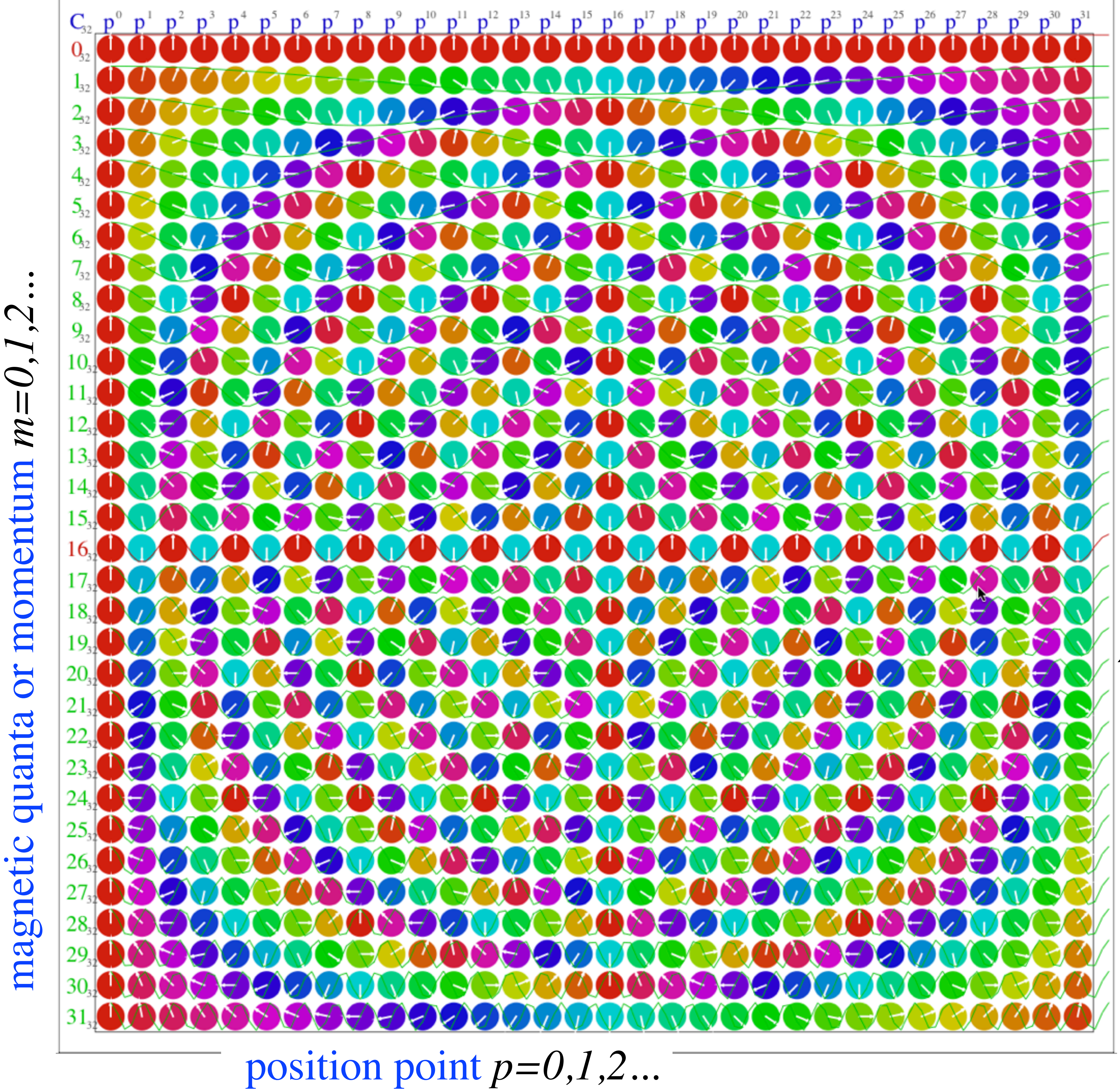
C_N Plane wave function

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



WaveIt

C_{24} Phasors



C_{32}

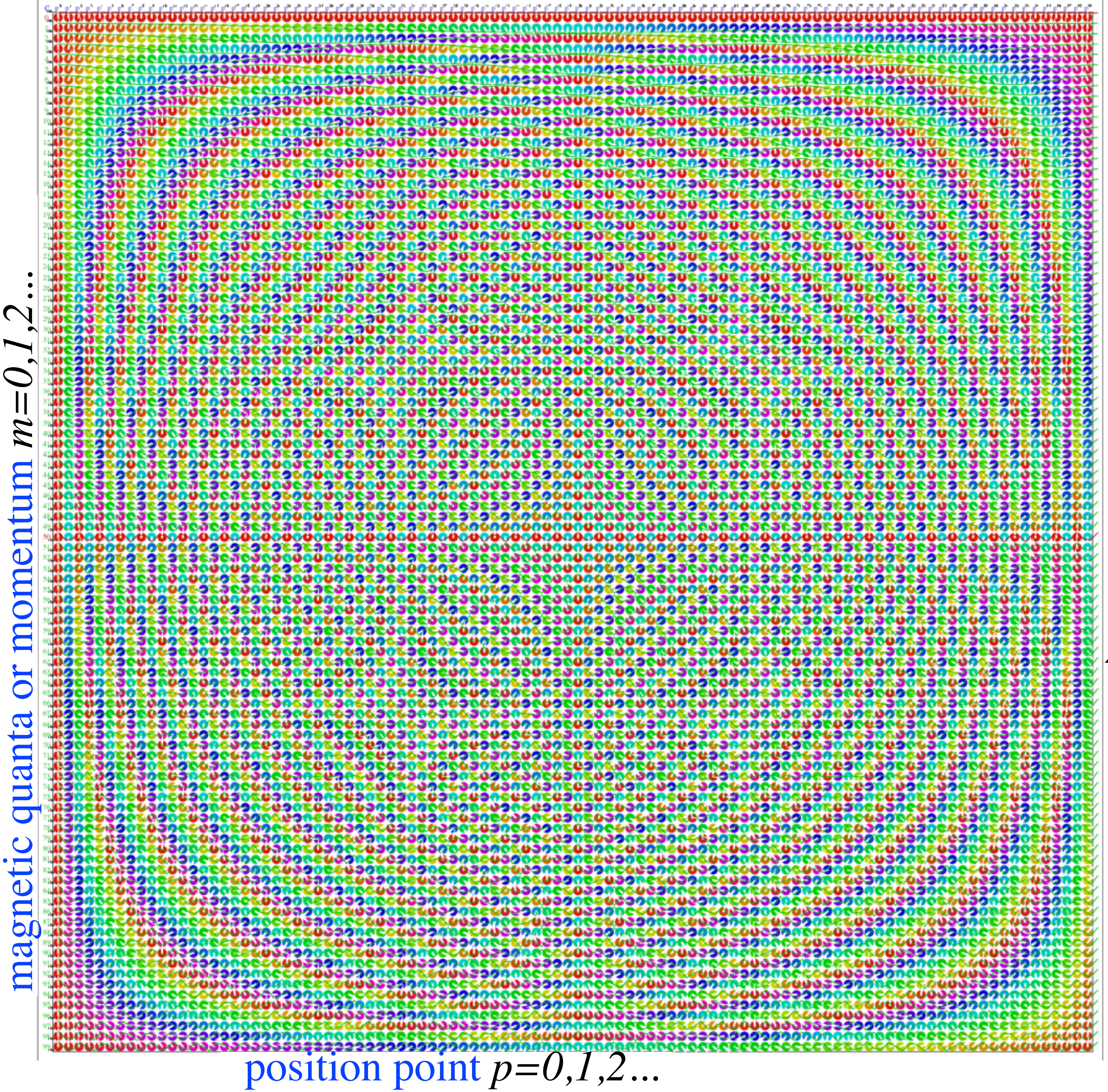
phasor character table

$$\chi_p^m = e^{-ik_m r^p}$$

$$= e^{\frac{-2\pi imp}{32}}$$

WaveIt

C_{32} Phasors



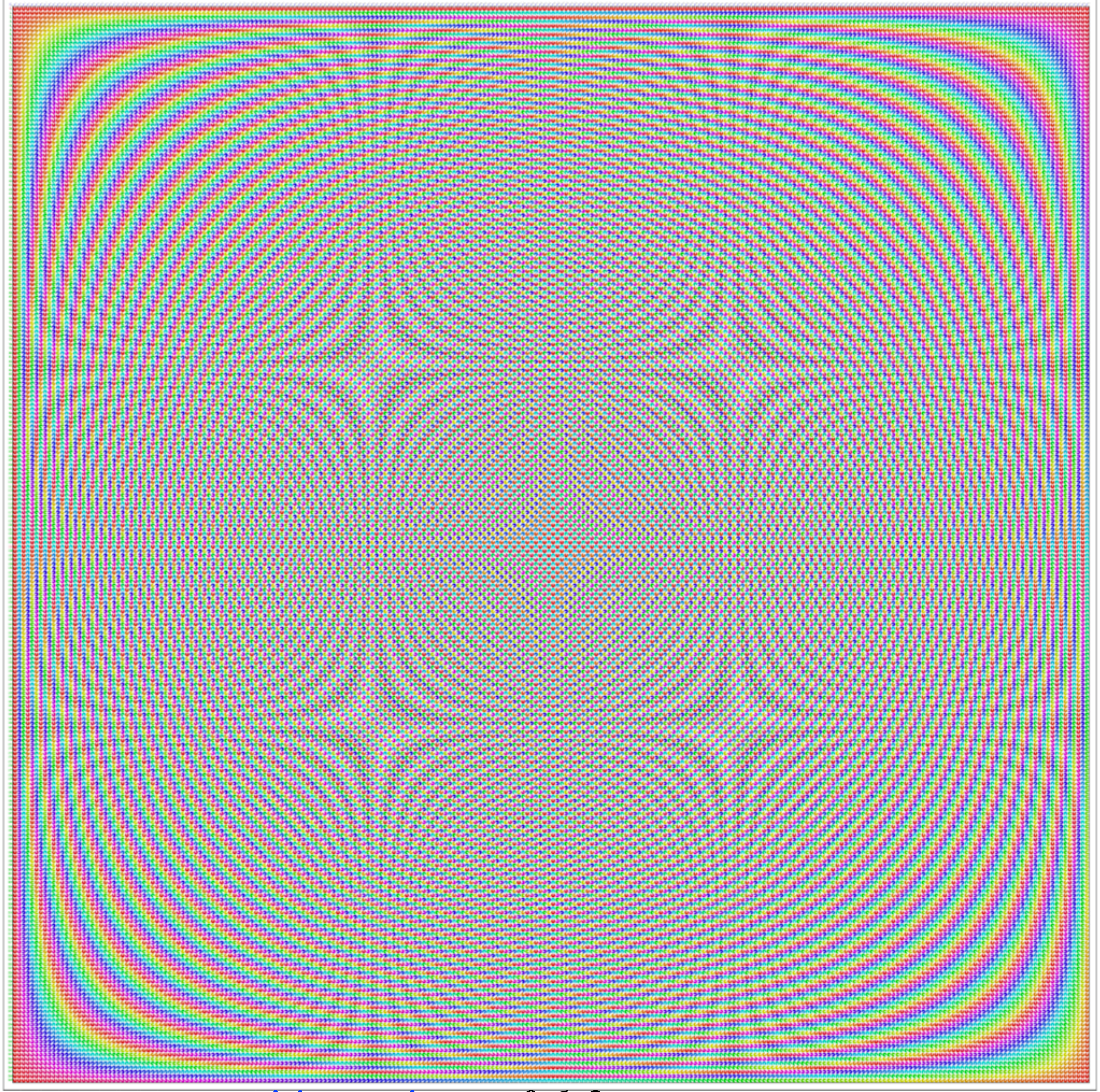
C_{100}

phasor character table

$$\chi_p^m = e^{-ik_m r^p}$$

$$= e^{\frac{-2\pi imp}{100}}$$

Invariant phase "Uncertainty" hyperbolas: $m \cdot p = const.$



magnetic quanta or momentum $m=0,1,2...$

position point $p=0,1,2...$

C_{256}

phasor
character
table

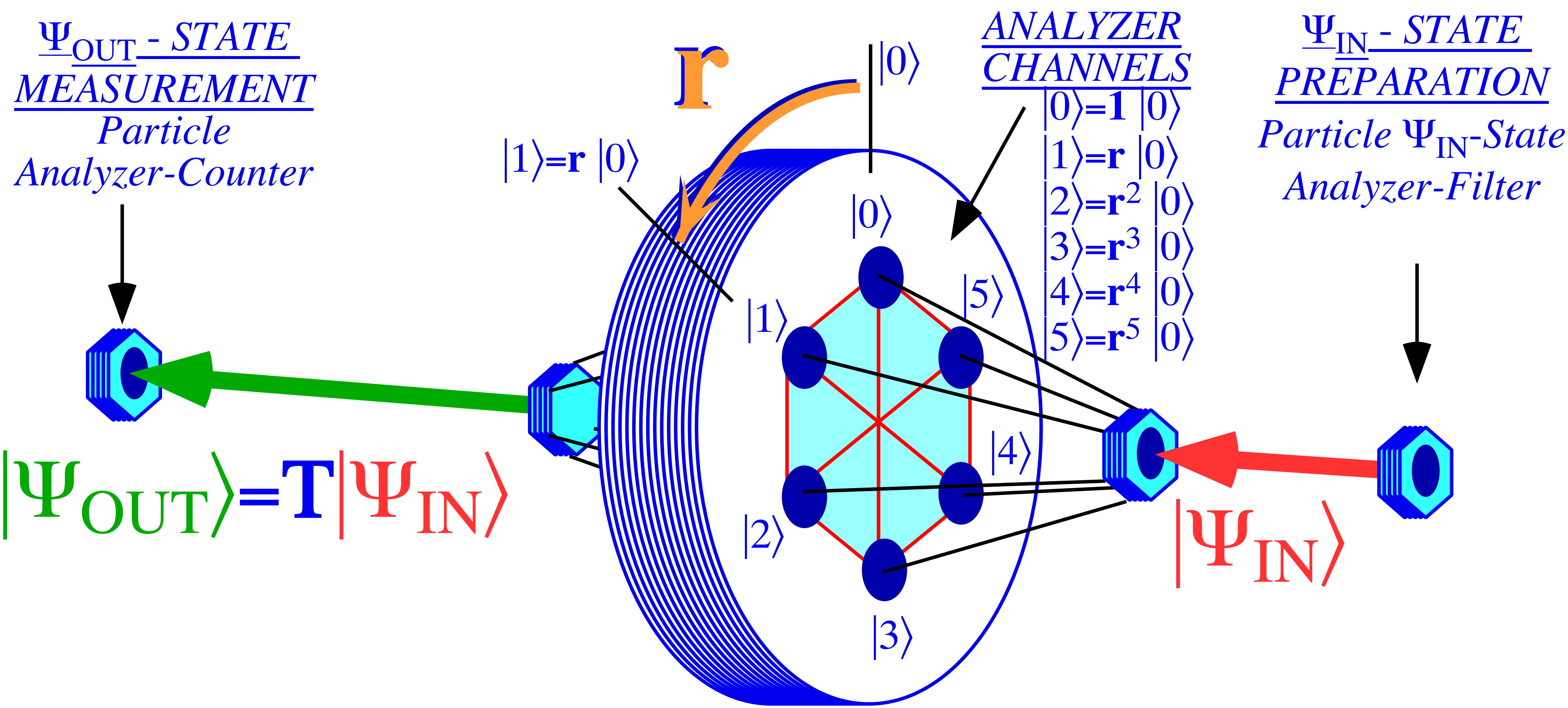
$$\chi_p^m = e^{-ik_m r^p}$$

$$= e^{\frac{-2\pi imp}{256}}$$

Invariant phase
"Uncertainty"
hyperbolas:
$m \cdot p = const.$

[WaveIt C_{256} Character Phasors Web Simulation]

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



QTforCA Fig. 8.1.1

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$
=>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

$\mathscr{G}$ = C_2 = Cyclic (or Circle) group of order 2

Basic Projection operators GThLect.4 p.31-46 *1st page*

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U(2) *beat phase dynamics for 2D oscillator GThLect.6 p.52-56*

$\mathscr{G}$ = C_3 = Cyclic (or Circle) group of order 3

C_3 *Basic group representation theory. GThLect.11 p6-12.* *1st page*

C_3 *group spectral resolution. GThLect.11 p14-27* *1st page*

C_3*Operator/State-Ortho-completeness GThLect.11 p29-38* *1st page*

C_3*Wavefunction bra-kets GThLect.11 p40-45.* *1st page*

C_3 *quantum number Mod-3 formulae GThLect.11 p47-52.* *1st page*

C_3 *character or irrep tables GThLect.11 p54-58.* *1st page*

C_3 *wave dispersion functions GThLect.11 p60-68.* *1st page*

Moving vs standing waves p71-73.

Radial vs transverse waves p71-73.

$\mathscr{G}$ = C_6 = Cyclic (or Circle) group of order *6*

1st Step: Find C_6 *symmetric* **H** *by* C_6 *product table of regular reps and coupling params* $\{r_0,r_1\ldots r_5\}$ *GThLect12 p3-9* *1st page*

2nd Step: Find **H** *eigenfunctions by spectral resolution of* $C_6=\{\mathbf{1}=\mathbf{r}^0,\mathbf{r}^1,\mathbf{r}^2,\mathbf{r}^3,\mathbf{r}^4,\mathbf{r}^5\}$ *GThLect12 p11-16* *1st page*

Character tables of C_2, C_3, C_4, C_5, *....* C_{144} *GThLect12 p18-24* *1st page*

3rd Step: Dispersion functions and eigenvalues for various coupling parameter sets GThLect12 p27-30 *1st page*

Ortho-complete eigenvalue/parameters p32-38 *1st page*

Gauge shifting complex coupling p40-48 *1st page*

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

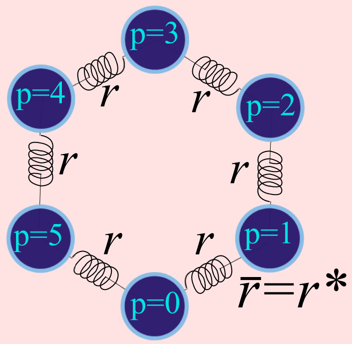
$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$ *(Dispersion functions)*

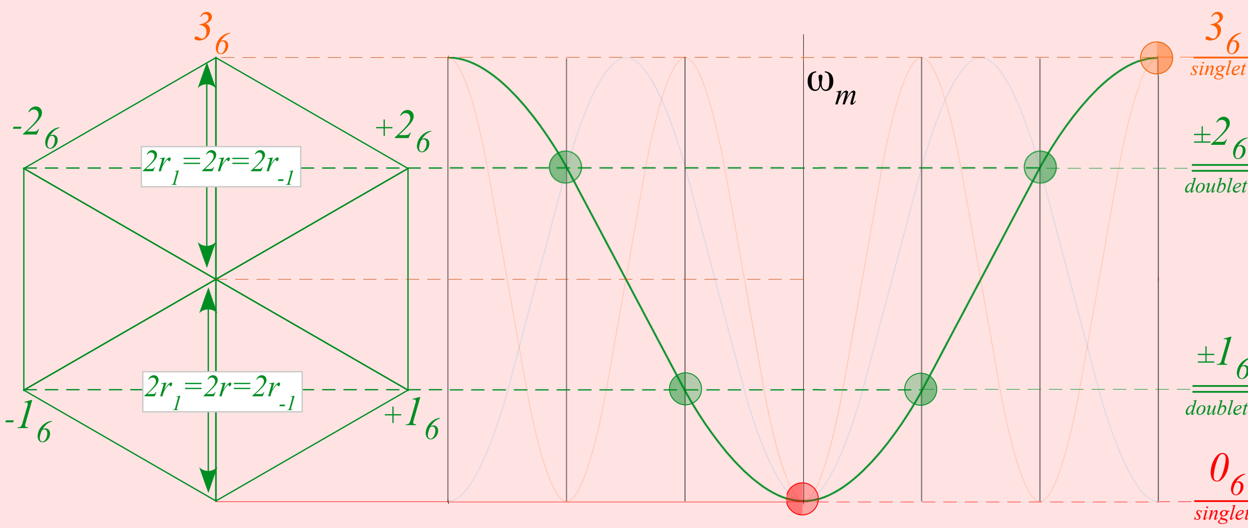
3^{rd} Step *Display all eigensolutions of all possible C_6 symmetric real H*

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

Elementary Bloch Model

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





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

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

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

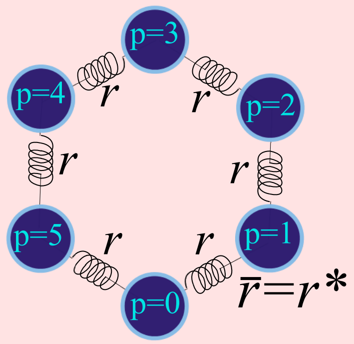
r_1 equals conjugate of r_5: ($r_1 = r_5^* = -r$)

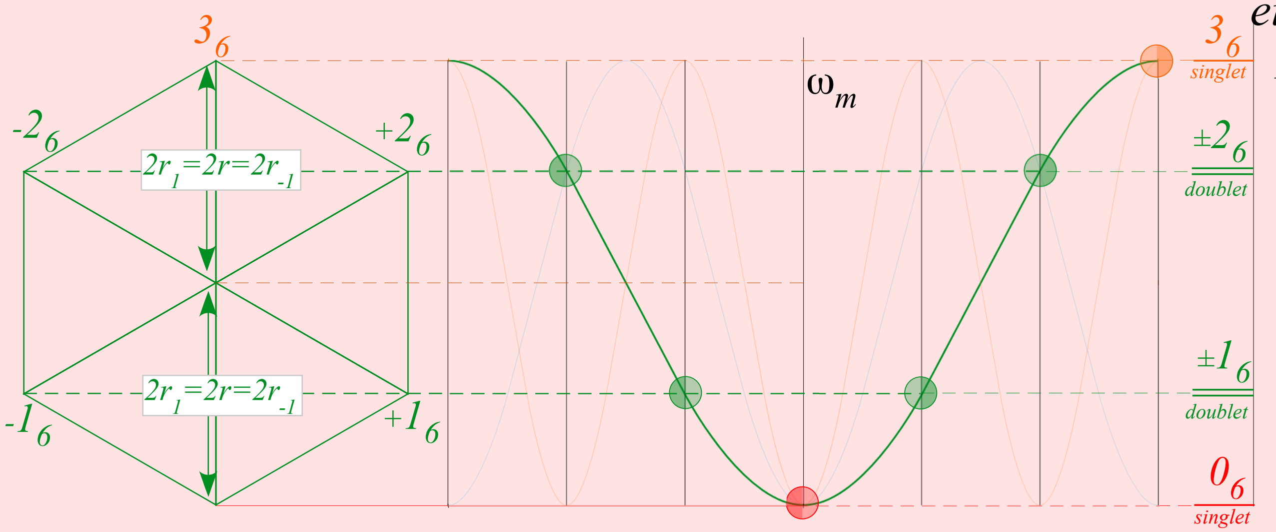
3^{rd} Step *Display all eigensolutions of all possible C_6 symmetric real H*

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

Elementary Bloch Model

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





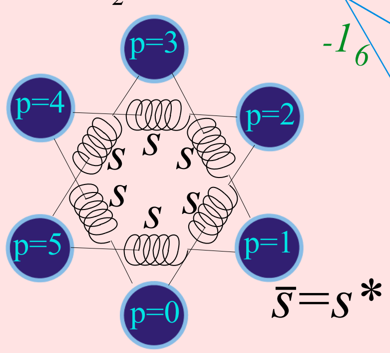
eigenvalues of $\mathbf{H}^{B1(6)}$

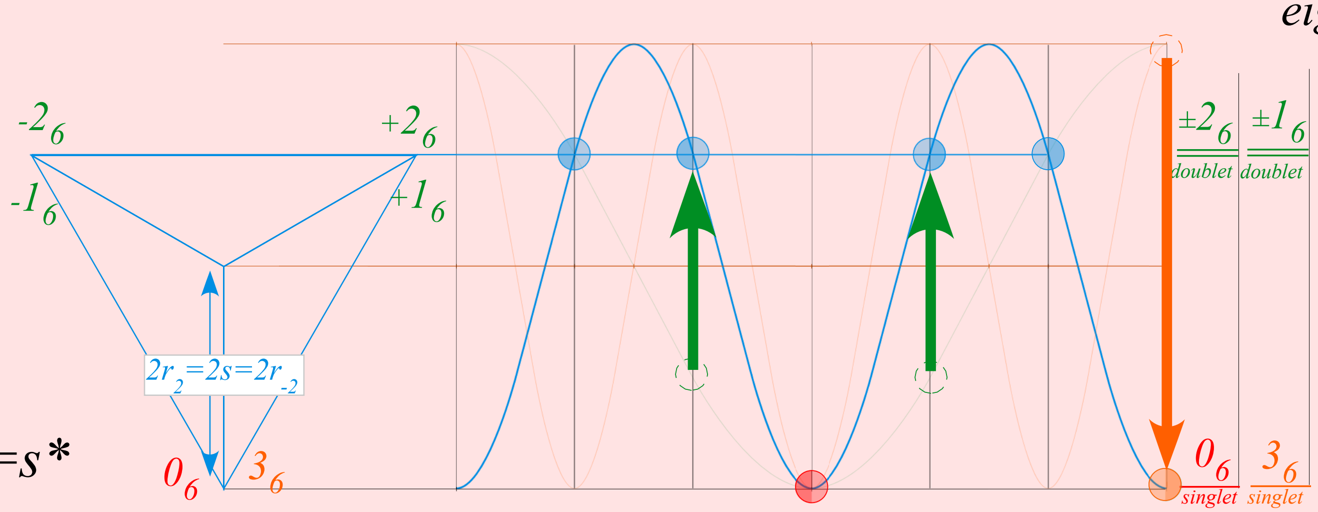
$$\begin{array}{c|c} \begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array} & \\ \begin{pmatrix} H_1 & -r & \cdot & \cdot & \cdot & -r \\ -r & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -r & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -r & H_1 & -r & \cdot \\ \cdot & \cdot & \cdot & -r & H_1 & -r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

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

2^{nd} Neighbor coupling

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





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

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

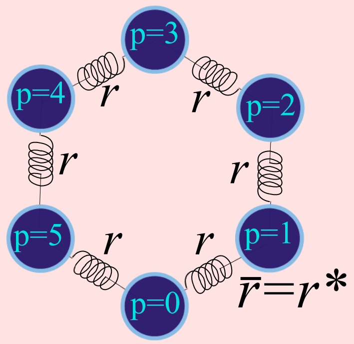
$$\omega^{B2(n)}(k_m) = r_0\chi_0^m + r_2\chi_2^m + r_{-2}\chi_{-2}^m = H_2 - 2s\,cos(4\pi m/6)$$

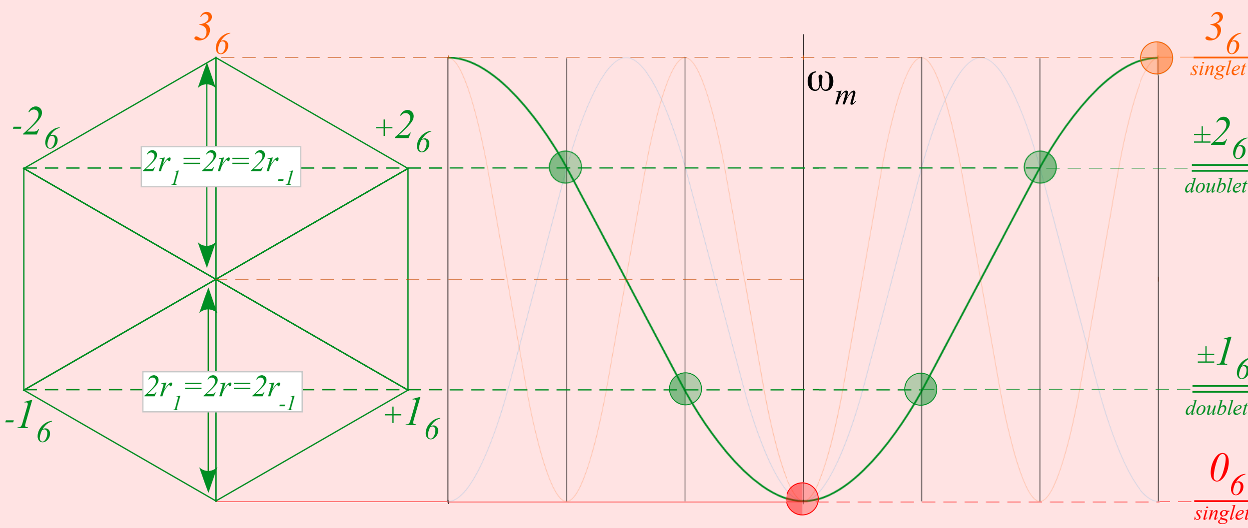
3^{rd} Step *Display all eigensolutions of all possible C_6 symmetric real H*

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

Elementary Bloch Model

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





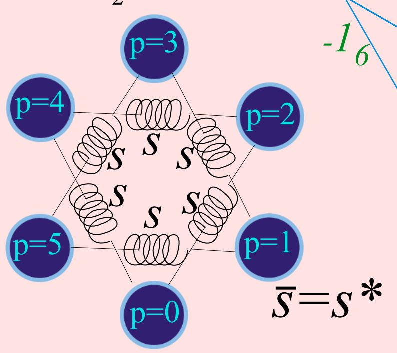
eigenvalues of $\mathbf{H}^{B1(6)}$

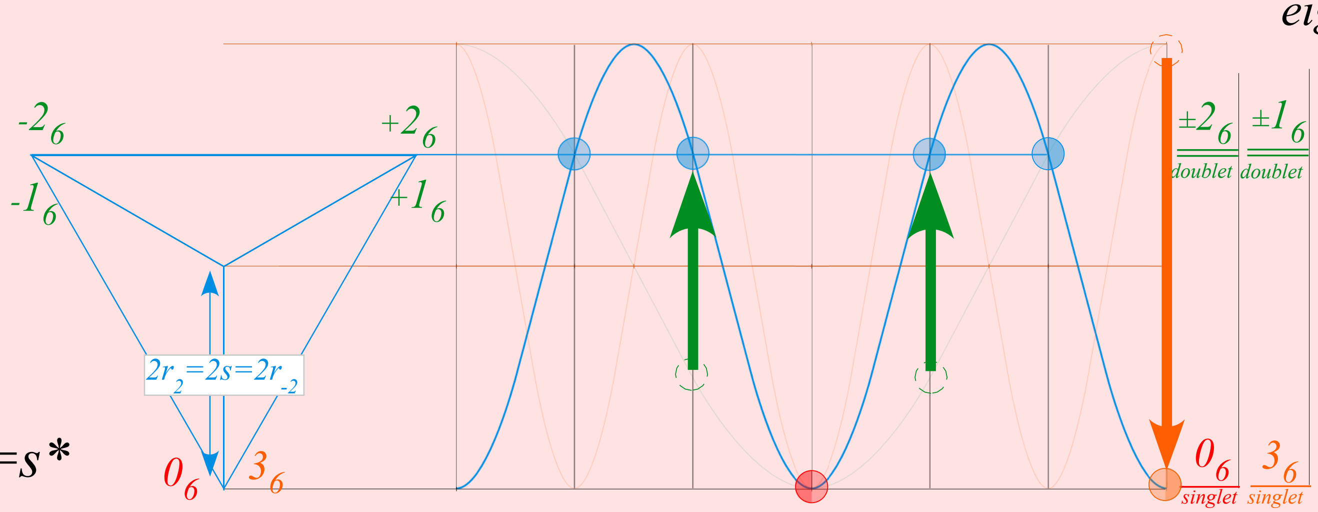
$$\begin{array}{c c} \begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array} & \\ \left(\begin{array}{cccccc} H_1 & -r & \cdot & \cdot & \cdot & -r \\ -r & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -r & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -r & H_1 & -r & \cdot \\ \cdot & \cdot & \cdot & -r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

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

2^{nd} Neighbor coupling

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





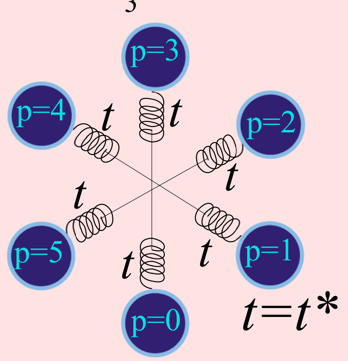
eigenvalues of $\mathbf{H}^{B2(6)}$

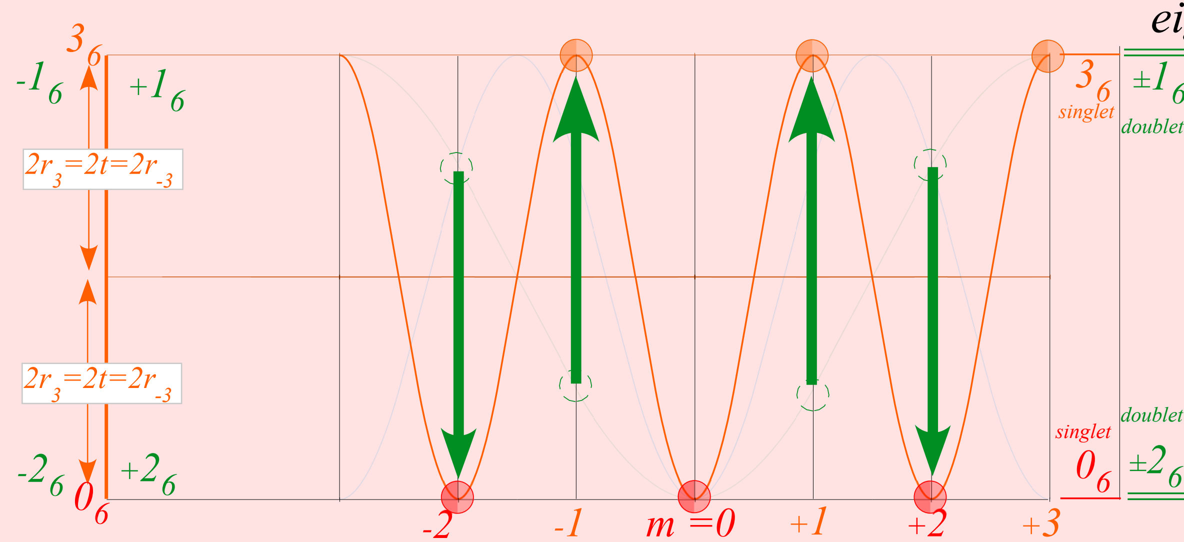
$$\begin{array}{c c} \begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array} & \\ \left(\begin{array}{cccccc} H_2 & \cdot & -s & \cdot & -s & \cdot \\ \cdot & H_2 & \cdot & -s & \cdot & -s \\ -s & \cdot & H_2 & \cdot & -s & \cdot \\ \cdot & -s & \cdot & H_2 & \cdot & -s \\ -s & \cdot & -s & \cdot &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

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

3^{rd} Neighbor coupling

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





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

$$\begin{array}{c c} \begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5 \end{array} & \\ \left(\begin{array}{cccccc} H_3 & \cdot & \cdot & -t & \cdot & \cdot \\ \cdot & H_3 & \cdot & \cdot & -t & \cdot \\ \cdot & \cdot & H_3 & \cdot & \cdot & -t \\ -t & \cdot & \cdot & H_3 & \cdot & \cdot \\ \cdot & -t & \cdot & \cdot & H_3 & \cdot \\ \cdot & \cdot & -t & \cdot & \cdot & H_3 \end{array}\right) & \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \end{array}$$

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

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$
=>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

Complete sets of C_6 coupling parameters and Fourier dispersion

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

C_6 Bloch $\mathbf{H}^{\mathrm{GB}(N)}$ eigenvalues are Fourier series

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero ($\phi_p = 0$)

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

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

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero (ϕ_p =0)

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

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

$$\omega_m(\mathbf{H}_{real}{}^{GB(6)}) = r_0 + r_1(e^{i\pi\frac{m\cdot 1}{3}} + e^{-i\pi\frac{m\cdot 1}{3}}) \quad + r_2(e^{i\pi\frac{m\cdot 2}{3}} + e^{-i\pi\frac{m\cdot 2}{3}}) \quad + r_3(e^{i\pi\frac{m\cdot 3}{3}})$$

(for real: $r_p = r_{-p} = r_p^*$)

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero ($\phi_p = 0$)

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

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

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

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

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero (ϕ_p =0)

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

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

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

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

giving 4 ω_m-levels:

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

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero (ϕ_p =0)

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

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

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

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

giving 4 ω_m-levels:

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

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

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

Complete sets of C_6 coupling parameters and Fourier dispersion

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

Setting gauge to zero ($\phi_p=0$)

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

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

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

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

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

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

Nonzero gauge ϕ_p, or complex: $r_{-p} = r_p^*$

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

Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

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

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

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

or complex: $r_{-p} = r_p^*$.

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

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

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

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

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

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

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

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

giving 6 ω_m-levels:

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

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

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

Nonzero gauge ϕ_p ,

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

or complex: $r_{-p} = r_p^*$.

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

or 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...

3rd Step (contd.)

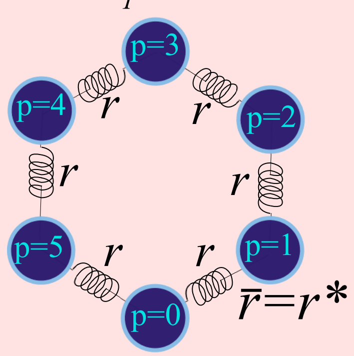
...eigensolutions for all possible C_6 symmetric complex H

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

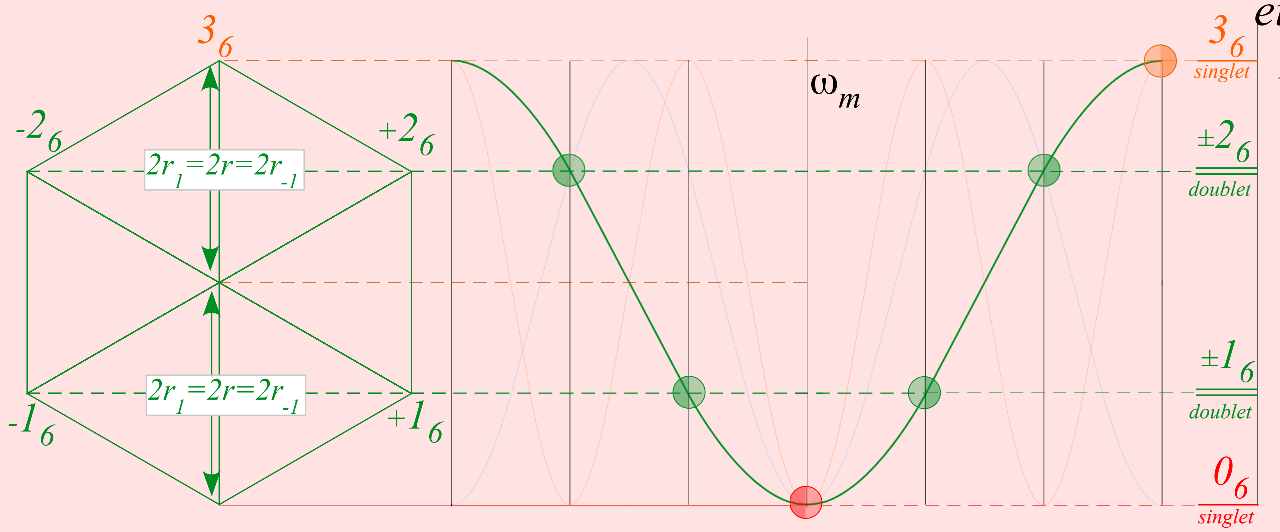
(Dispersion function)

Elementary Bloch Model

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



$\bar{r}=r^*$



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

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

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

Nearest neighbor coupling

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

3rd Step (contd.)

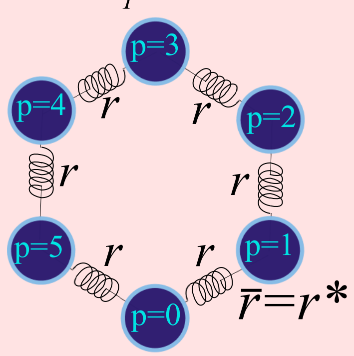
...eigensolutions for all possible C_6 symmetric complex H

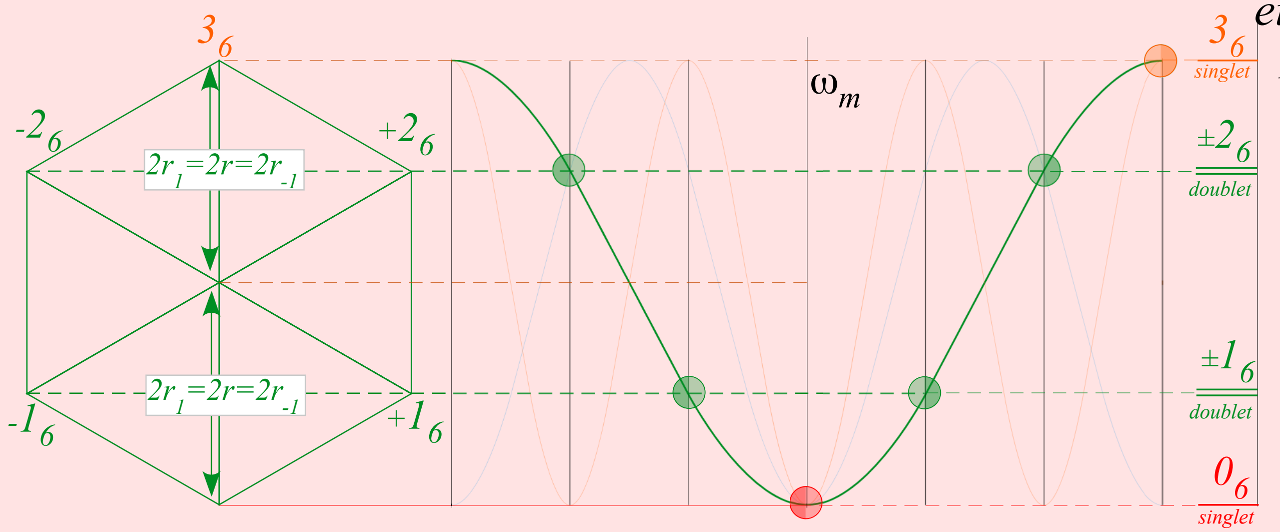
$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1}\chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1}\omega^{(m)}\mathbf{P}^{(m)} \quad where:\ \omega^{(m)}=\sum_{p=0}^{n-1} r_p\chi_p^m = \omega(k_m)$$

(Dispersion function)

Elementary Bloch Model

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





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

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

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

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.)

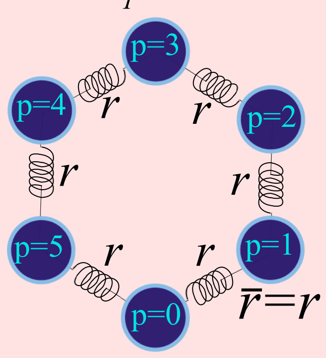
...eigensolutions for all possible C_6 symmetric complex H

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

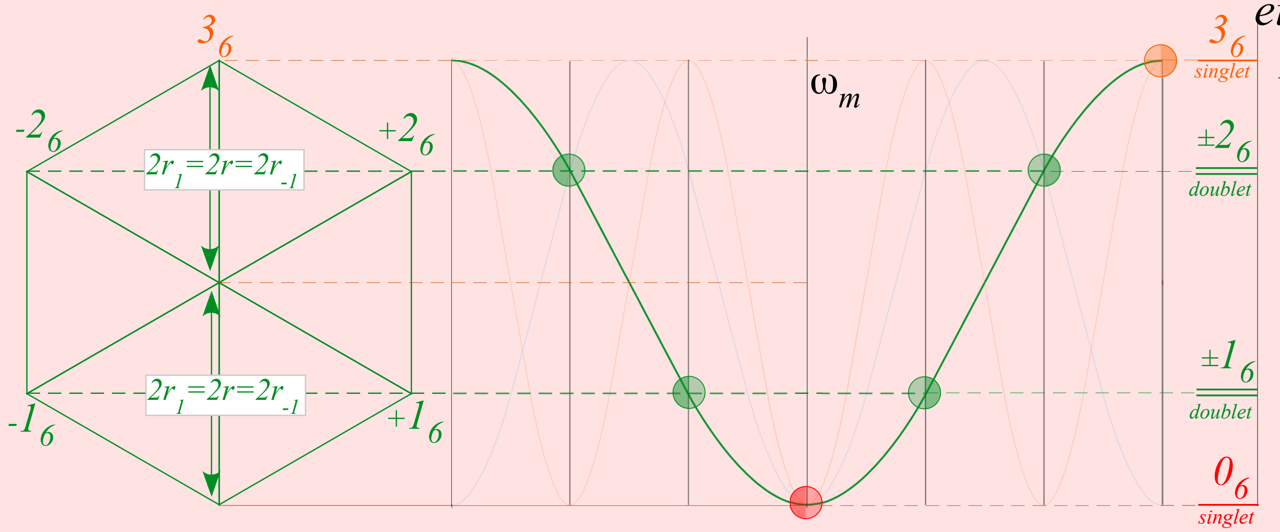
(Dispersion function)

Elementary Bloch Model

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



$\bar{r} = r^*$



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

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

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

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

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

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

3^{rd} Step (contd.)

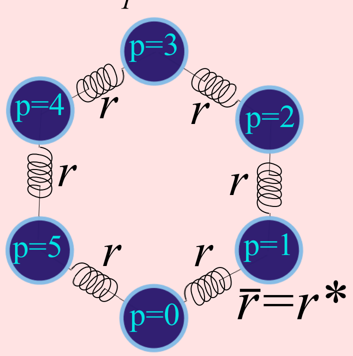
...eigensolutions for all possible C_6 symmetric complex H

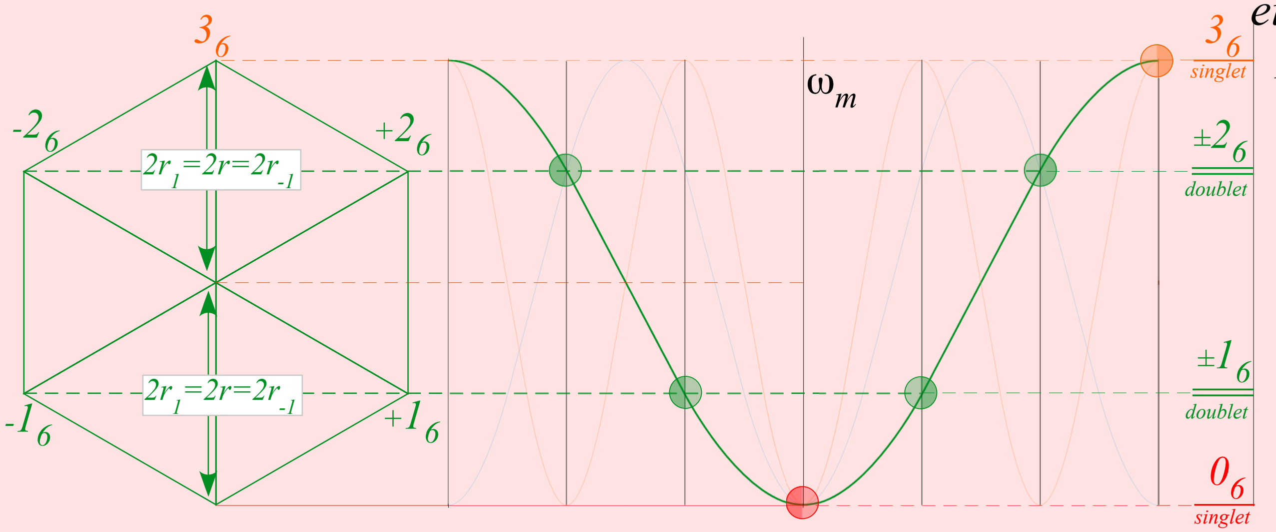
$$\mathbf{H} = \sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where:\ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$

(Dispersion function)

Elementary Bloch Model

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





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

$$\begin{array}{c} \quad p=0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \\ \left(\begin{array}{cccccc} H_1 & r_{-1} & \cdot & \cdot & \cdot & r_1 \\ r_1 & H_1 & r_{-1} & \cdot & \cdot & \cdot \\ \cdot & r_1 & H_1 & r_{-1} & \cdot & \cdot \\ \cdot & \cdot & r_1 & H_1 & r_{-1} & \cdot \\ \cdot & \cdot & \cdot & r_1 & H_1 & r_{-1} \\ r_{-1} & \cdot & \cdot & \cdot & r_1 & H_1 \end{array}\right) \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \end{array}$$

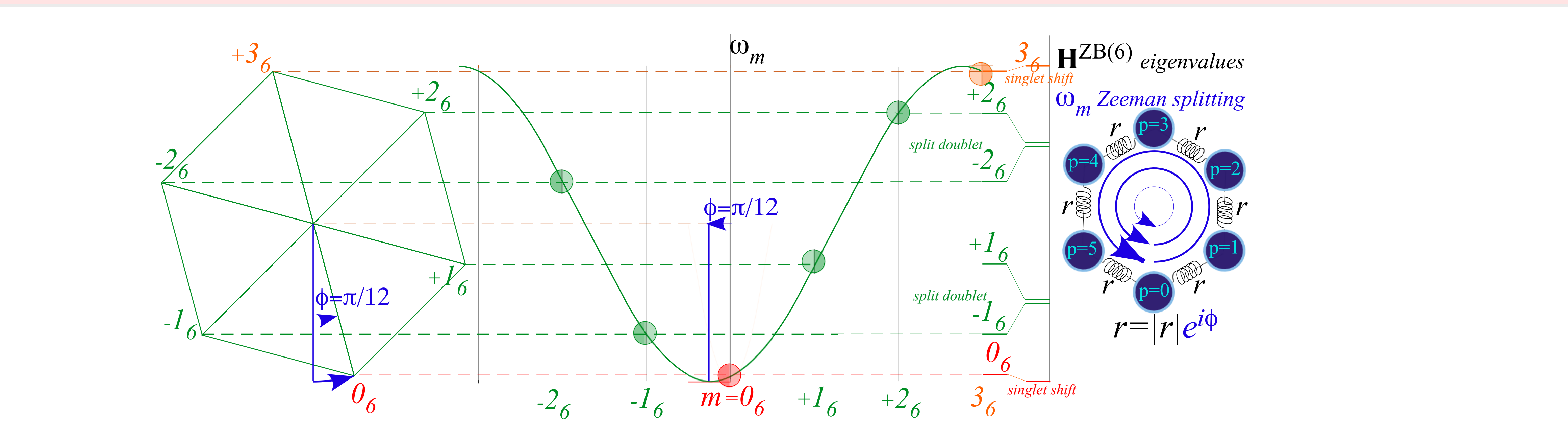
$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\cos(2\pi m/6)$$

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

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



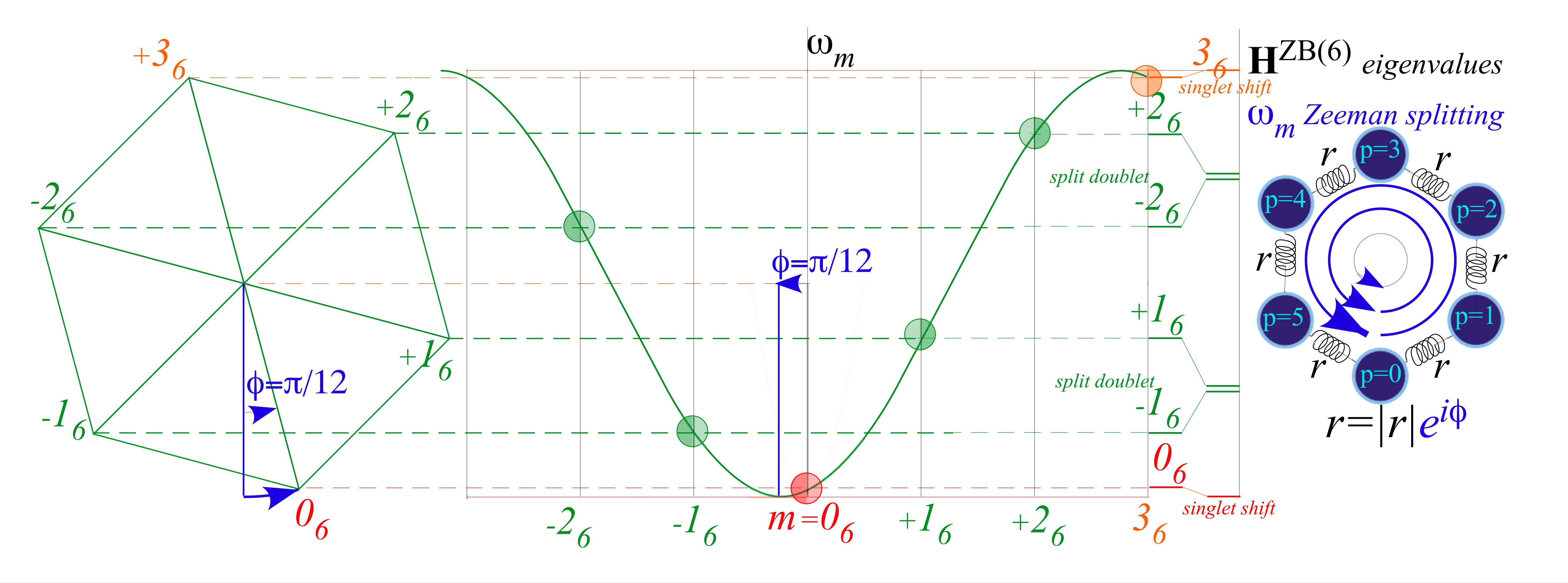
3^{rd} Step (contd.)

...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 <u>required</u> to be <u>moving</u> waves $e^{ik_m \cdot x_p}$



Symmetry group $\mathscr{G}$ representations=>*AMOP* Hamiltonian **H** (or K) matrices, irreps $\mathscr{D}^{(\alpha)}$ =>*AMOP* wave functions $\Psi^{(\alpha)}$, eigensolution projectors $\mathbf{P}^{(\alpha)}$

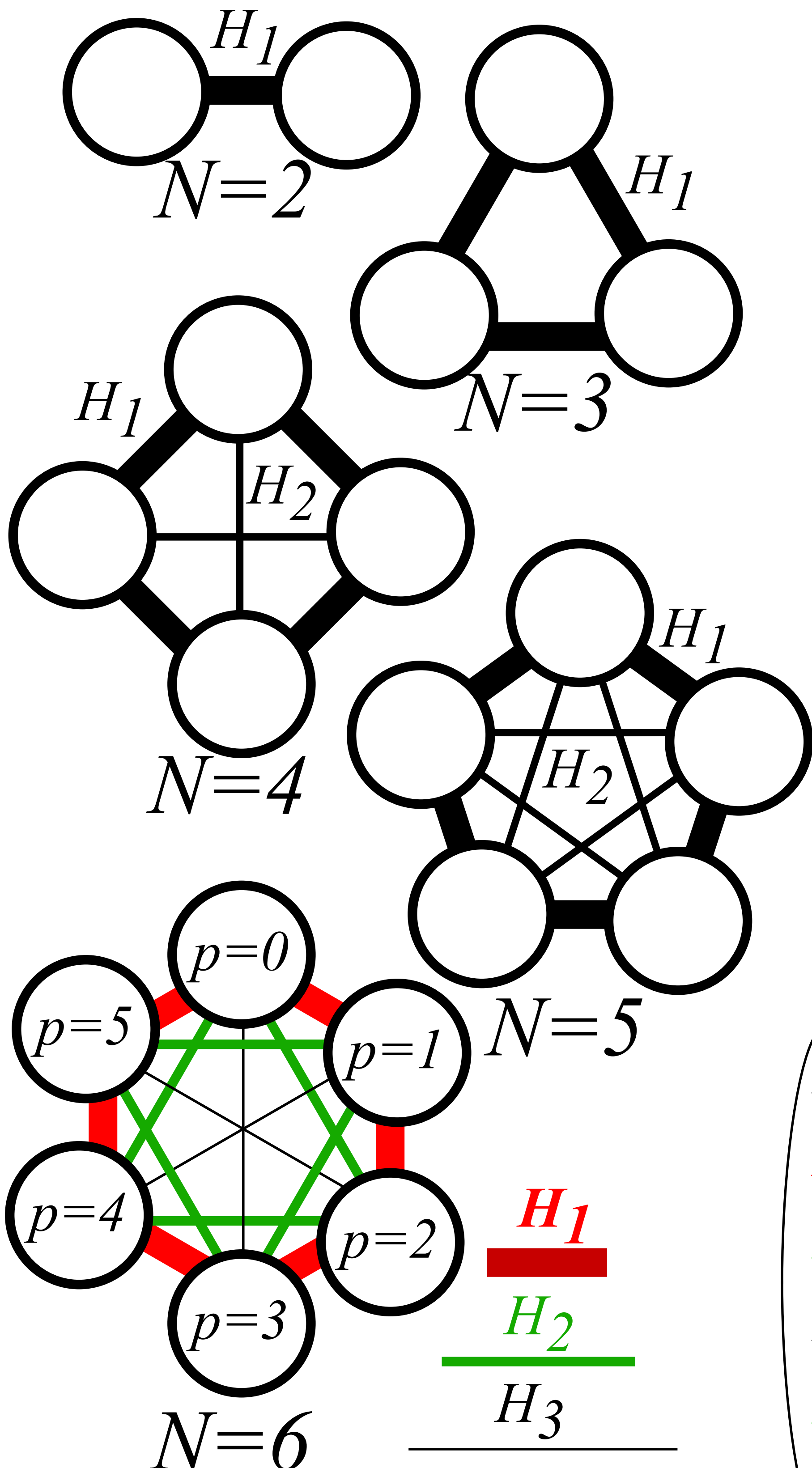
$\mathscr{G} = C_2$ = Cyclic (or Circle) group of order 2

$\mathscr{G} = C_3$ = Cyclic (or Circle) group of order 3

$\mathscr{G} = C_6$ = Cyclic (or Circle) group of order *6*

Simulating Complex Systems With Simpler Ones

Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots

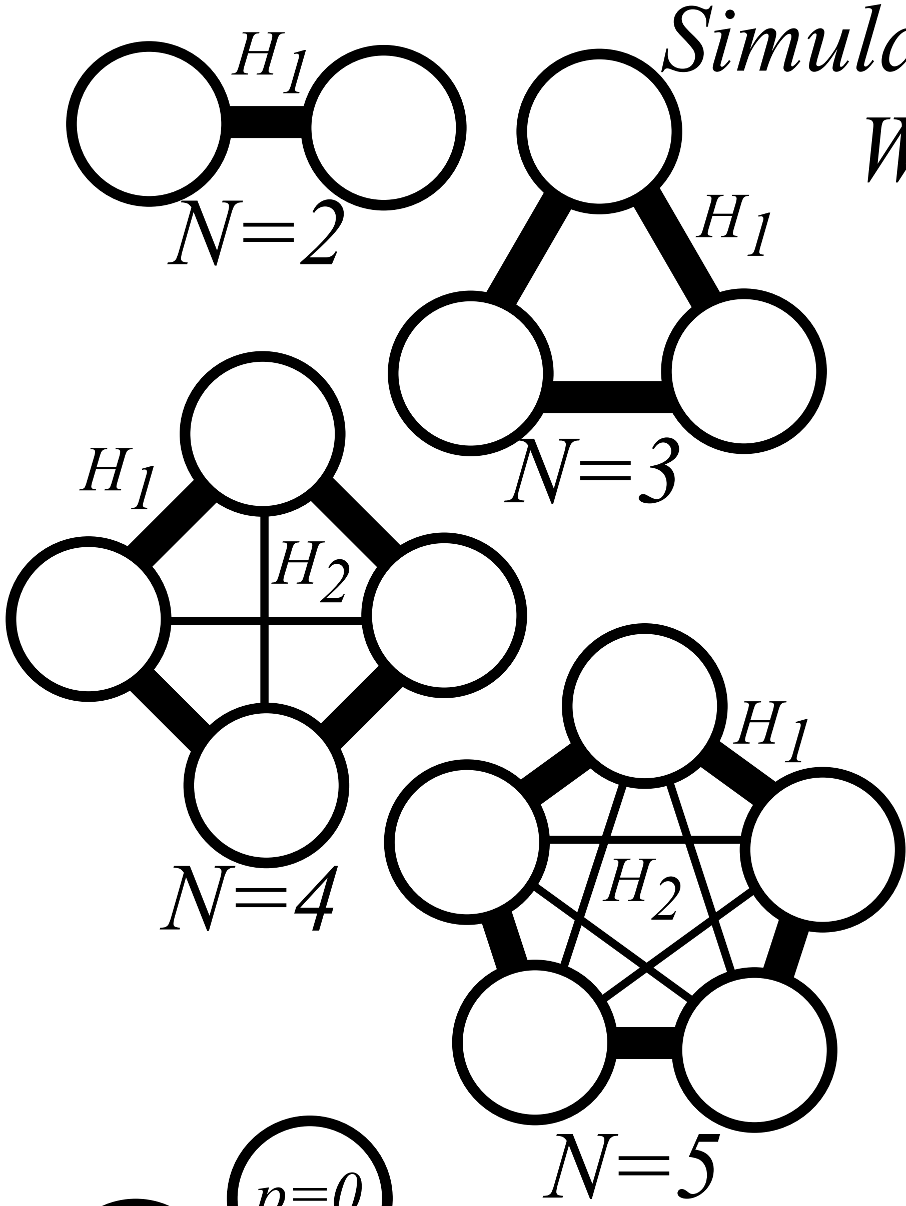


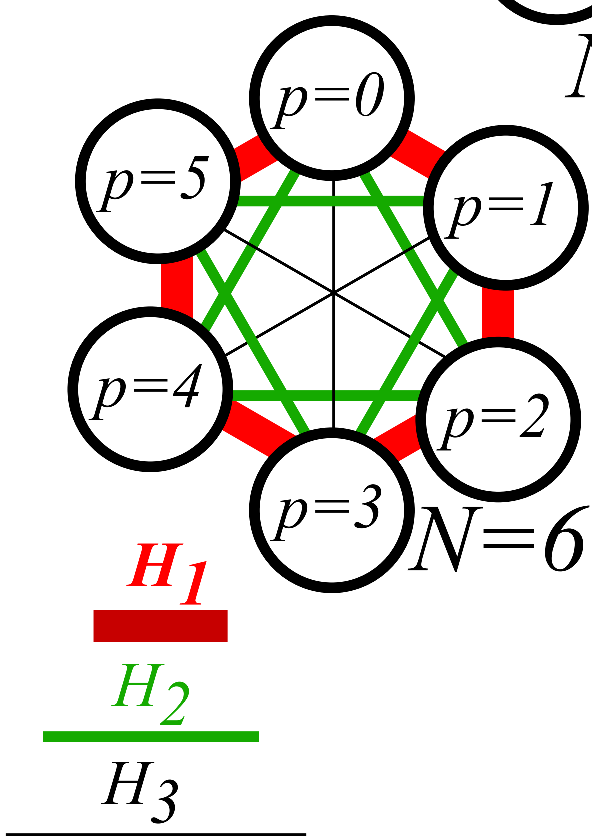
$$\begin{pmatrix} H_0 & H_1 & H_2 & H_3 & H_2 & H_1 \\ H1 & H_0 & H_1 & H_2 & H_3 & H_2 \\ H_2 & H_1 & H_0 & H_1 & H_2 & H_3 \\ H_3 & H_2 & H_1 & H_0 & H_1 & H_2 \\ H_2 & H_3 & H_2 & H_1 & H_0 & H_1 \\ H_1 & H_2 & H_3 & H_2 & H_1 & H_0 \end{pmatrix}$$

Simulating Complex Systems With Simpler Ones

Made of Quantum Dots

[Harter, J. Mol. Spec. 210, 166-182 (2001)]

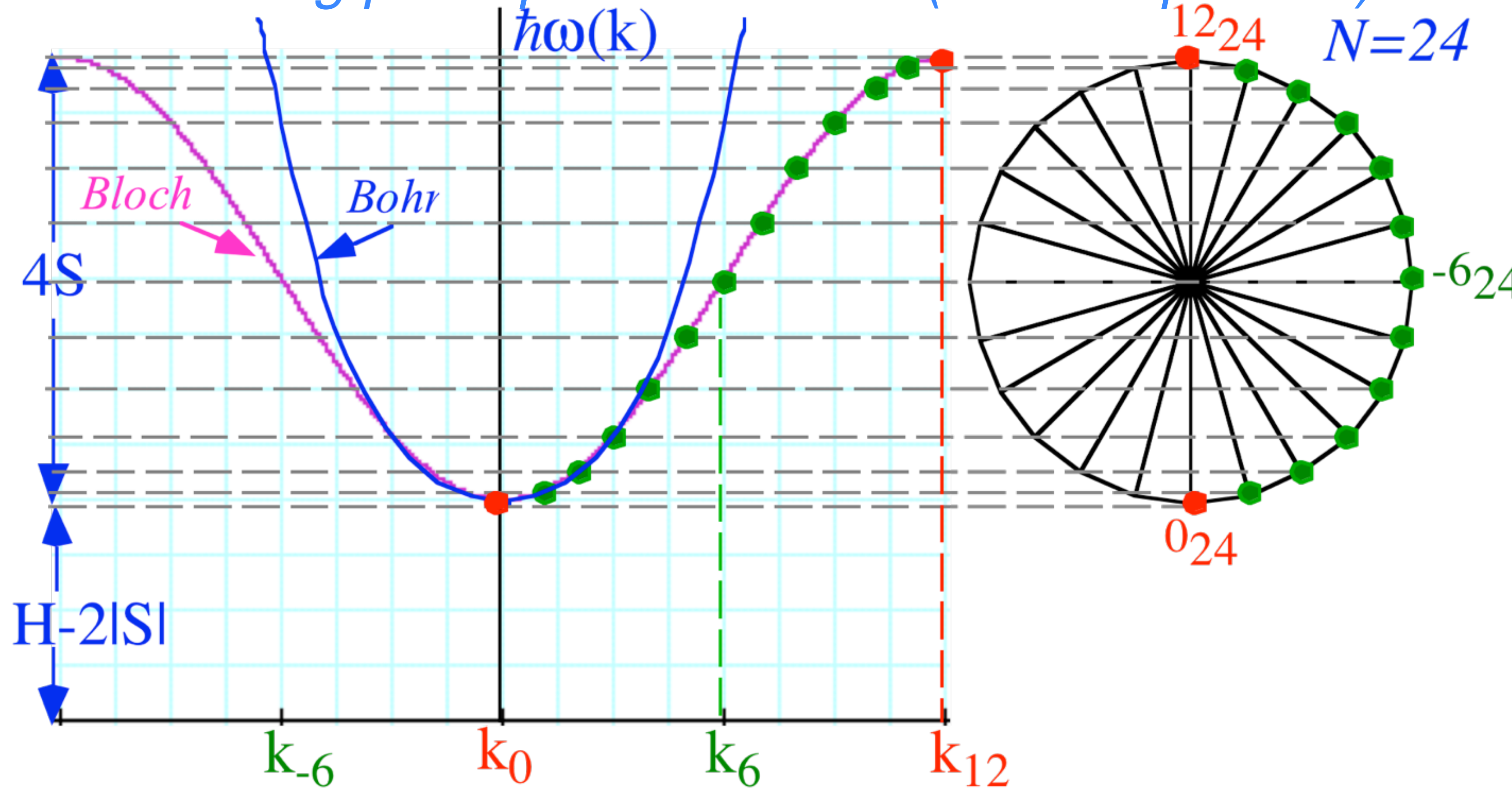




Hexagonal 2D Rotor

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

Making pure quadratic $\omega = ck^2$ (Bohr dispersion)



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Made of Quantum Dots

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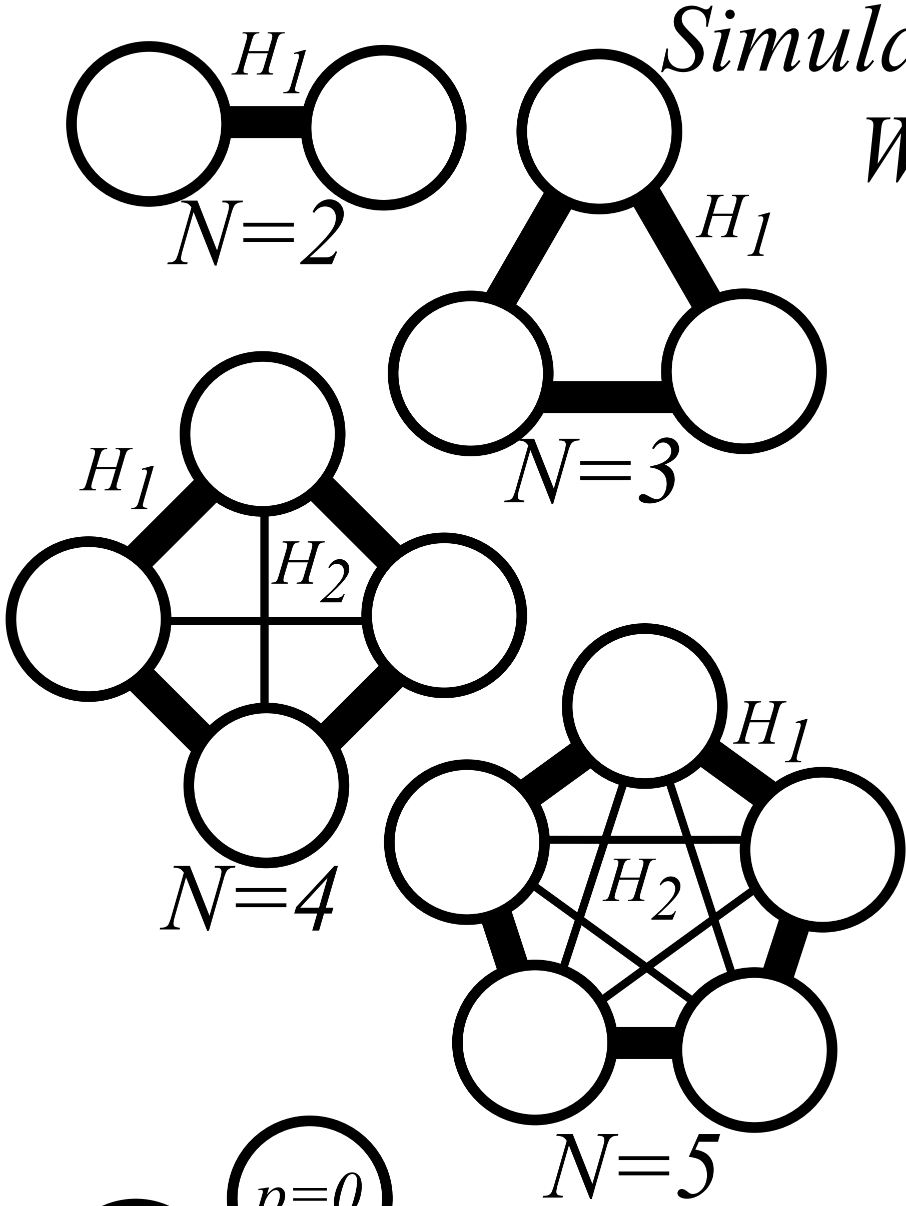
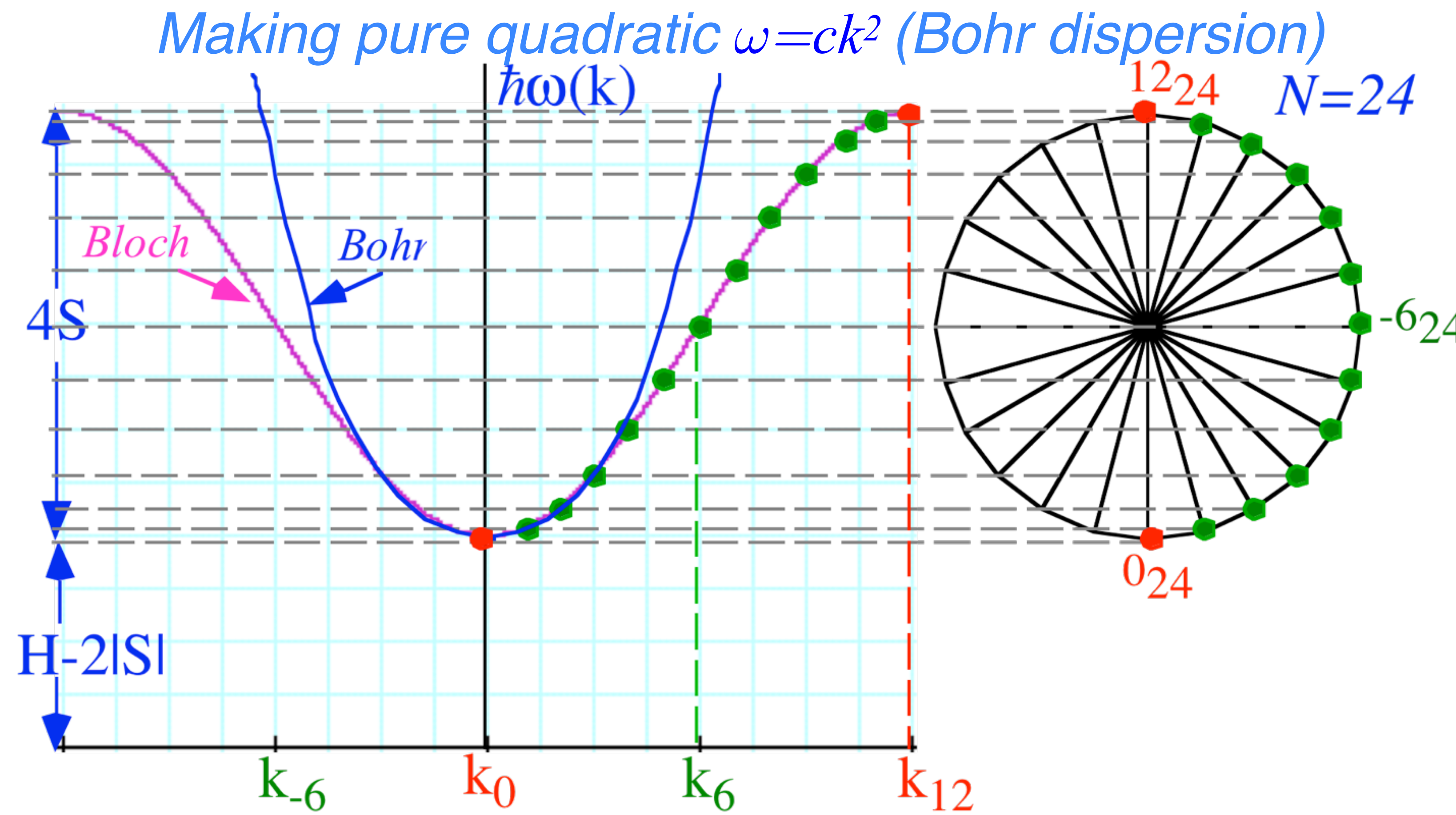
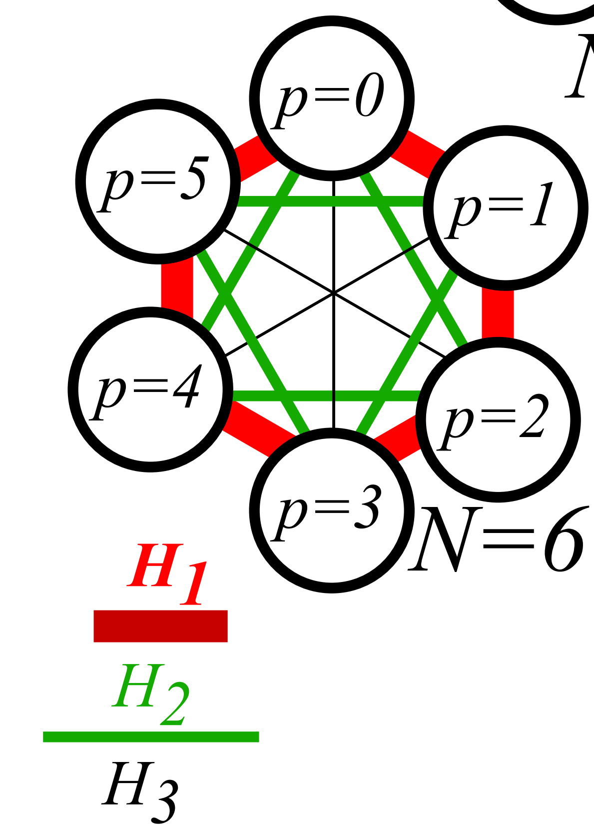




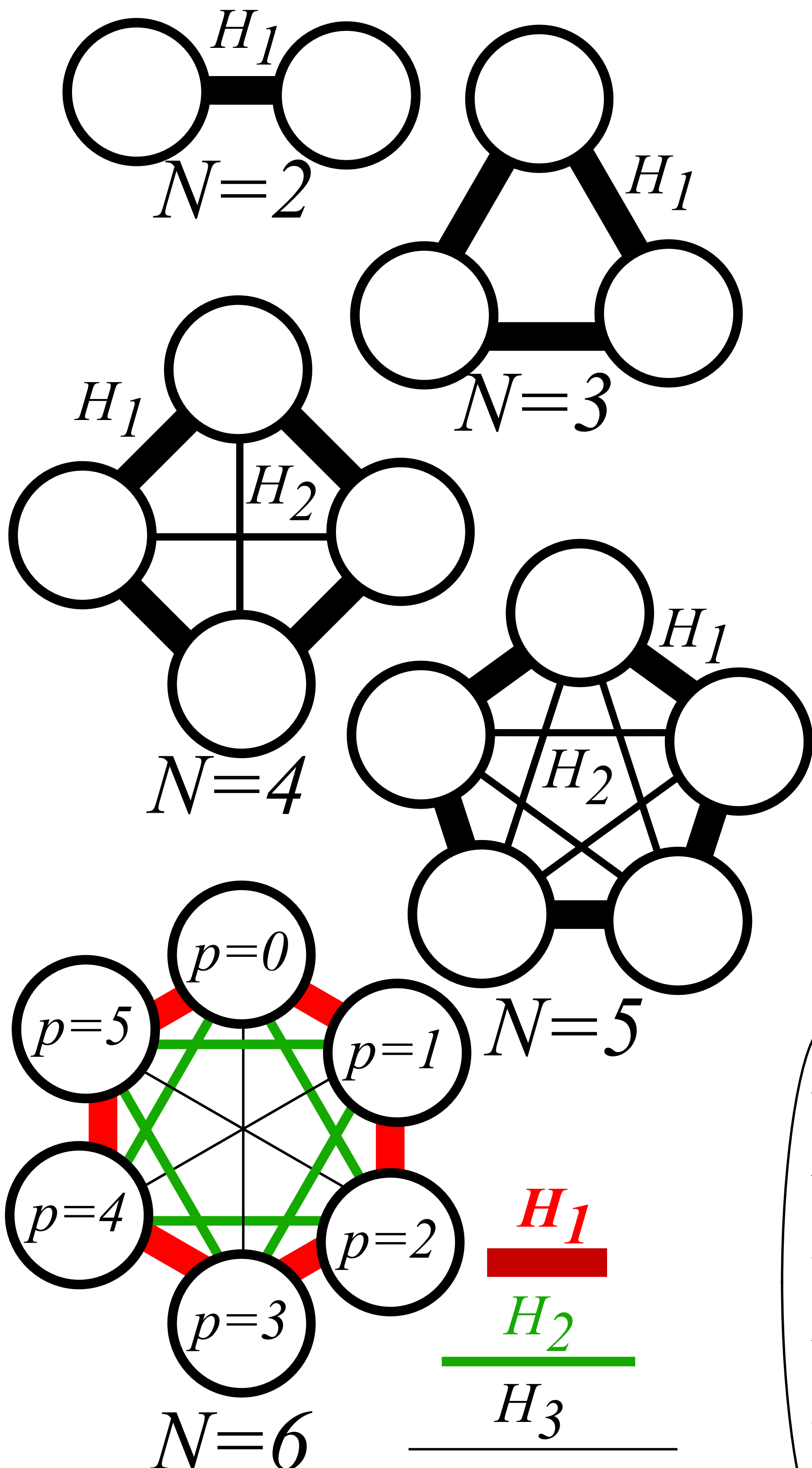


Hexagonal 2D Rotor

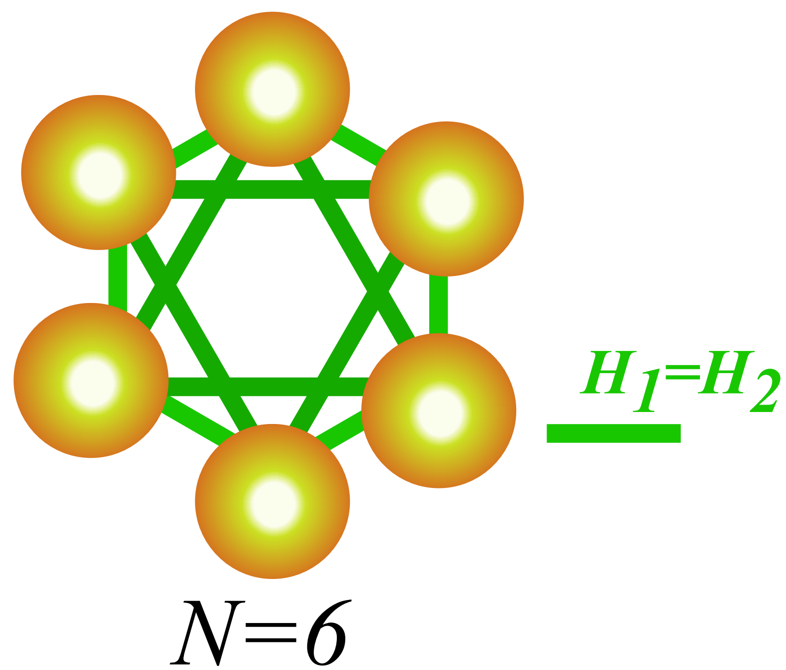
$$\begin{pmatrix} H_0 & H_1 & H_2 & H_3 & H_2 & H_1 \\ H_1 & H_0 & H_1 & H_2 & H_3 & H_2 \\ H_2 & H_1 & H_0 & H_1 & H_2 & H_3 \\ H_3 & H_2 & H_1 & H_0 & H_1 & H_2 \\ H_2 & H_3 & H_2 & H_1 & H_0 & H_1 \\ H_1 & H_2 & H_3 & H_2 & H_1 & H_0 \end{pmatrix}$$

	H_0	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8
N=2	1/2	-1/2							
N=3	2/3	-1/3							
N=4	3/2	-1	1/2						
N=5	2	-1.1708	0.1708						
N=6	19/6	-2	2/3	-1/2					
N=7	4	-2.393	0.51	-0.1171					
N=8	11/2	-3.4142	1	-0.5858	1/2				
N=9	20/3	-4.0165	0.9270	-1/3	0.0895				
N=10	17/2	-5.2361	1.4472	-0.7639	0.5528	-1/2			
N=11	10	-6.0442	1.4391	-0.5733	0.2510	-0.0726			
N=12	73/6	-7.4641	2	-1	2/3	-0.5359	1/2		
N=13	14	-8.4766	2.0500	-0.8511	0.4194	-0.2028	0.06116		
N=14	33/2	-10.098	2.6560	-1.2862	0.8180	-0.6160	0.5260	-1/2	
N=15	57/3	-11.314	2.7611	-1.1708	0.6058	-1/3	0.1708	-0.0528	
N=16	43/2	-13.137	3.4142	-1.6199	1	-0.7232	0.5858	-0.5198	1/2
N=17	24	-14.557	3.5728	-1.5340	0.81413	-0.4732	0.2781	-0.1479	0.0465

Simulating Complex Systems With Simpler Ones



Discrete Rotor Waves
Bohr-Rotors Made of Quantum Dots



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

Hexagonal becomes Octahedral

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