Group Theory in Quantum Mechanics

Lecture 14 *(3.02.17)*

C_N symmetry systems coupled, uncoupled, and re-coupled

(Geometry of U(2) characters - Ch. 6-12 of Unit 3)
(Principles of Symmetry, Dynamics, and Spectroscopy - Sec. 1-12 of Ch. 2)

Bohr-rotor wave dynamics and group vs. phase velocity
- *Gaussian wave-packet bandwidth and uncertainty*
  - *Gaussian Bohr-rotor revivals and quantum fractals*

Understanding quantum fractals using geometry of fractions (Rationalizing rationals)
- *Farey-Sums and Ford-products*
- *Discrete C_N beat phase dynamics (Characters gone wild!)*
- *The classical bouncing-ball Monster-Mash*

Breaking C_N cyclic coupling into linear chains
- *Breaking C_{2N+2} to approximate linear N-chain*
  - *Band-It simulation: Intro to scattering approach to quantum symmetry*

Breaking C_{2N} cyclic coupling down to C_N symmetry
- *Acoustical modes vs. Optical modes*
- *Intro to other examples of band theory*
- *Type-AB avoided crossing view of band-gaps*

[John Farey, Phil. Mag.(1816) Wolfram]

[Lester Ford, Am. Math. Mnthly 45,586(1938)]

Quantum Revivals of
Morse Oscillators and
Farey-Ford Geometry

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

[*Harter, Li, ArXiv, (2013)*]

[Harter, Li, UAF, (2013)]

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Review of 1D-Bohr-ring related to infinite square well (and review of revival)

∞-Square well paths analyzed using Bohr rotor paths

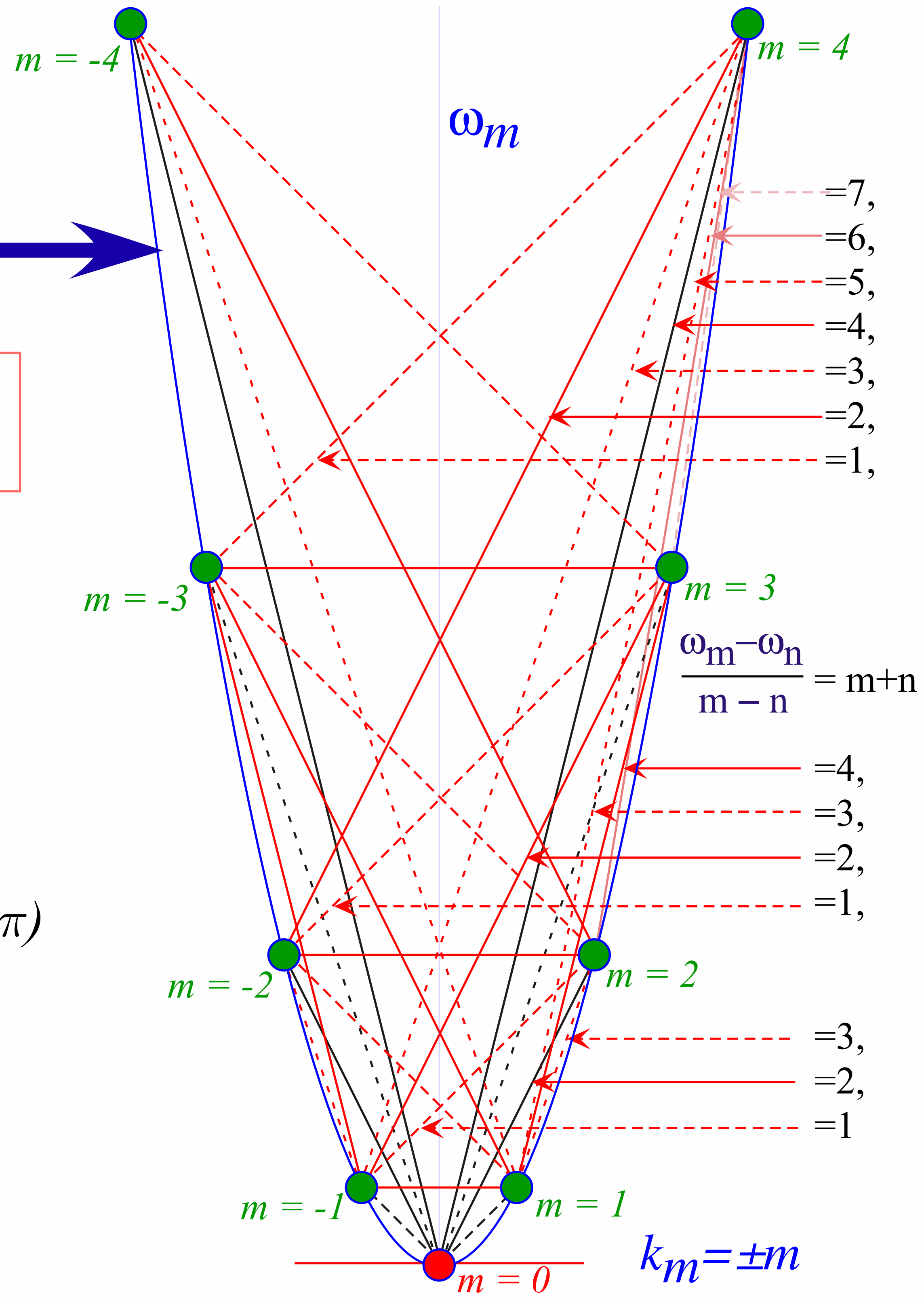
Breaking C_{2N+2} to approximate linear N-chain

Band-It simulation: Intro to scattering approach to quantum symmetry

Possible wave velocities for Quadratic (Bohr-Rotor) Spectrum

$$\omega_m = Bm^2$$

$$k_m = \pm m$$



$$V_{phase} = \frac{\omega_m}{k_m} = \frac{Bm^2}{m} = mB$$

$$V_{group} = \frac{\omega_m - \omega_n}{k_m - k_n} = \frac{m^2 - n^2}{m \pm n} B = (m \pm n)B$$

Note: V_{group} usually faster than V_{phase}
(That happens if we ignore Mc^2 !)

$m = 0, \pm 1, \pm 2, \pm 3, \ldots$ are momentum quanta
in wavevector formula: $k_m = 2\pi m / L \quad (k_m = m \quad if{:}\ L = 2\pi)$

$$E_m = (\hbar k_m)^2/2M = m^2[h^2/2ML^2] = m^2 h\upsilon_1 = m^2 \hbar\omega_1$$

fundamental Bohr ∠−frequency $\omega_1 = 2\pi\upsilon_1$
and lowest *transition (beat) frequency* $\upsilon_1 = (E_1 - E_0)/h$

Possible wave velocities for Quadratic (Bohr-Rotor) Spectrum

$\omega_m = Bm^2$

$k_m = \pm m$

$$V_{phase} = \frac{\omega_m}{k_m} = \frac{Bm^2}{m} = mB$$

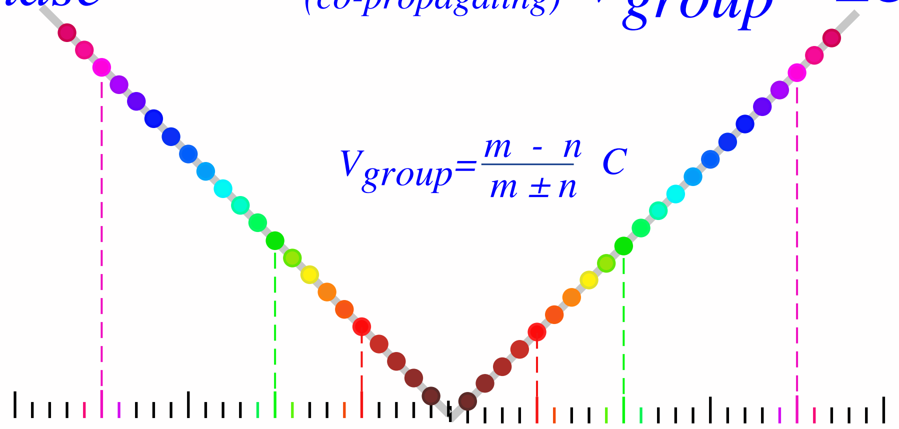
$$V_{group} = \frac{\omega_m - \omega_n}{k_m - k_n} = \frac{m^2 - n^2}{m \pm n} B = (m \pm n)B$$

Possible wave velocities for Linear (Optical) Spectrum

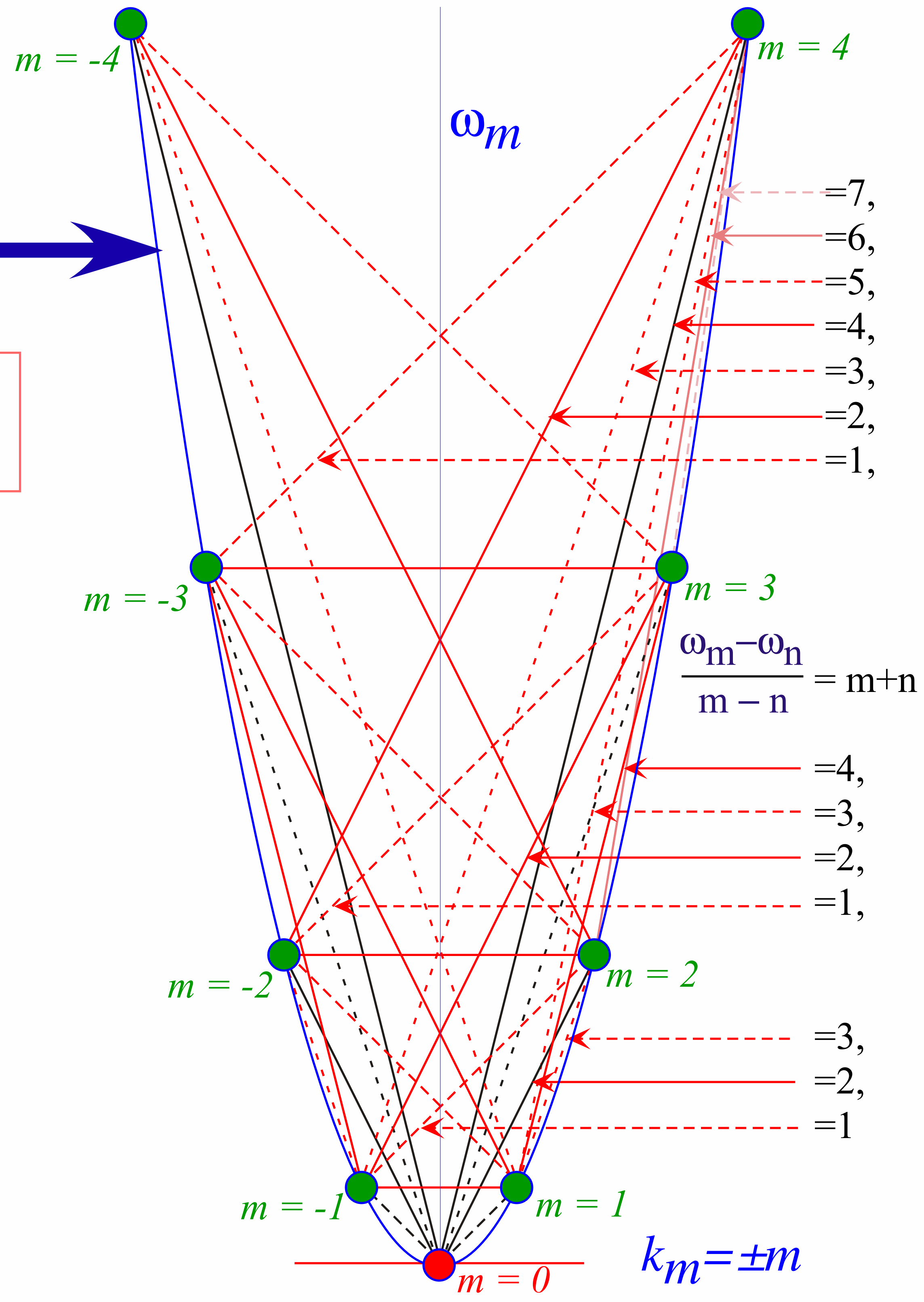
$\omega_m = C|m|^1$

$k_m = m$

$V_{phase} = \pm C$ (co-propagating) $V_{group} = \pm C$

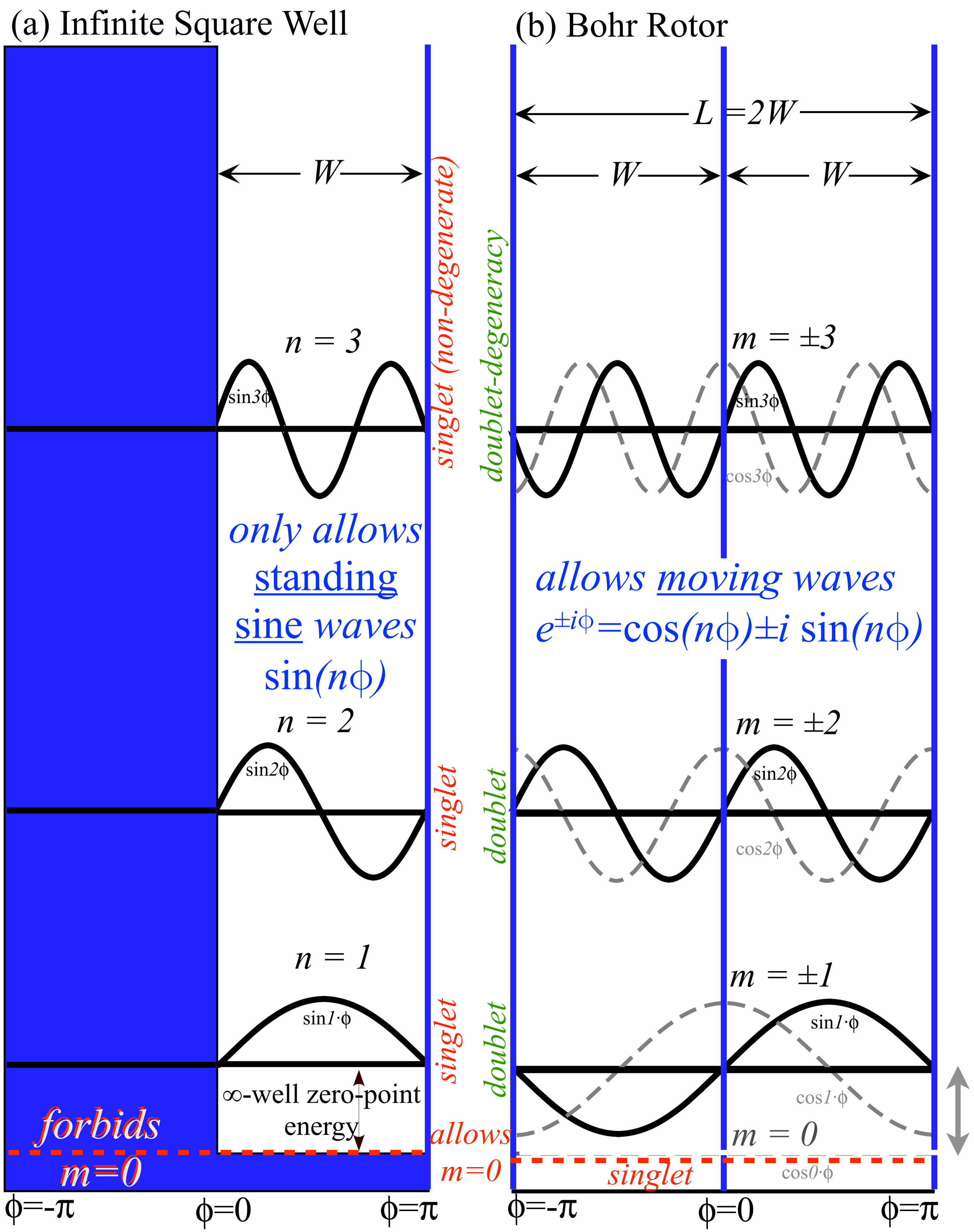


$$V_{group} = \frac{m - n}{m \pm n} C$$



$$\frac{\omega_m - \omega_n}{m - n} = m+n$$

Review: ∞-*Square well PE & Bohr rotor*



only allows standing sine *waves* sin*(nϕ)*

allows moving waves
$e^{\pm i\phi}=\cos(n\phi)\pm i\sin(n\phi)$

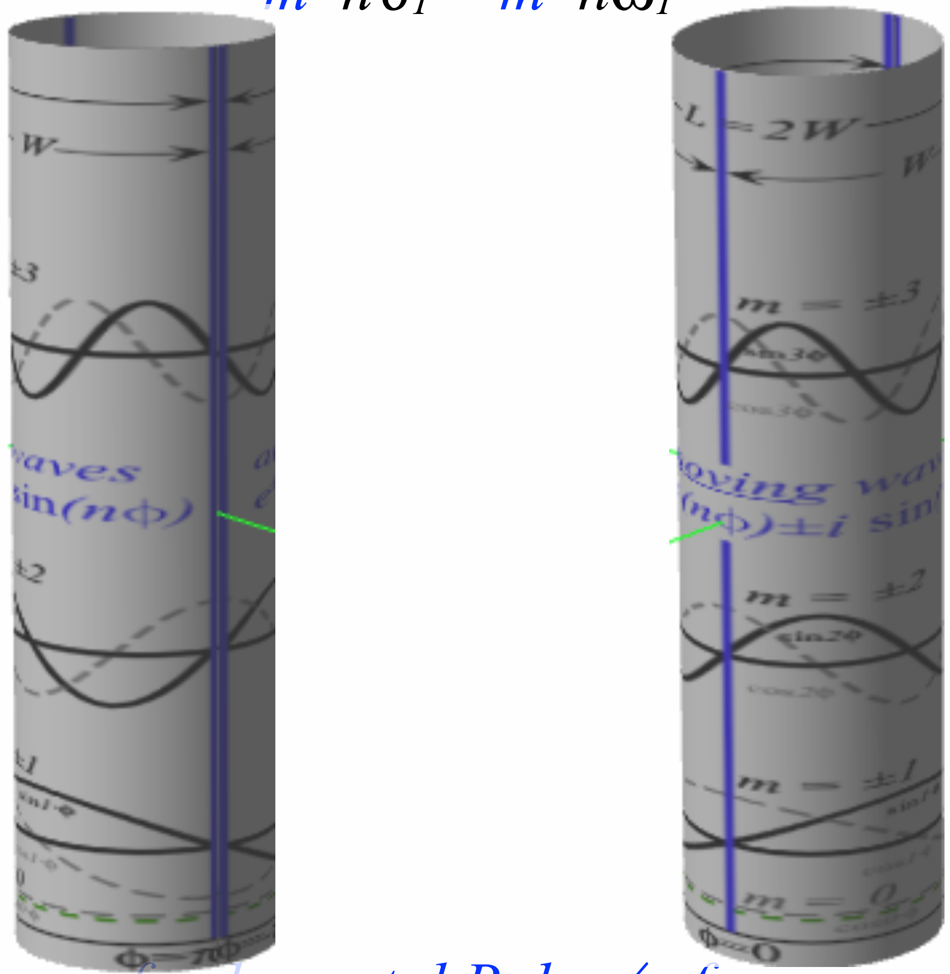
Fig. 12.2.6 Comparison of eigensolutions for (a) Infinite square well, and (b) Bohr rotor.

From QTCA Unit 5 Ch. 12

$m=0, \pm 1, \pm 2, \pm 3$,...are momentum quanta in wavevector formula: $k_m=2\pi m/L$

$(k_m=m \quad \text{if: } L=2\pi)$

$$E_m=(\hbar k_m)^2/2M = m^2[h^2/2ML^2]$$
$$= m^2\, h\upsilon_1 = m^2\, \hbar\omega_1$$



fundamental Bohr ∠*−frequency*

$\omega_1=2\pi\upsilon_1$

lowest *transition (beat) frequency*

$\upsilon_1=(E_1-E_0)/h$ (E_0 is defined as zero)

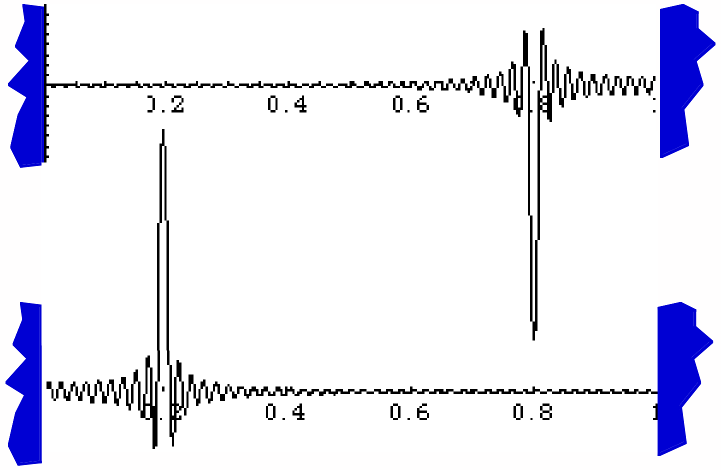
Review: ∞-Square well PE paths analyzed using Bohr rotor paths

$t = 0.5000\tau_1$

$= 1.5\tau_{beat}$

$t = 1.0000\tau_1$

$= 3.0\tau_{beat}$

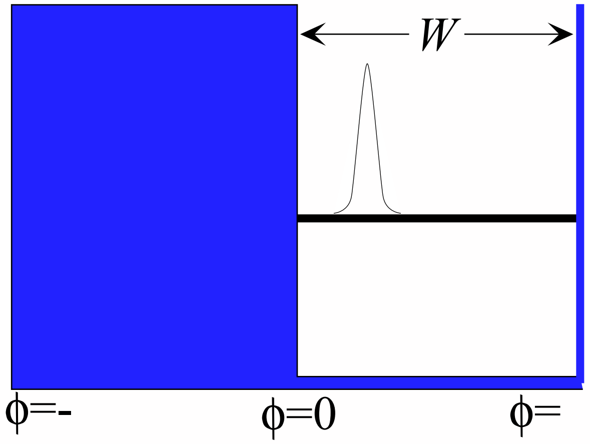


After only 50 round-trips *M*'s wave does a *partial revival* as it makes an upside down-delta function around *x=0.8W*.

1.
All ∞-well peak must be made of sine wave components.

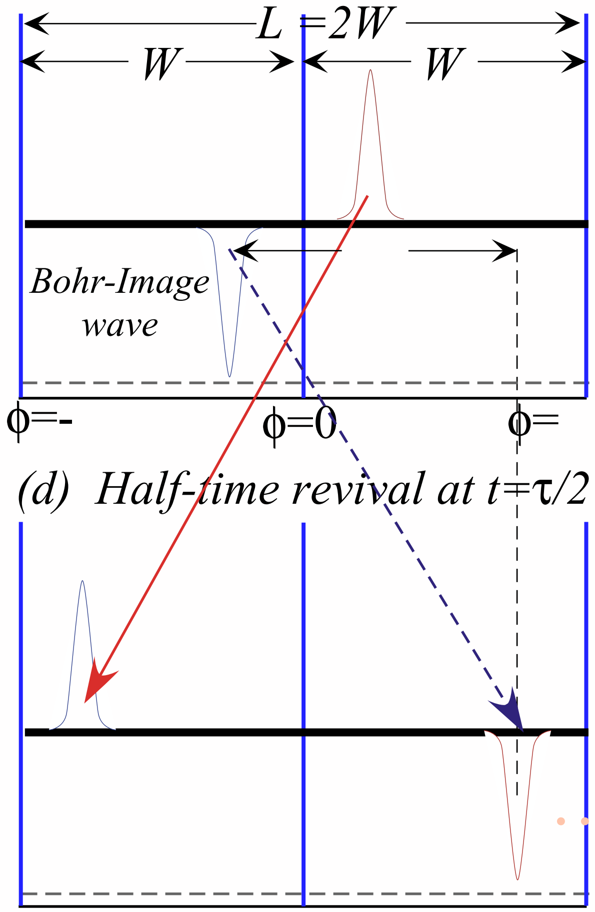
2. Bohr rotor peak made of *sine* wave components is *anti*-symmetric, so an *upside-down mirror* image peak must accompany any peak.

(a) Infinite Square Well at t=0

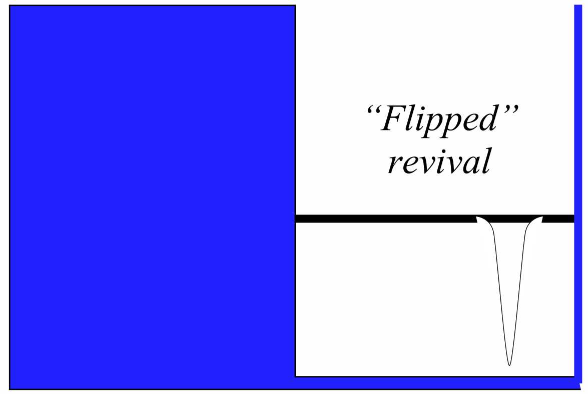


(b) Bohr Rotor at t=0

(d) Half-time revival at t=τ/2



(c) Half-time revival at t=τ/2



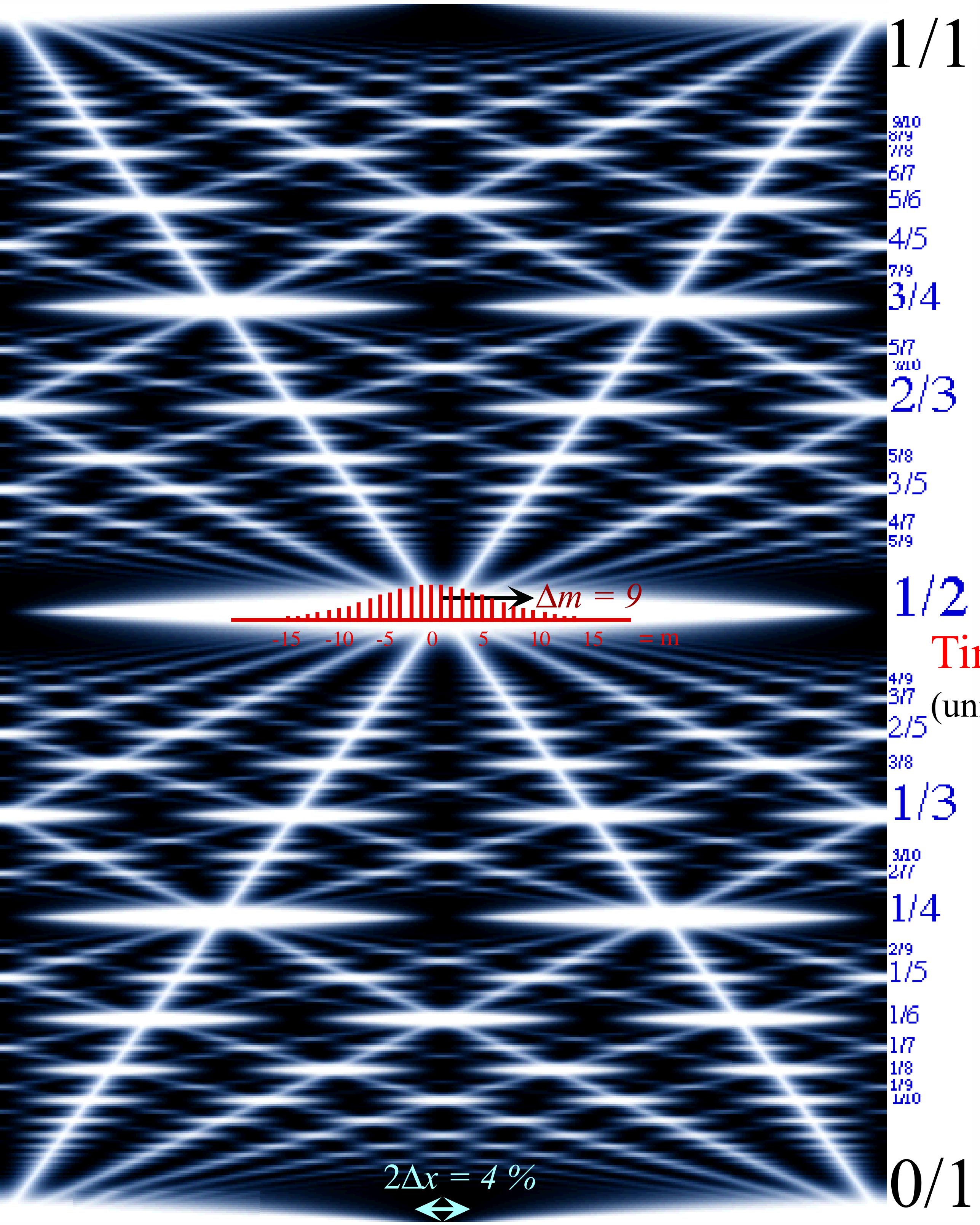
3. So how is the ∞-well "flipped revival explained?

4. Bohr rotor half-time revival is *same*-side-up copy of initial peak on *opposite* side of ring. So that upside-down Bohr-image will appear upside-down on the other side at half-time revival.

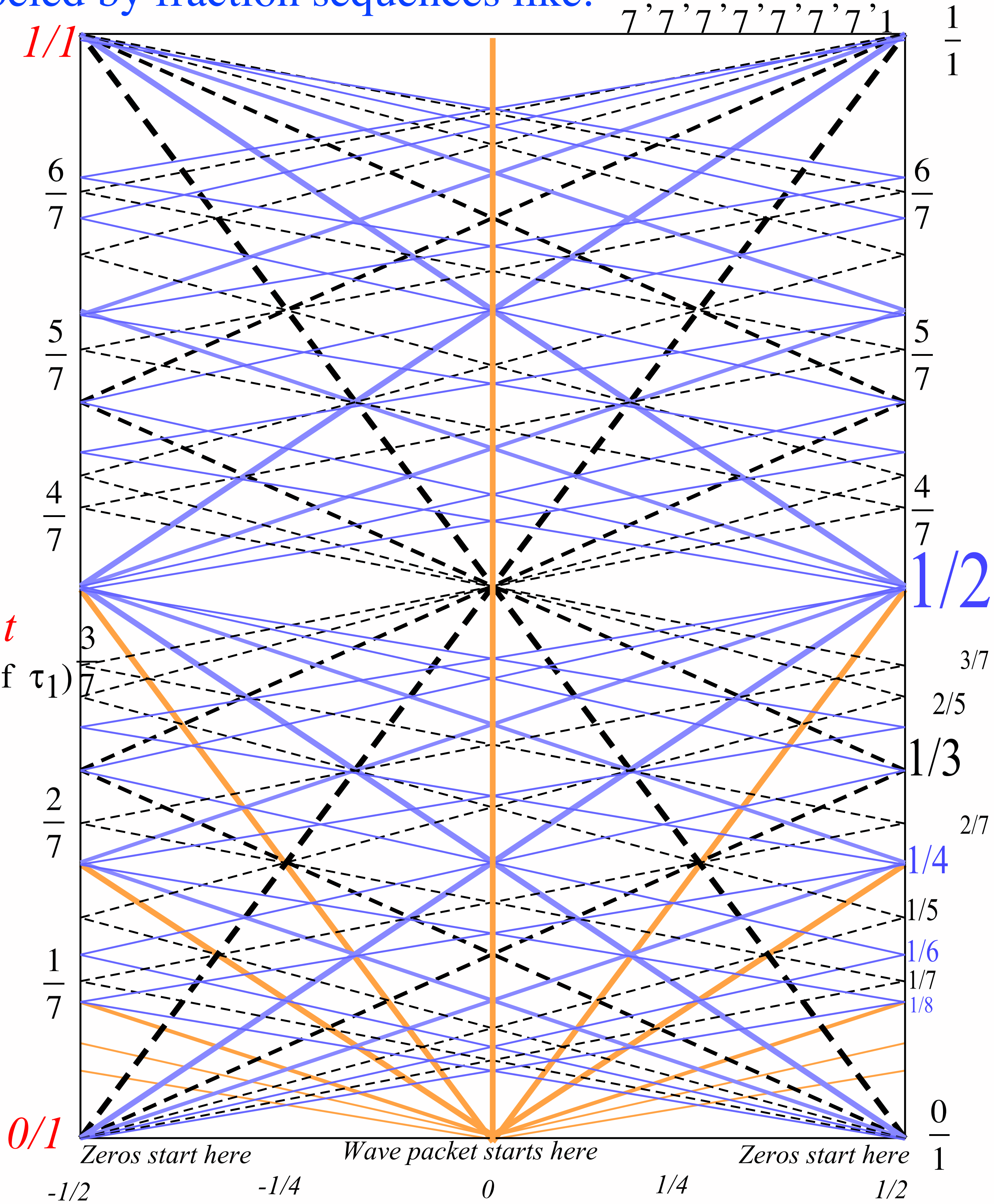
Review: ∞-Square well PE paths analyzed using Bohr rotor paths

(9 or10-levels (0, ±1, ±2, ±3, ±4,..., ±9, ±10, ±11...) excited)

Zeros (clearly) and "particle-packets" (faintly) have paths labeled by fraction sequences like: $\frac{0}{7},\frac{1}{7},\frac{2}{7},\frac{3}{7},\frac{4}{7},\frac{5}{7},\frac{6}{7},\frac{1}{1}$



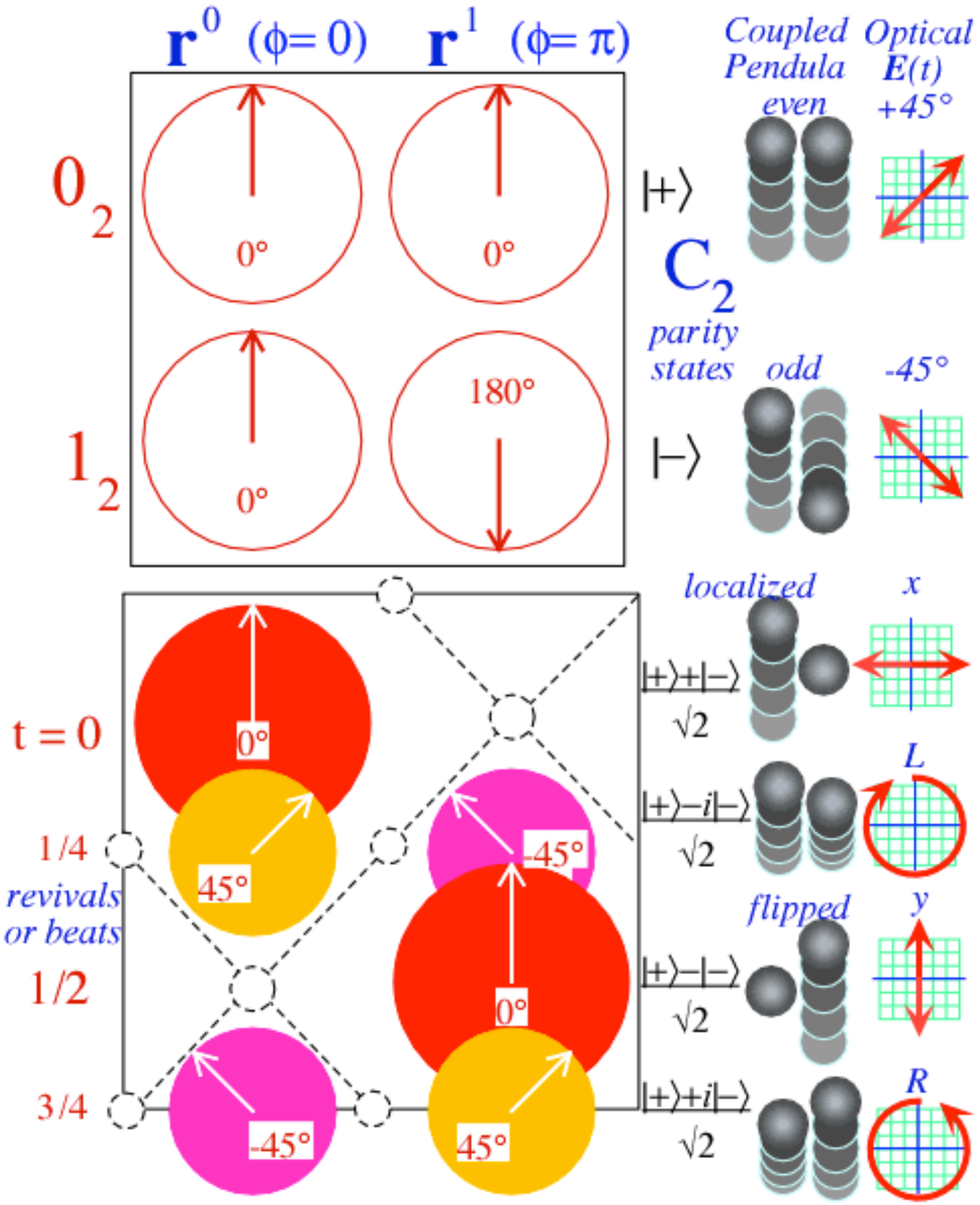
Time t
(units of τ_1)



Coordinate ϕ
(units of 2π)

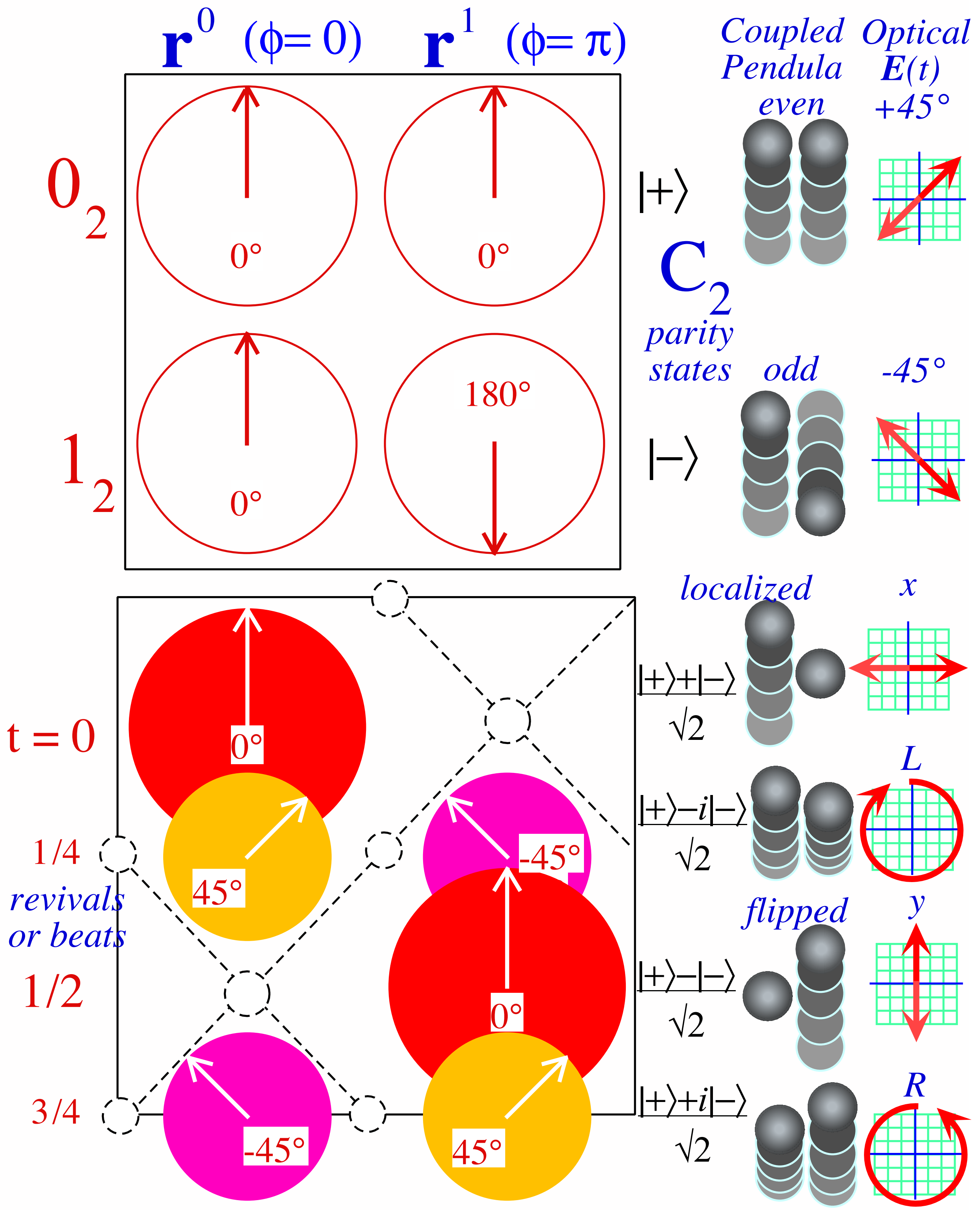
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry
[Harter, Li, UAF, (2013)]

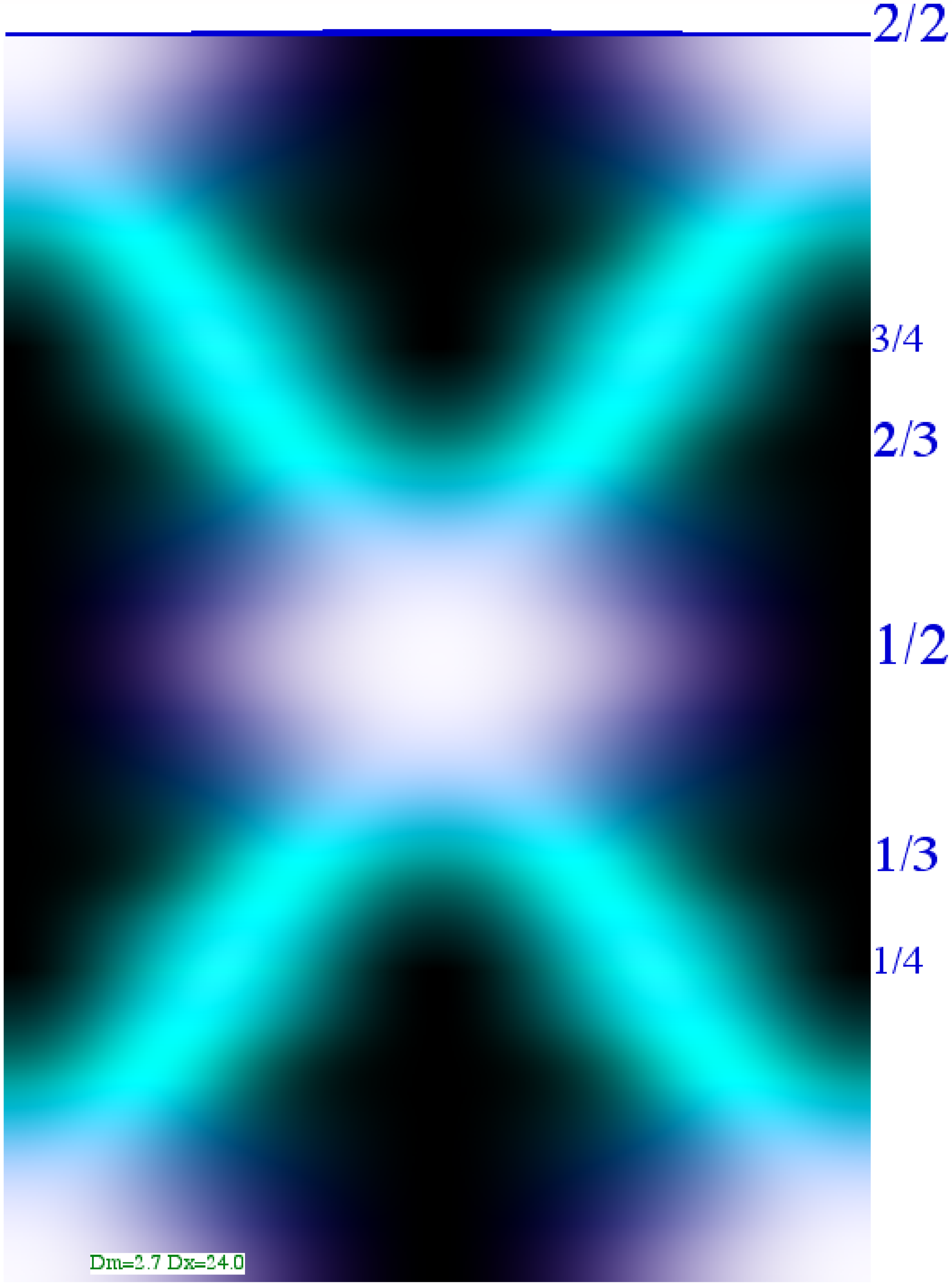
C_2
Fourier transformation matrix
and
dynamics

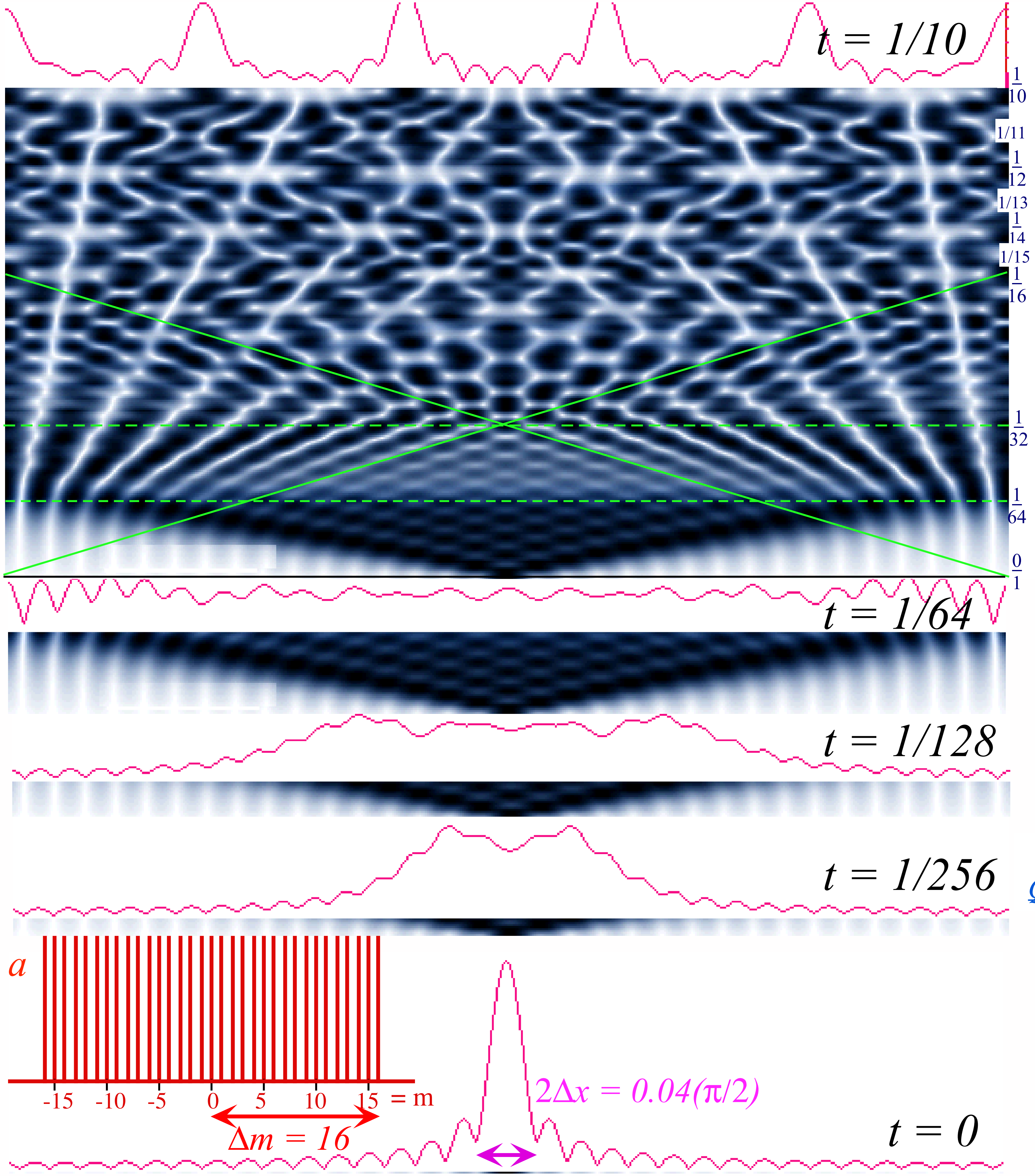


Quantum Revivals of Morse Oscillators and Farey-Ford Geometry
[Harter, Li, UAF, (2013)]

Fundamental Beats and 2-Level Transitions: The "Mother of all symmetry" is C_2



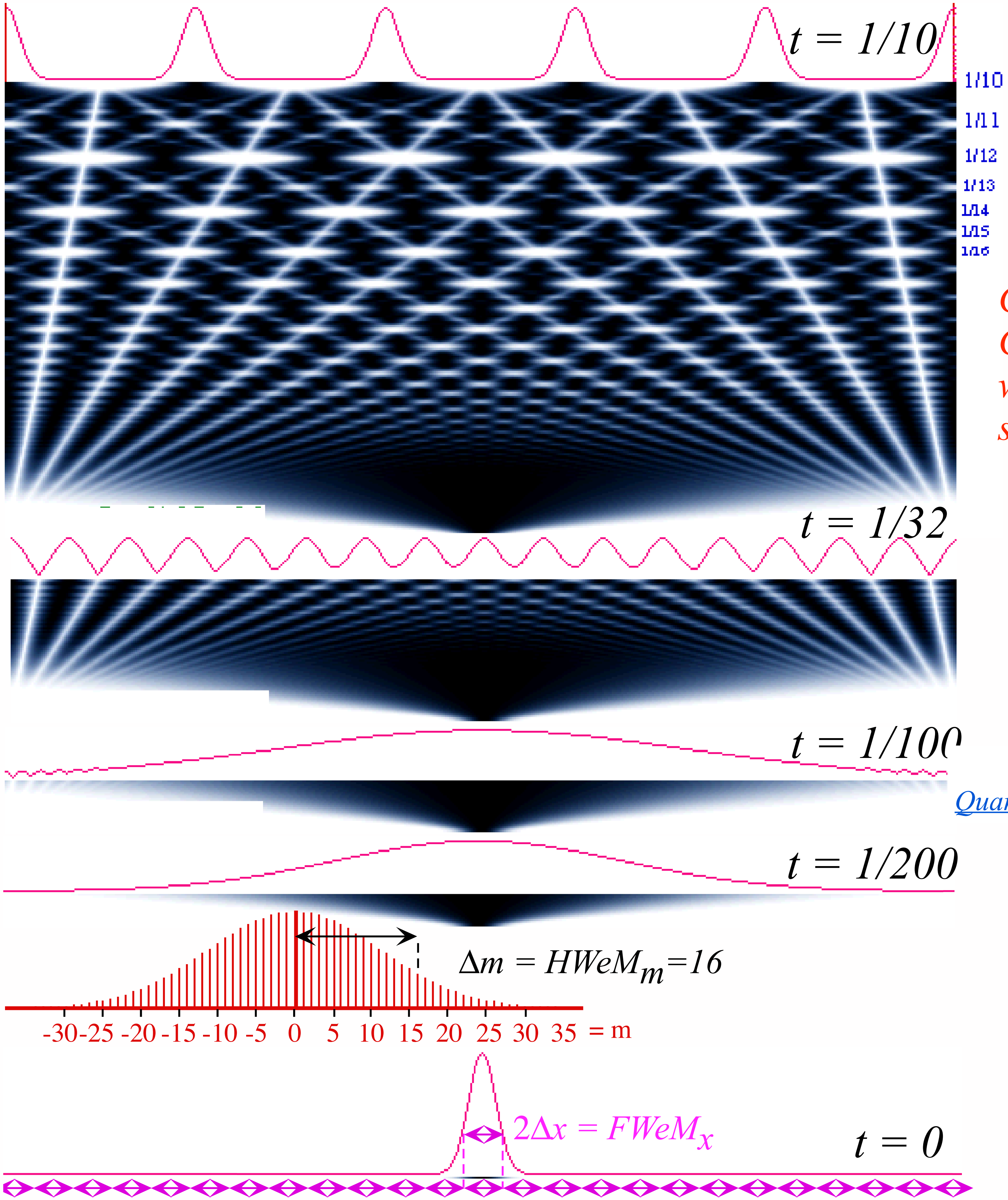




(sinNx)/x has a
"boxcar spectrum"
with very complicated
space-time revival paths

Known as a
"boxcar"
spectrum

WaveIt Web Simulation
Quantum Carpet Boxcar distribution



Gaussian wave has a Gaussian spectrum with comparatively simple space-time revival paths

(Gaussian wave properties are derived in several pages below…)

WaveIt Web Simulation
Quantum Carpet Gaussian distribution

WaveIt Web Simulation
1 PW Gaussian distribution
w/ Linear Dispersion

WaveIt Web Simulation
Gaussian distribution
w/ component waves

[Harter, Li, UAF, (2013)]

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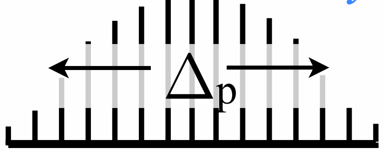
Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p *be momentum-**m** "spread" or uncertainty*



Suppose we excite a Gaussian combination of Bohr momentum-*m* plane waves:

$$\Psi(\phi,t{=}0)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2} e^{im\phi}$$

Gaussian wave-packet bandwidth and uncertainty

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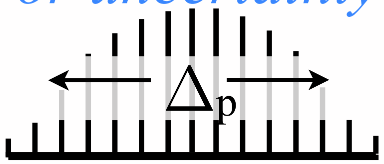

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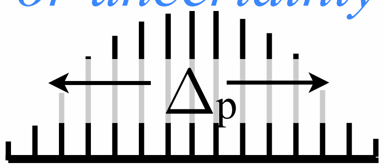
Complete the square in exponent to simplify ϕ*-angle wavefunction.*

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p be momentum-m "spread" or uncertainty



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$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_\mathrm{p}}\right)^2+im\phi+\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}$$

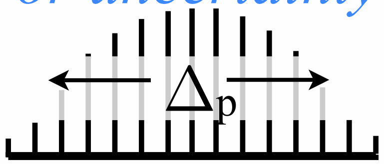
Complete the square in exponent to simplify ϕ-angle wavefunction.

Add and subtract : $\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2$

in exponent…

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_{p} *be momentum-**m** "spread" or uncertainty*



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$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}\right)^2+im\phi+\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2} \quad e^{-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ*-angle wavefunction.*

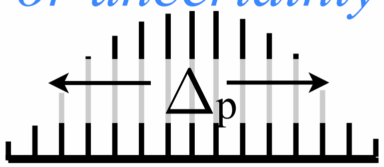
Add and subtract : $\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2$

in exponent…

Extract binomial : $-\left(\frac{m}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2$

Gaussian wave-packet bandwidth and uncertainty

*Let constant Δ_p be momentum-**m** "spread" or uncertainty*



Suppose we excite a Gaussian combination of Bohr momentum-*m* plane waves:

$$\Psi(\phi,t{=}0)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2}e^{im\phi}=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2+im\phi}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2+im\phi+\left(\frac{\Delta_p}{2}\phi\right)^2-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Add and subtract : $\left(\frac{\Delta_p}{2}\phi\right)^2 - \left(\frac{\Delta_p}{2}\phi\right)^2$

in exponent…

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}\quad e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Extract binomial : $-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2$

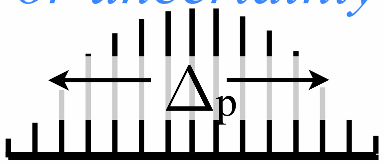
$$=\qquad\frac{A\left(\Delta_p,\phi\right)}{2\pi}\qquad e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

where:

$$A\left(\Delta_p,\phi\right)=\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}$$

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p be momentum-m "spread" or uncertainty



Suppose we excite a Gaussian combination of Bohr momentum-*m* plane waves:

$$\Psi(\phi,t{=}0) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2} e^{im\phi} = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2 + im\phi}$$

$$= \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2 + im\phi + \left(\frac{\Delta_p}{2}\phi\right)^2 - \left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$= \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2} \quad e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$= \frac{A\left(\Delta_p,\phi\right)}{2\pi} \quad e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

Add and subtract : $\left(\frac{\Delta_p}{2}\phi\right)^2 - \left(\frac{\Delta_p}{2}\phi\right)^2$

in exponent…

Extract binomial : $-\left(\frac{m}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2$

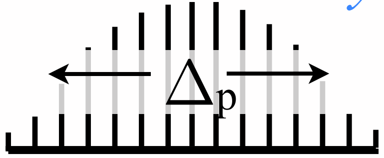
where:

$$A\left(\Delta_p,\phi\right) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2} \xrightarrow[\Delta_p >> 1]{} \int_{-\infty}^{\infty} dk \; e^{-\left(\frac{k}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2}$$

*m=0, ±1, ±2, ±3,…*are momentum quanta in wavevector formula: $k_m = 2\pi m/L$ ($k_m = m$ *if:* $L = 2\pi$)

Gaussian wave-packet bandwidth and uncertainty

*Let constant Δ_p be momentum-**m** "spread" or uncertainty*



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$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_\mathrm{p}}\right)^2+im\phi+\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_\mathrm{p}}-i\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}\quad e^{-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}$$

$$=\frac{A\left(\Delta_\mathrm{p},\phi\right)}{2\pi}\quad e^{-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

Add and subtract : $\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2-\left(\frac{\Delta_\mathrm{p}}{2}\phi\right)^2$

in exponent...

Extract binomial : $-\left(\frac{m}{\Delta_\mathrm{p}}-i\frac{\Delta_\mathrm{p}}{2}\phi\right)^2$

where:

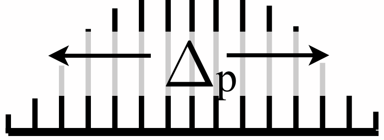
$$A\left(\Delta_\mathrm{p},\phi\right)=\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_\mathrm{p}}-i\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}\xrightarrow[\Delta_\mathrm{p}>>1]{}\int_{-\infty}^{\infty}dk\ e^{-\left(\frac{k}{\Delta_\mathrm{p}}-i\frac{\Delta_\mathrm{p}}{2}\phi\right)^2}$$

$$\left[\text{let: }K=\frac{k}{\Delta_\mathrm{p}}-i\frac{\Delta_\mathrm{p}}{2}\phi\ \text{ so: } dk=\Delta_\mathrm{p}dK\right]$$

$m=0, \pm1, \pm2, \pm3,$...are momentum quanta in wavevector formula: $k_m=2\pi m/L$ $\quad(k_m=m$ *if:* $L=2\pi)$

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_{p} be momentum-m "spread" or uncertainty



Suppose we excite a Gaussian combination of Bohr momentum-m plane waves:

$$\Psi(\phi,t{=}0)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}\right)^2}e^{im\phi}=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}\right)^2+im\phi}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}\right)^2+im\phi+\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}\quad e^{-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

$$=\frac{A\left(\Delta_{\mathrm{p}},\phi\right)}{2\pi}\quad e^{-\left(\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

Gaussian integral:

$$\int_{-\infty}^{\infty}e^{-K^2}dK=\sqrt{\int_{-\infty}^{\infty}e^{-x^2}dx}\sqrt{\int_{-\infty}^{\infty}e^{-y^2}dy}=\sqrt{\iint e^{-(x^2+y^2)}dx\,dy}$$

$$=\sqrt{\int_0^{2\pi}\int_0^{\infty}e^{-r^2}r\,dr\,d\theta}=\sqrt{2\pi\int_0^{\infty}e^{-r^2}\frac{dr^2}{2}}=\sqrt{\pi}$$

$$\text{since:}\int_0^{\infty}e^{-r^2}dr^2=1$$

where:

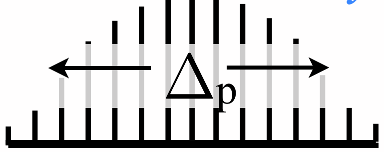
$$A\left(\Delta_{\mathrm{p}},\phi\right)=\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}\xrightarrow[\Delta_{\mathrm{p}}>>1]{}\int_{-\infty}^{\infty}dk\;e^{-\left(\frac{k}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\right)^2}$$

$$\left[\text{let: }K=\frac{k}{\Delta_{\mathrm{p}}}-i\frac{\Delta_{\mathrm{p}}}{2}\phi\quad\text{so: }dk=\Delta_{\mathrm{p}}dK\right]$$

$m=0, \pm 1, \pm 2, \pm 3,\ldots$ are momentum quanta in wavevector formula: $k_m=2\pi m/L$ ($k_m=m$ *if:* $L=2\pi$)

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p be momentum-m "spread" or uncertainty



Suppose we excite a Gaussian combination of Bohr momentum-m plane waves:

$$\Psi(\phi,t{=}0)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2}e^{im\phi}=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2+im\phi}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}\right)^2+im\phi+\left(\frac{\Delta_p}{2}\phi\right)^2-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$=\frac{A\left(\Delta_p,\phi\right)}{2\pi}e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

$$\Psi(\phi,t{=}0)=\frac{\Delta_p}{2\sqrt{\pi}}e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

It is a Gaussian distribution, too

Gaussian integral:

$$\int_{-\infty}^{\infty}e^{-K^2}dK=\sqrt{\int_{-\infty}^{\infty}e^{-x^2}dx}\sqrt{\int_{-\infty}^{\infty}e^{-y^2}dy}=\sqrt{\iint e^{-(x^2+y^2)}dx\,dy}$$

$$=\sqrt{\int_0^{2\pi}\int_0^{\infty}e^{-r^2}r\,dr\,d\theta}=\sqrt{2\pi\int_0^{\infty}e^{-r^2}\frac{dr^2}{2}}=\sqrt{\pi}$$

$$\text{since:}\int_0^{\infty}e^{-r^2}dr^2=1$$

where:

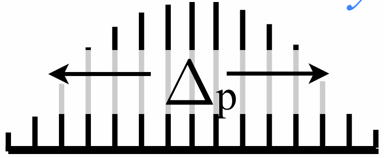
$$A\left(\Delta_p,\phi\right)=\sum_{m=-\infty}^{\infty}e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}\xrightarrow[\Delta_p>>1]{}\int_{-\infty}^{\infty}dk\,e^{-\left(\frac{k}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}$$

$$\left[\text{let: }K=\frac{k}{\Delta_p}-i\frac{\Delta_p}{2}\phi\quad\text{so: }dk=\Delta_p dK\right]\quad\text{then: }A\left(\Delta_p,\phi\right)\simeq\Delta_p\int_{-\infty}^{\infty}dK\,e^{-(K)^2}=\Delta_p\sqrt{\pi}$$

m=0, ±1, ±2, ±3,... are momentum quanta in wavevector formula: $k_m=2\pi m/L$ ($k_m=m$ *if:* $L=2\pi$)

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p be momentum-m "spread" or uncertainty



Suppose we excite a Gaussian combination of Bohr momentum-*m* plane waves:

$$\Psi(\phi,t{=}0)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2} e^{im\phi}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2+im\phi+\left(\frac{\Delta_p}{2}\phi\right)^2-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2} e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$=\frac{A\left(\Delta_p,\phi\right)}{2\pi} e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

$$\Psi(\phi,t{=}0)=\frac{\Delta_p}{2\sqrt{\pi}} e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

It is a Gaussian distribution, too

$$\Psi(\phi,t{=}0)\simeq\frac{\Delta_p}{2\sqrt{\pi}} e^{-\left(\frac{\phi}{\Delta_\phi}\right)^2}$$

where: $\Delta_\phi=\frac{2}{\Delta_p}$ or: $\Delta_\phi\Delta_p=2$

where:

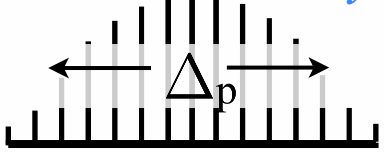
$$A\left(\Delta_p,\phi\right)=\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2} \xrightarrow[\Delta_p>>1]{} \int_{-\infty}^{\infty} dk\, e^{-\left(\frac{k}{\Delta_p}-i\frac{\Delta_p}{2}\phi\right)^2}$$

$\left[\text{let: } K=\frac{k}{\Delta_p}-i\frac{\Delta_p}{2}\phi \quad \text{so: } dk=\Delta_p dK\right]$ then: $A\left(\Delta_p,\phi\right)\simeq\Delta_p\int_{-\infty}^{\infty} dK\, e^{-(K)^2}=\Delta_p\sqrt{\pi}$

m=0, ±1, ±2, ±3,...are momentum quanta in wavevector formula: $k_m=2\pi m/L$ ($k_m=m$ *if:* $L=2\pi$)

Gaussian wave-packet bandwidth and uncertainty

Let constant Δ_p *be momentum-m "spread" or uncertainty*



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$$\Psi(\phi,t=0) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2} e^{im\phi}$$

$$= \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p}\right)^2 + im\phi + \left(\frac{\Delta_p}{2}\phi\right)^2 - \left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$= \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2} e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

$$= \frac{A\left(\Delta_p,\phi\right)}{2\pi} e^{-\left(\frac{\Delta_p}{2}\phi\right)^2}$$

Complete the square in exponent to simplify ϕ-angle wavefunction.

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It is a Gaussian distribution, too

$$\Psi(\phi,t=0) \simeq \frac{\Delta_p}{2\sqrt{\pi}} e^{-\left(\frac{\phi}{\Delta_\phi}\right)^2}$$

where: $\Delta_\phi = \frac{2}{\Delta_p}$ or: $\Delta_\phi \Delta_p = 2$

Gaussian uncertainty relation

(Compare to $\Delta x \cdot \Delta k = \pi$ *for ∞-Well)*

where:

$$A\left(\Delta_p,\phi\right) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2} \xrightarrow[\Delta_p>>1]{} \int_{-\infty}^{\infty} dk\, e^{-\left(\frac{k}{\Delta_p} - i\frac{\Delta_p}{2}\phi\right)^2}$$

$$\left[\text{let: } K = \frac{k}{\Delta_p} - i\frac{\Delta_p}{2}\phi \quad \text{so: } dk = \Delta_p dK\right] \quad \text{then: } A\left(\Delta_p,\phi\right) \simeq \Delta_p \int_{-\infty}^{\infty} dK\, e^{-(K)^2} = \Delta_p\sqrt{\pi}$$

m=0, ±1, ±2, ±3,...are momentum quanta in wavevector formula: $k_m = 2\pi m/L$ ($k_m = m$ *if:* $L = 2\pi$)

$$E_m = (\hbar k_m)^2/2M = m^2[h^2/2ML^2] = m^2 h\upsilon_1 = m^2 \hbar\omega_1$$

fundamental Bohr ∠−frequency $\omega_1 = 2\pi\upsilon_1$ and lowest *transition (beat) frequency* $\upsilon_1 = (E_1 - E_0)/h$

Bohr-rotor wave dynamics and group vs. phase velocity

Gaussian wave-packet bandwidth and uncertainty

→ *Gaussian Bohr-rotor revivals and quantum fractals* ←

Understanding quantum fractals using geometry of fractions (Rationalizing rationals)

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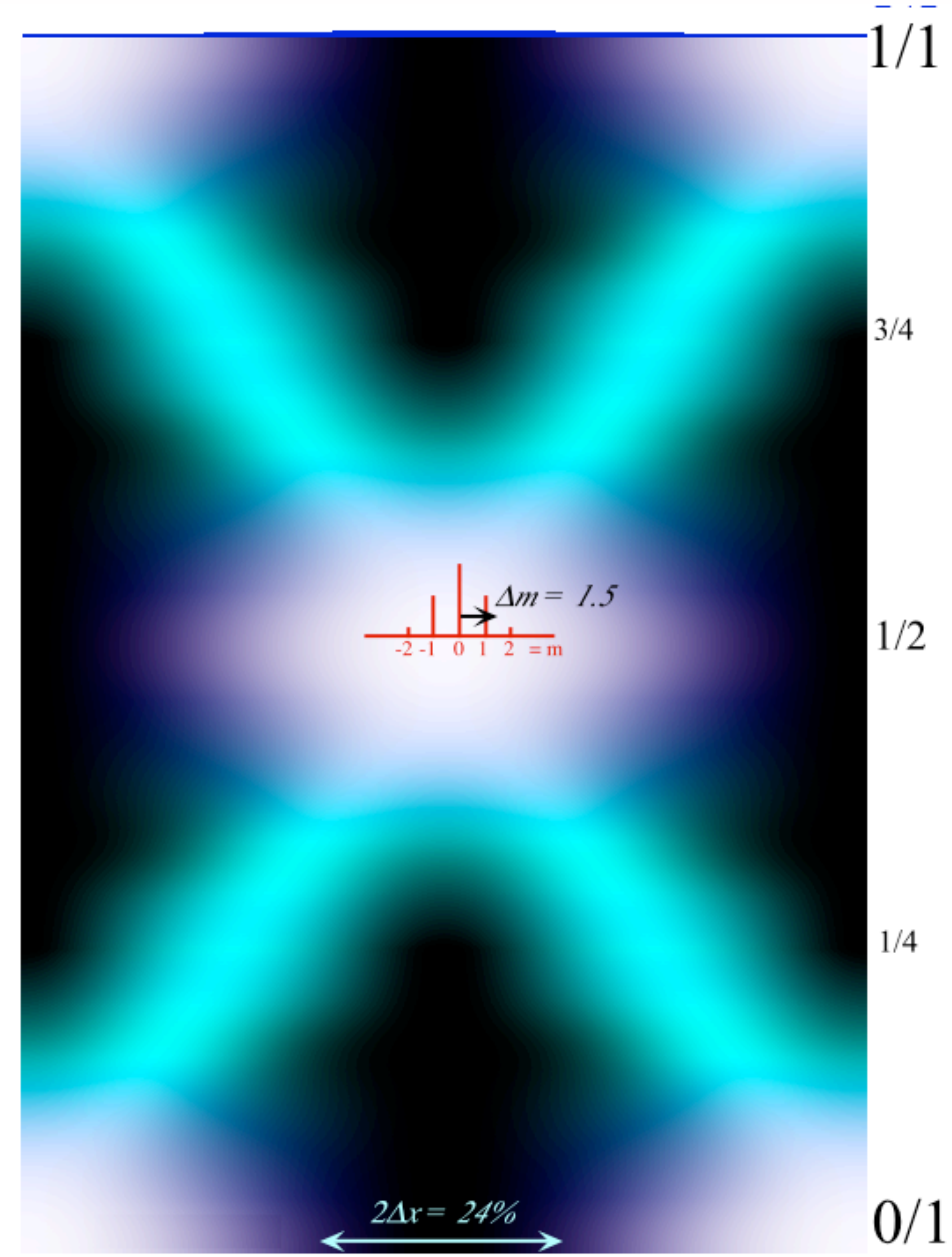
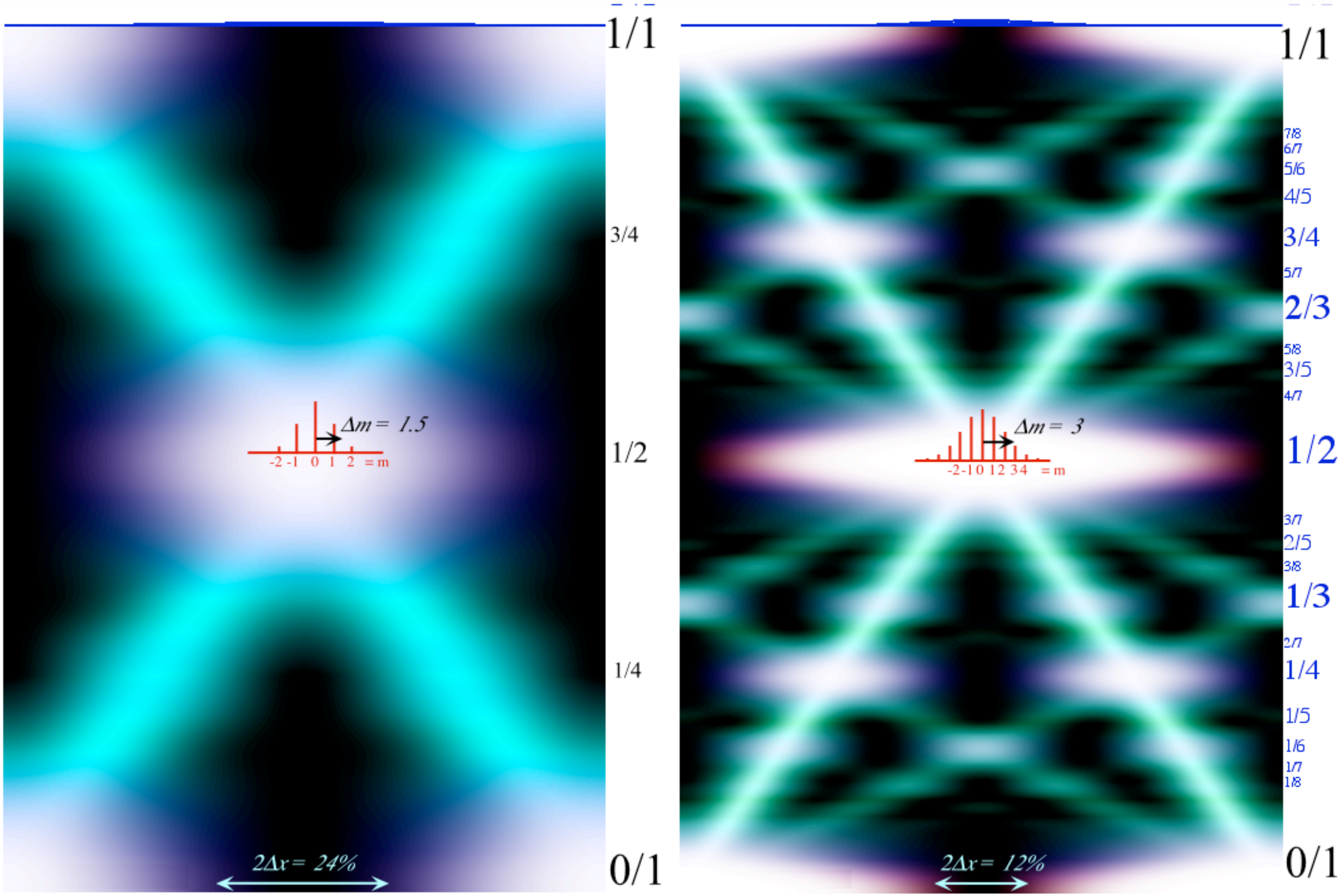
Band-It simulation: Intro to scattering approach to quantum symmetry



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



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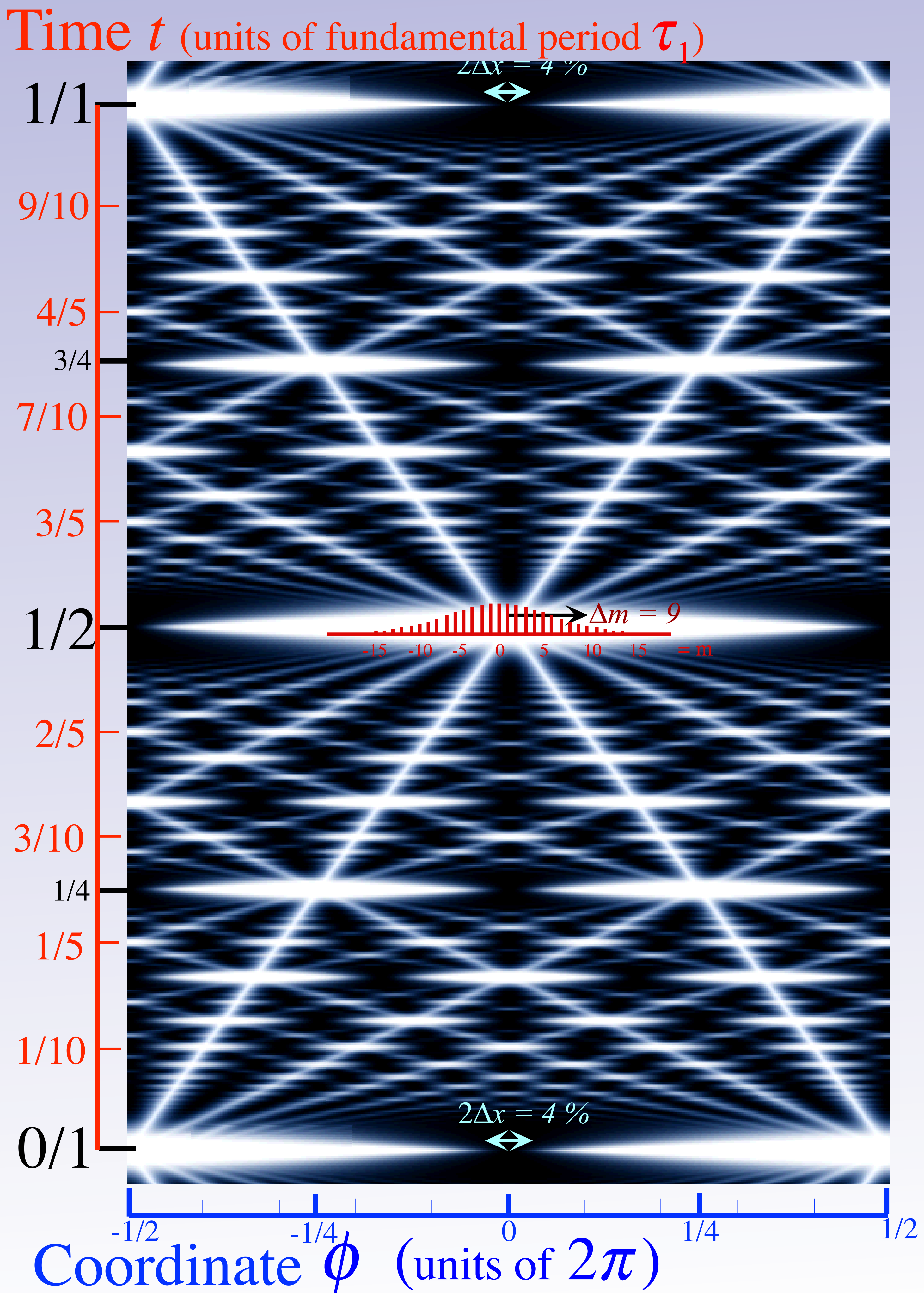
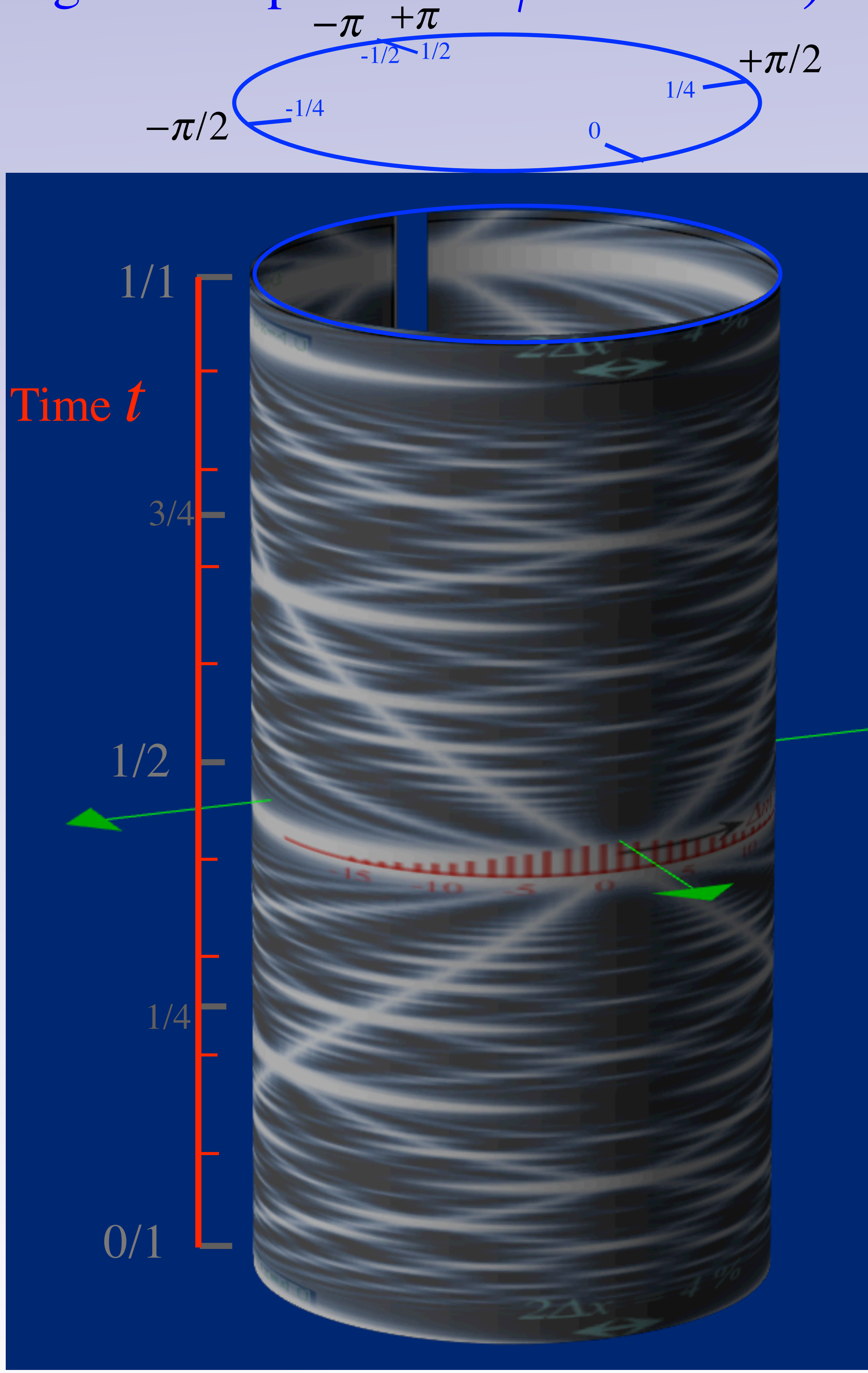


(Imagine "wrap-around" ϕ-coordinate)



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Web simulation

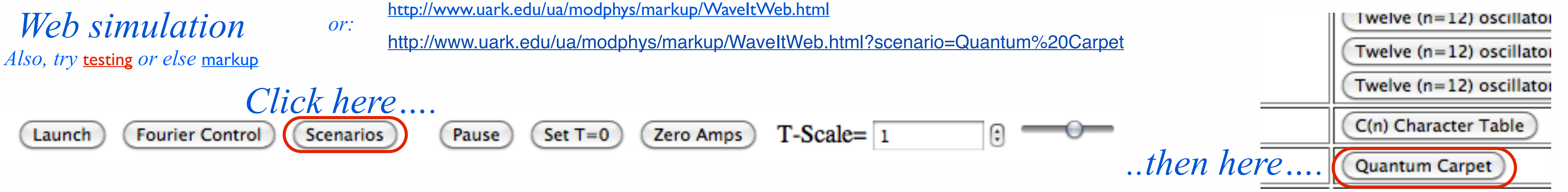
Also, try testing *or else* markup

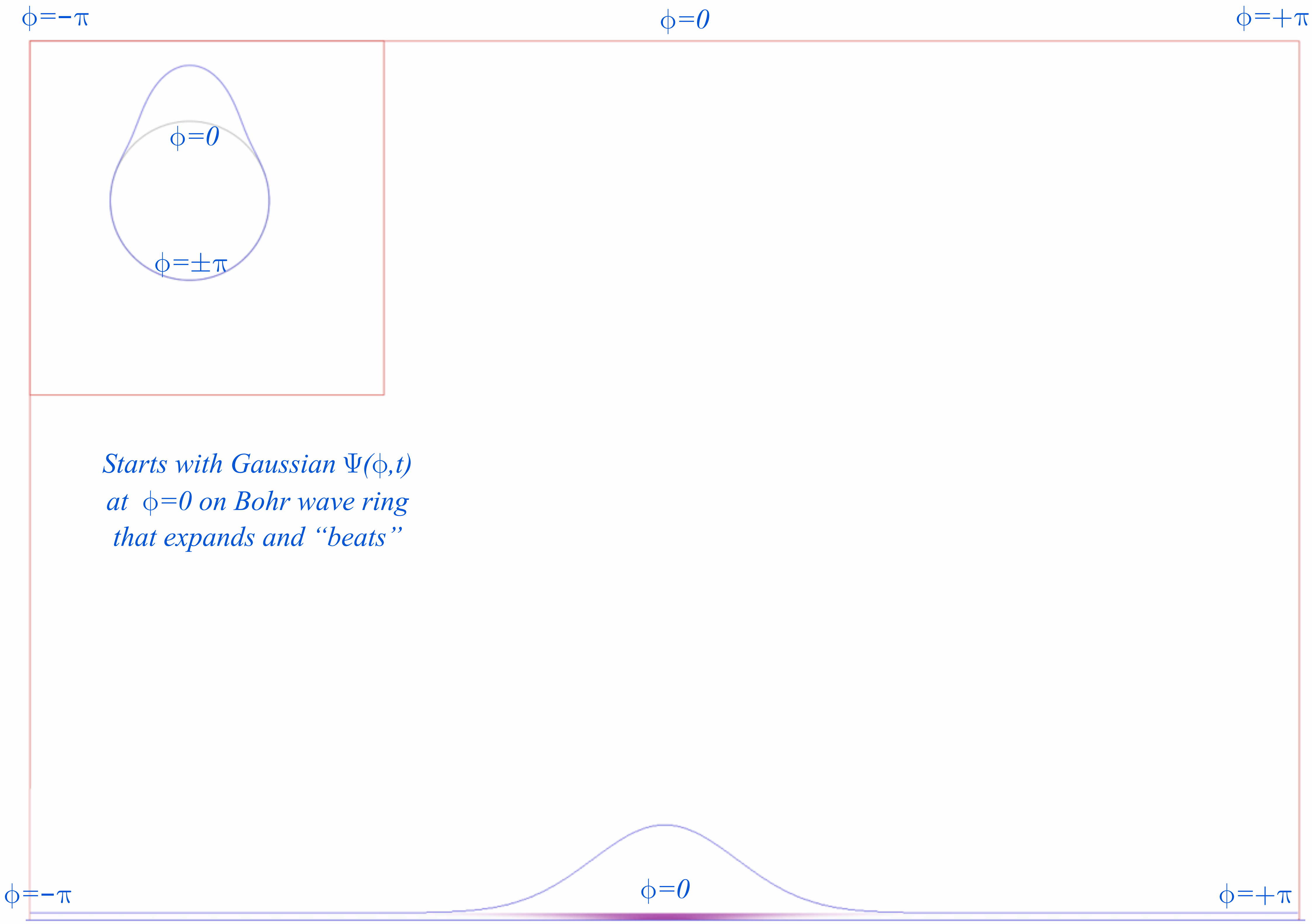
or: http://www.uark.edu/ua/modphys/markup/WaveItWeb.html

http://www.uark.edu/ua/modphys/markup/WaveItWeb.html?scenario=Quantum%20Carpet

Click here….

..then here….





Starts with Gaussian $\Psi(\phi,t)$
at $\phi=0$ on Bohr wave ring
that expands and "beats"

Web simulation

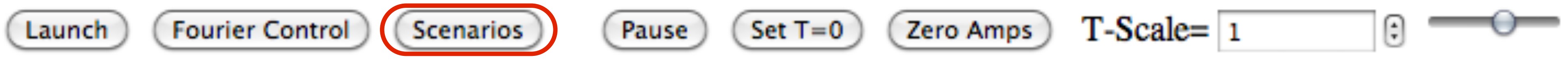
Also, try testing *or else* markup

or:

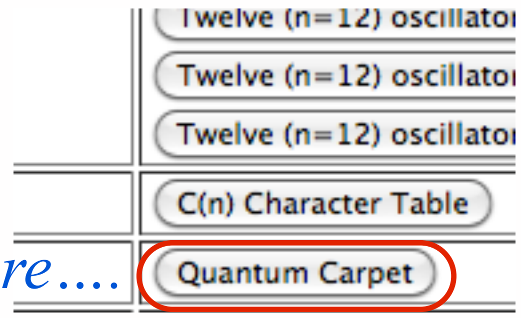
http://www.uark.edu/ua/modphys/markup/WaveltWeb.html

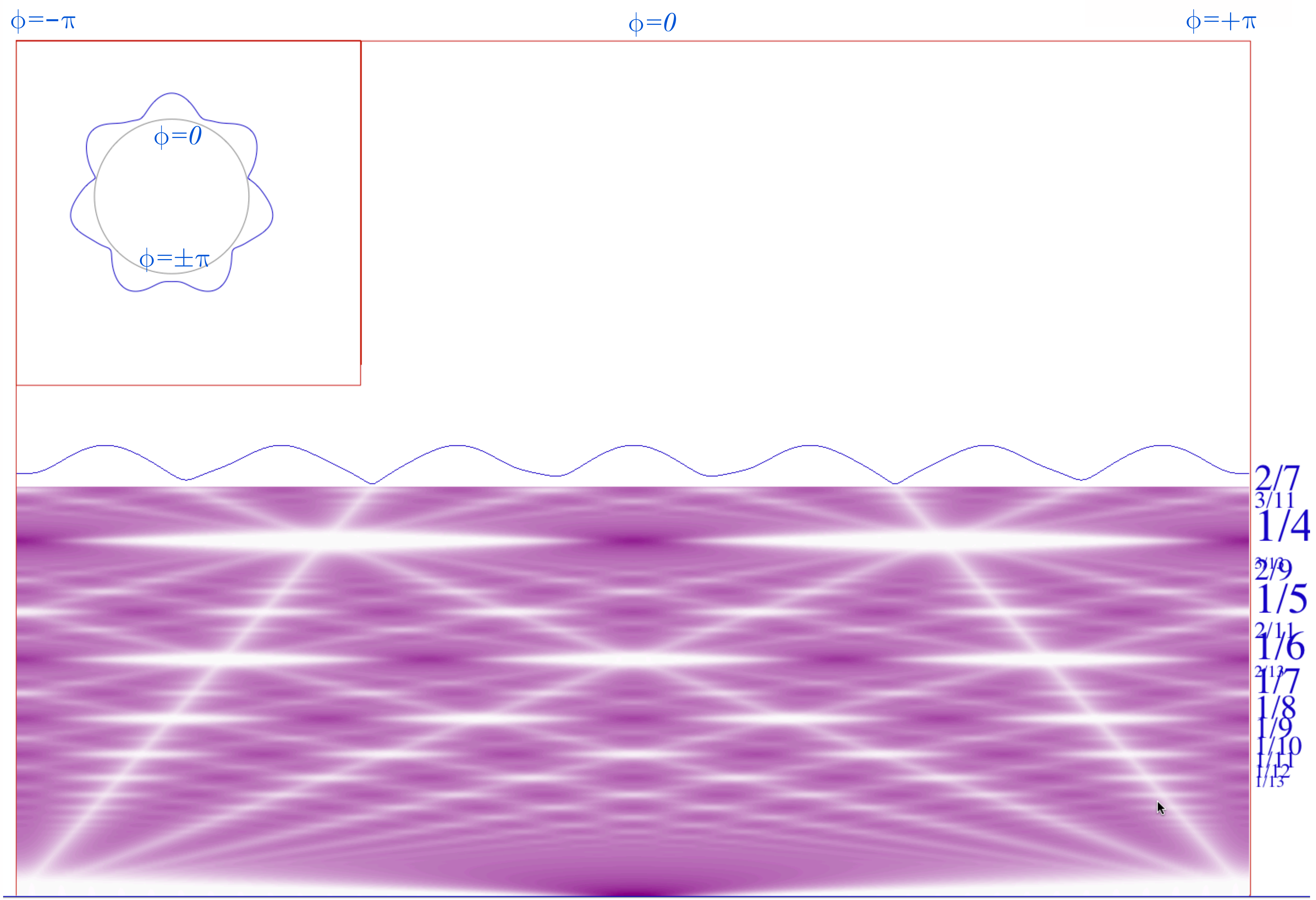
http://www.uark.edu/ua/modphys/markup/WaveltWeb.html?scenario=Quantum%20Carpet

Click here....



..then here....





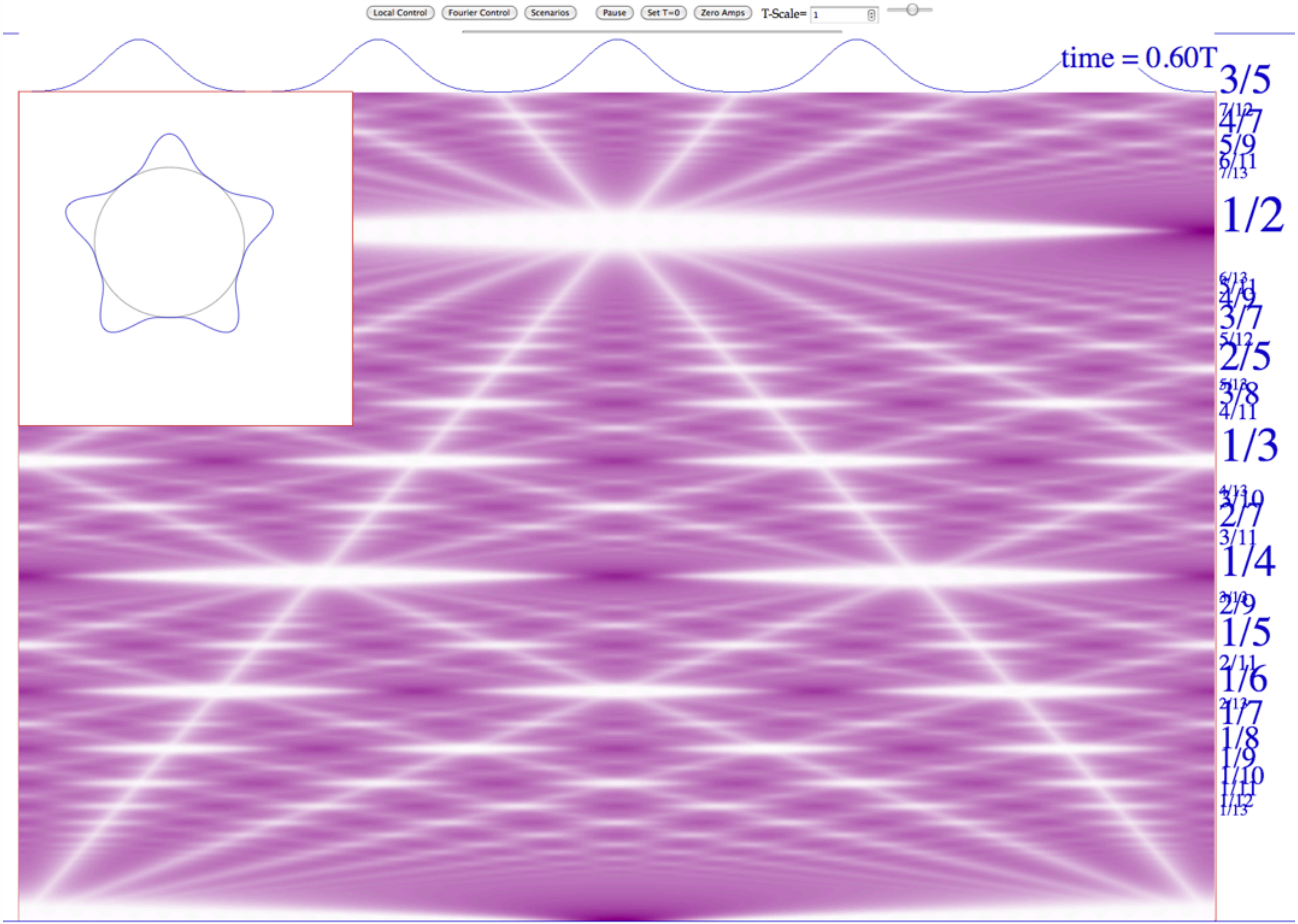
time

$t=0.29T_{max}$

$t=0.25T_{max}$

$t=0.20T_{max}$

$t=0.10T_{max}$


Local Control
Fourier Control
Scenarios
Pause
Set T=0
Zero Amps
T-Scale= 1
time = 0.60T
3/5
7/12
4/7
5/9
6/11
7/13
1/2
6/13
5/11
4/9
3/7
5/12
2/5
5/13
3/8
4/11
1/3
4/13
3/10
2/7
3/11
1/4
3/13
2/9
1/5
2/11
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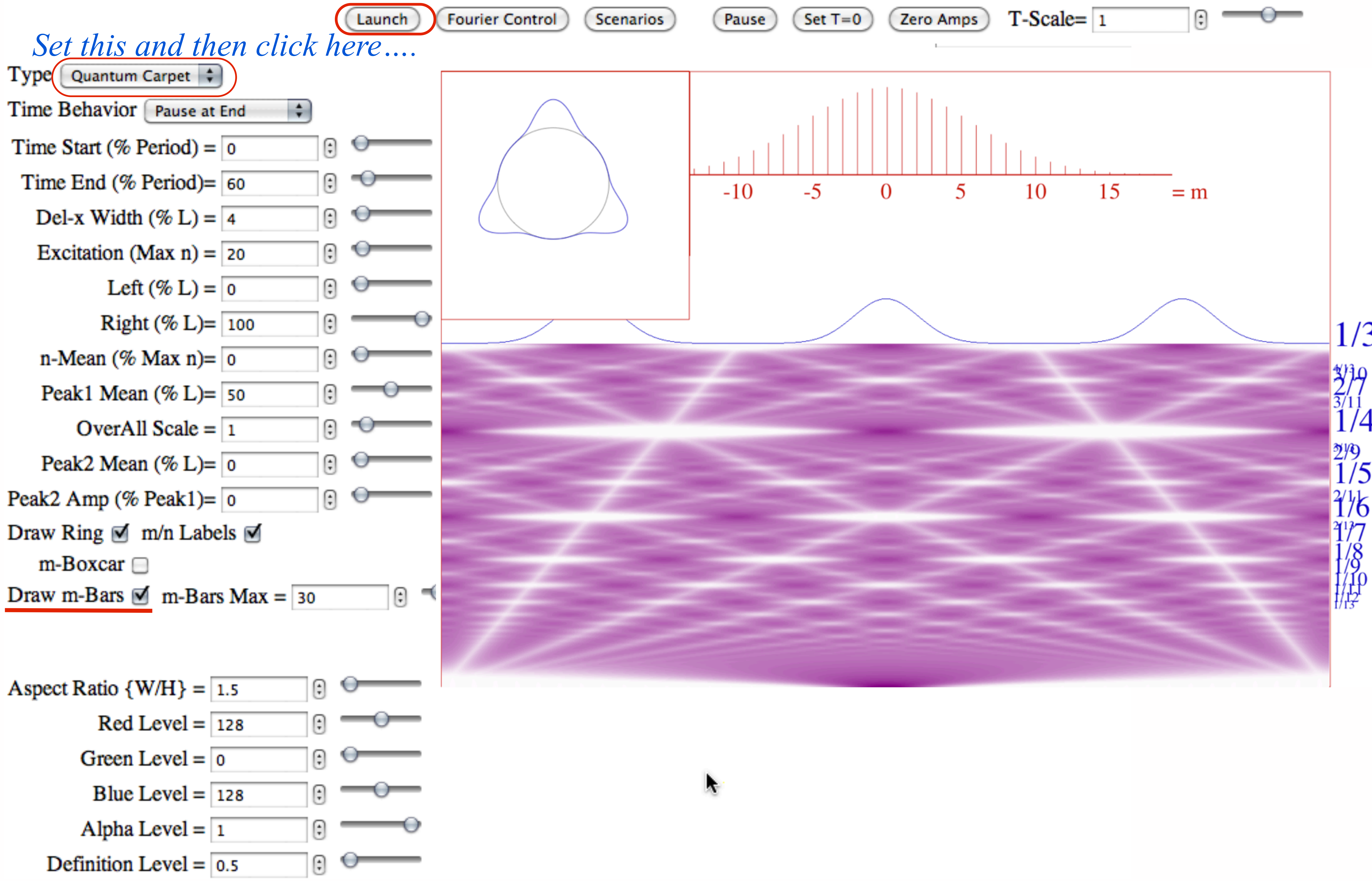
2/13
1/7
1/8
1/9
1/10
1/11
1/12
1/13

Set this and then click here….



T-Scale= 1

Type Quantum Carpet

Time Behavior Pause at End

Time Start (% Period) = 0

Time End (% Period)= 60

Del-x Width (% L) = 4

Excitation (Max n) = 20

Left (% L) = 0

Right (% L)= 100

n-Mean (% Max n)= 0

Peak1 Mean (% L)= 50

OverAll Scale = 1

Peak2 Mean (% L)= 0

Peak2 Amp (% Peak1)= 0

Draw Ring ☑ m/n Labels ☑

m-Boxcar ☐

Draw m-Bars ☑ m-Bars Max = 30

Aspect Ratio {W/H} = 1.5

Red Level = 128

Green Level = 0

Blue Level = 128

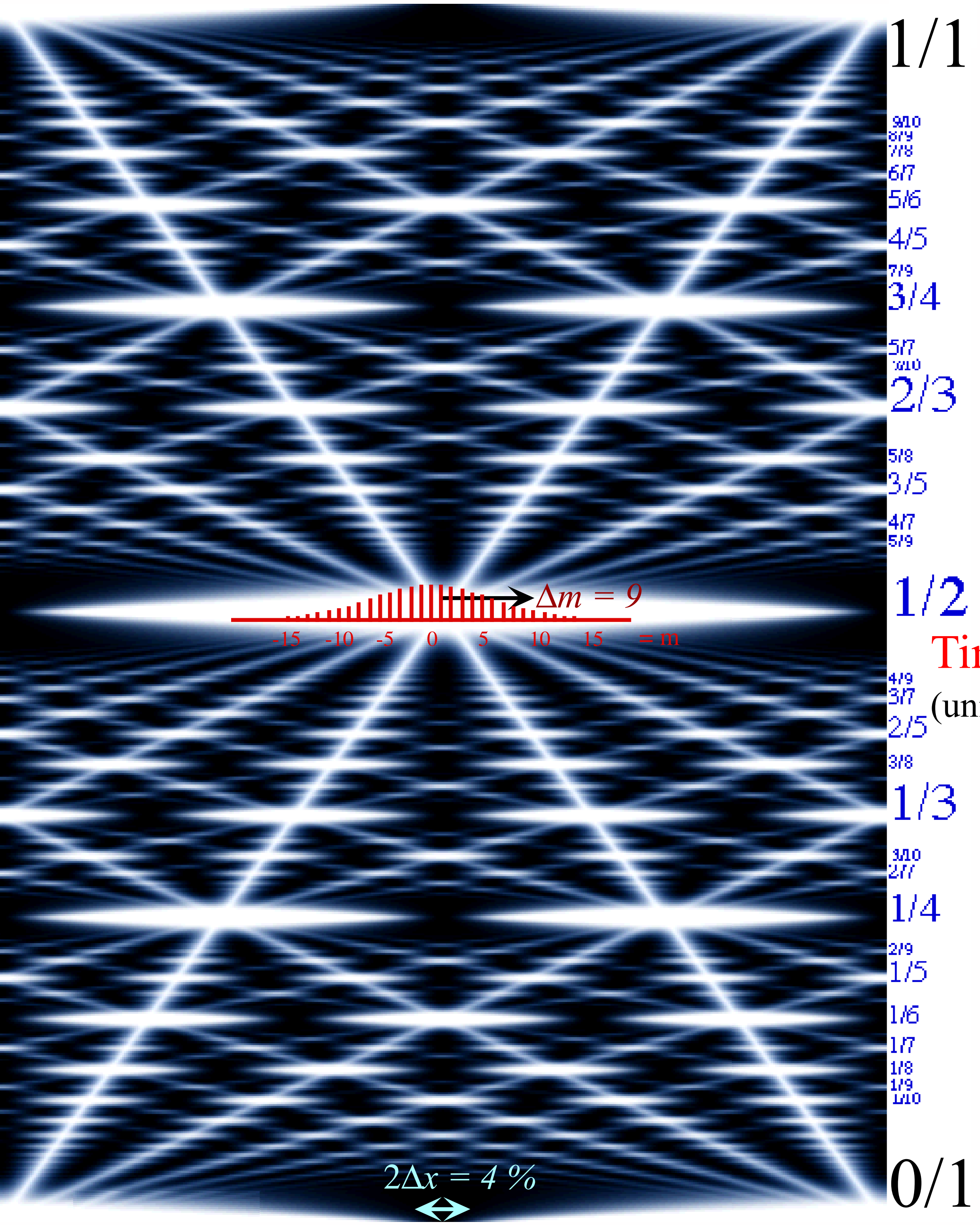
Alpha Level = 1

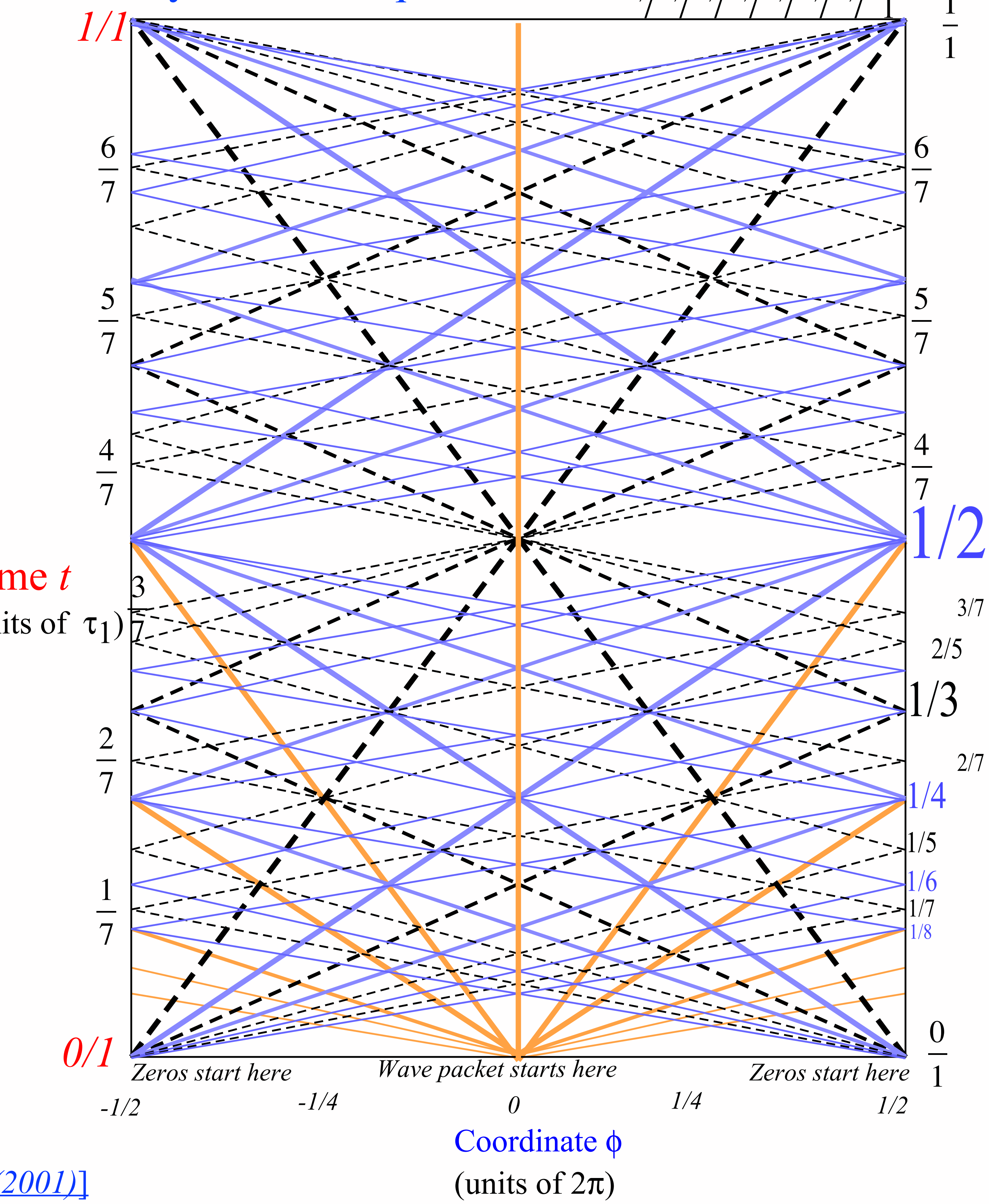
Definition Level = 0.5

N-level-system and revival-beat wave dynamics

(9 or10-levels (0, ±1, ±2, ±3, ±4,..., ±9, ±10, ±11...) excited)

Zeros (clearly) and “particle-packets” (faintly) have paths labeled by fraction sequences like: $\frac{0}{7},\frac{1}{7},\frac{2}{7},\frac{3}{7},\frac{4}{7},\frac{5}{7},\frac{6}{7},\frac{1}{1}$





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

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    - *Gaussian wave-packet bandwidth and uncertainty*
        - *Gaussian Bohr-rotor revivals and quantum fractals*
- *Understanding quantum fractals using geometry of fractions (Rationalizing rationals)*
    - *Farey-Sums and Ford-products*
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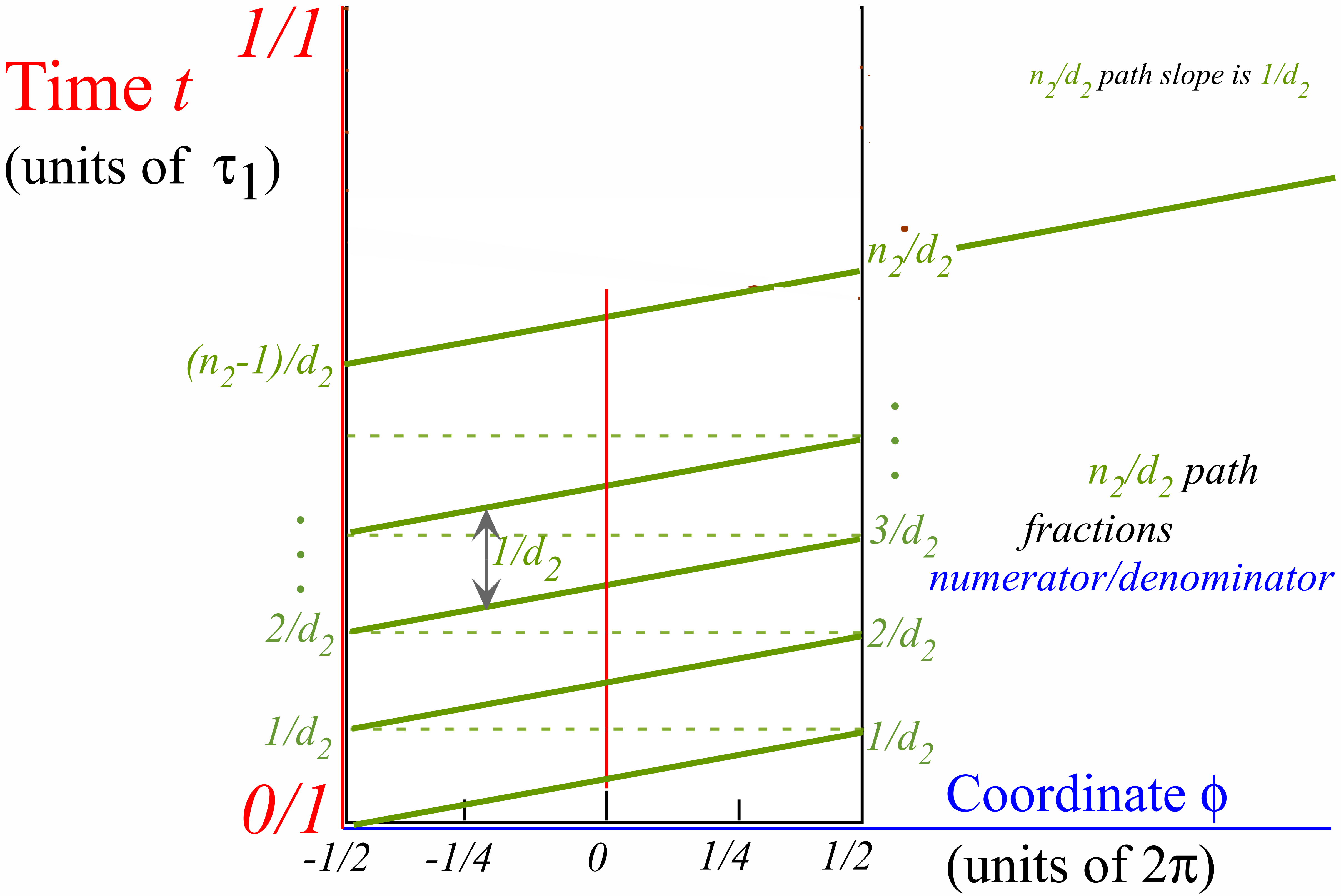
Farey Sum algebra of revival-beat wave dynamics

Label by *numerators N* and *denominators D* of rational fractions *N/D*



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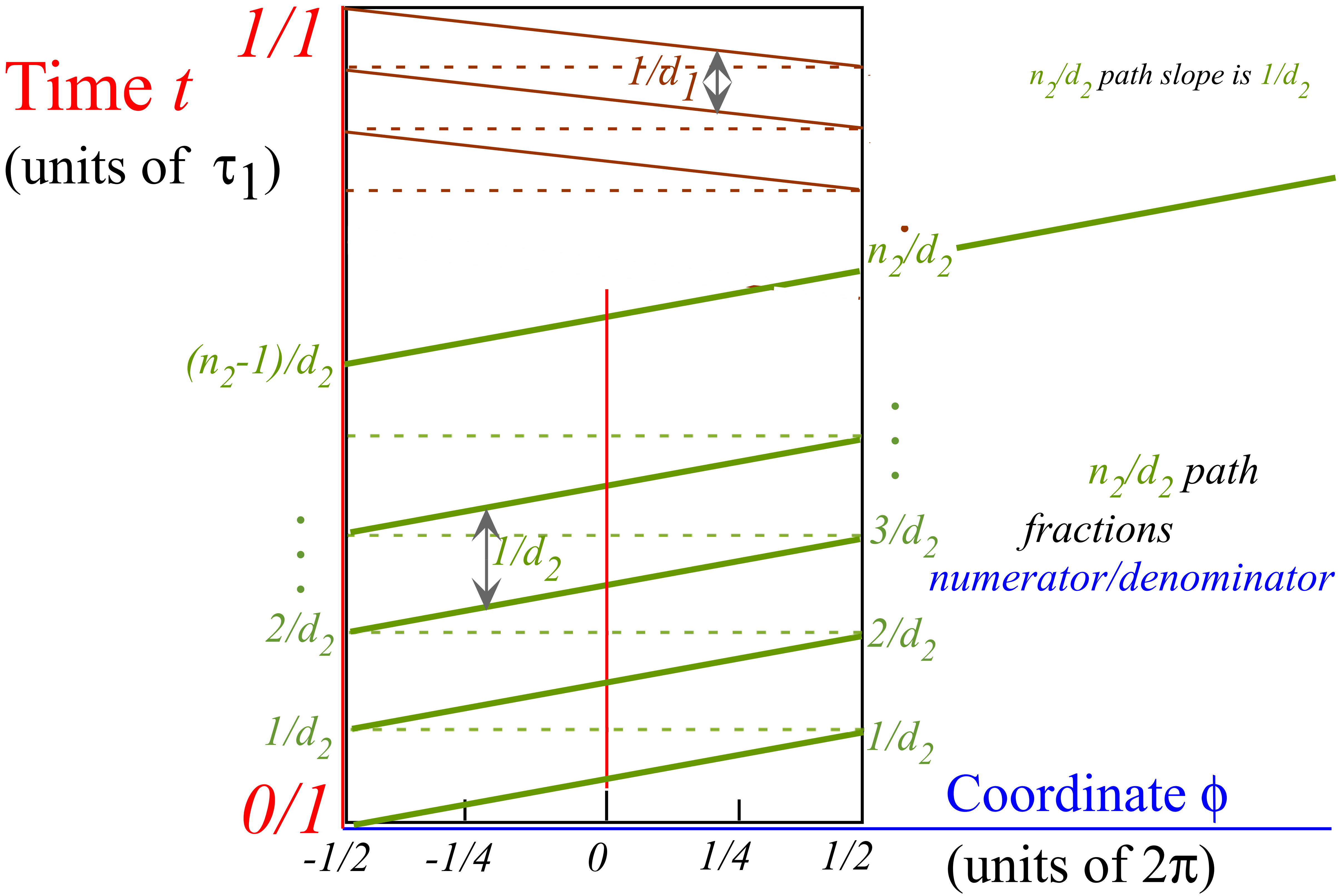

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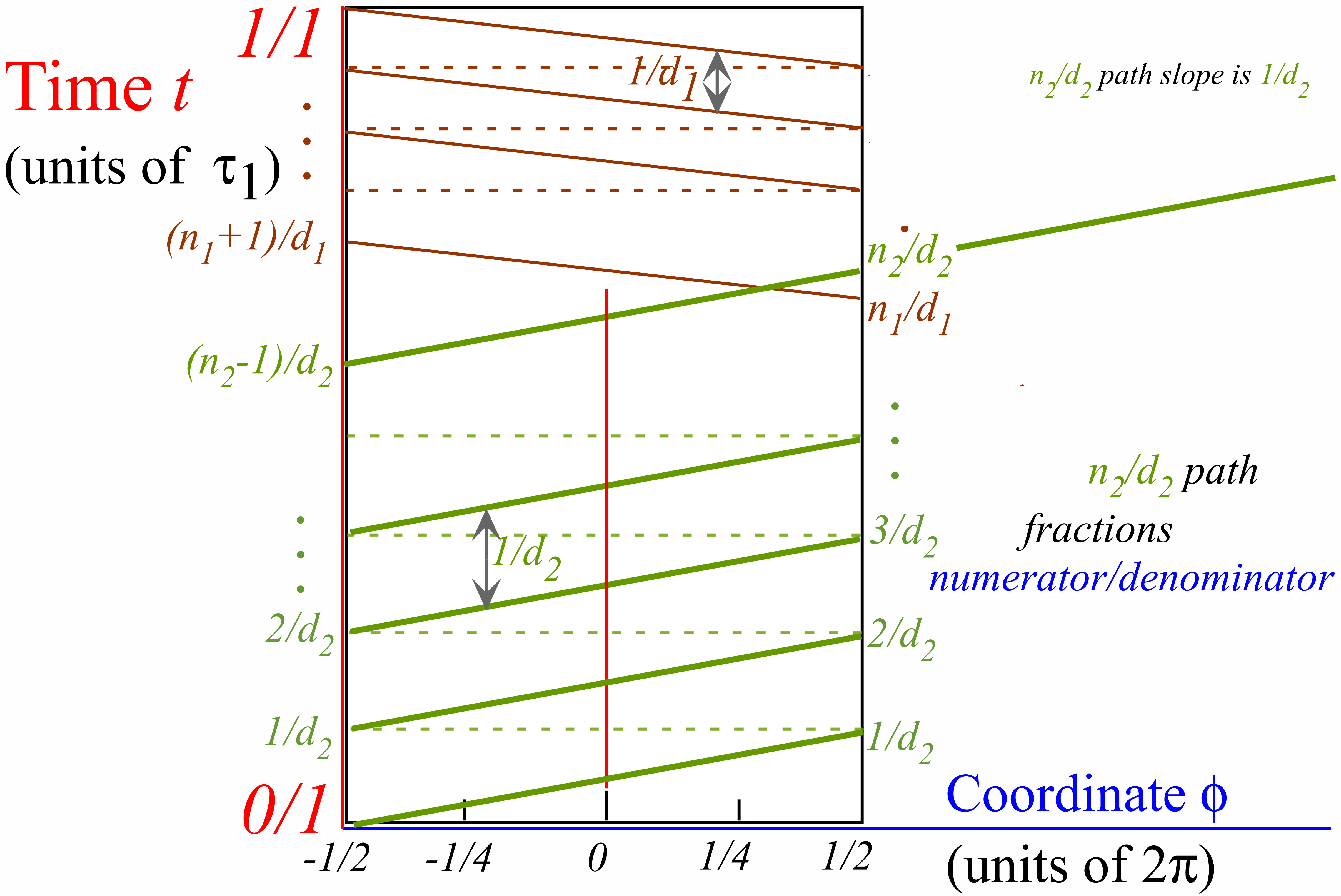

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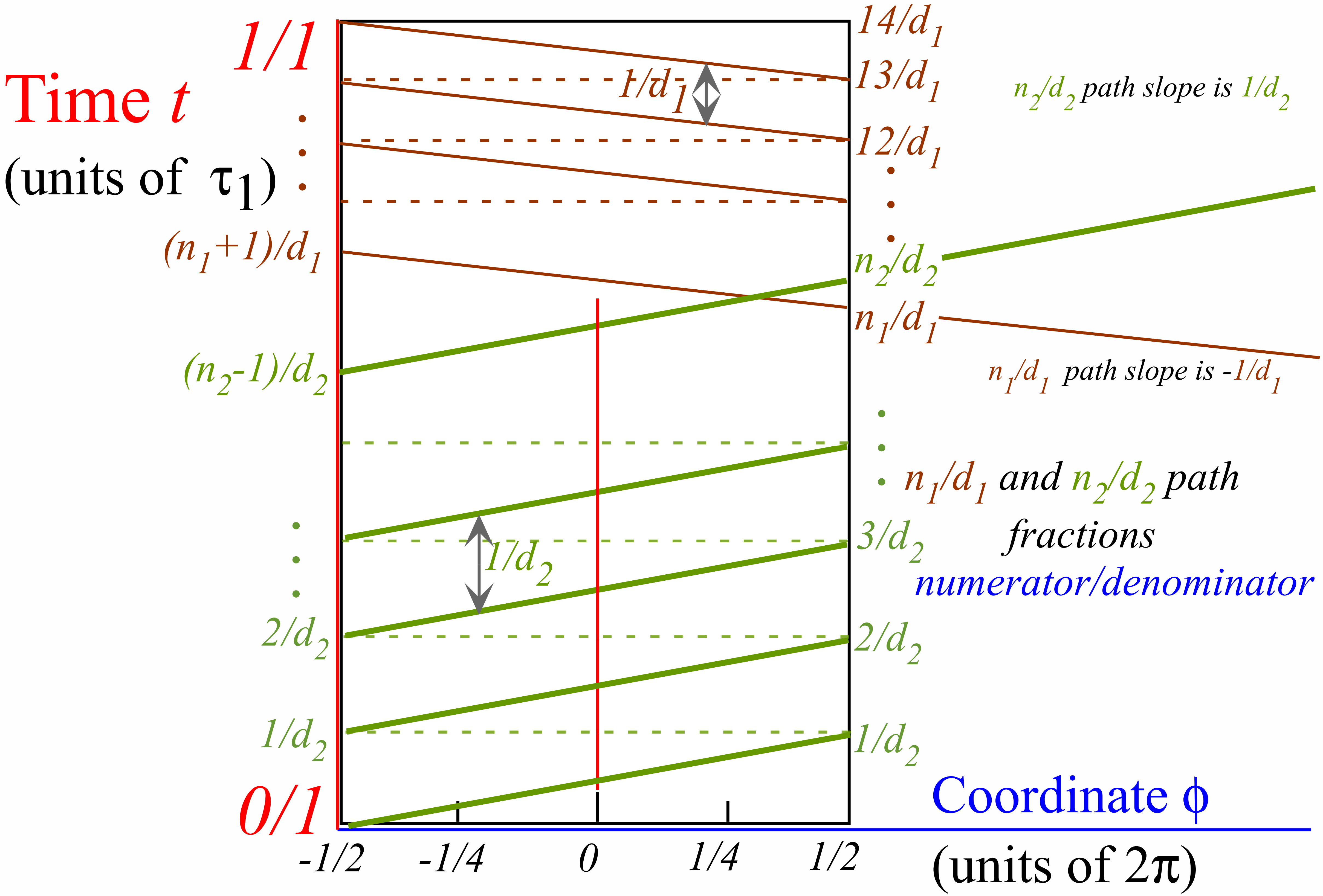

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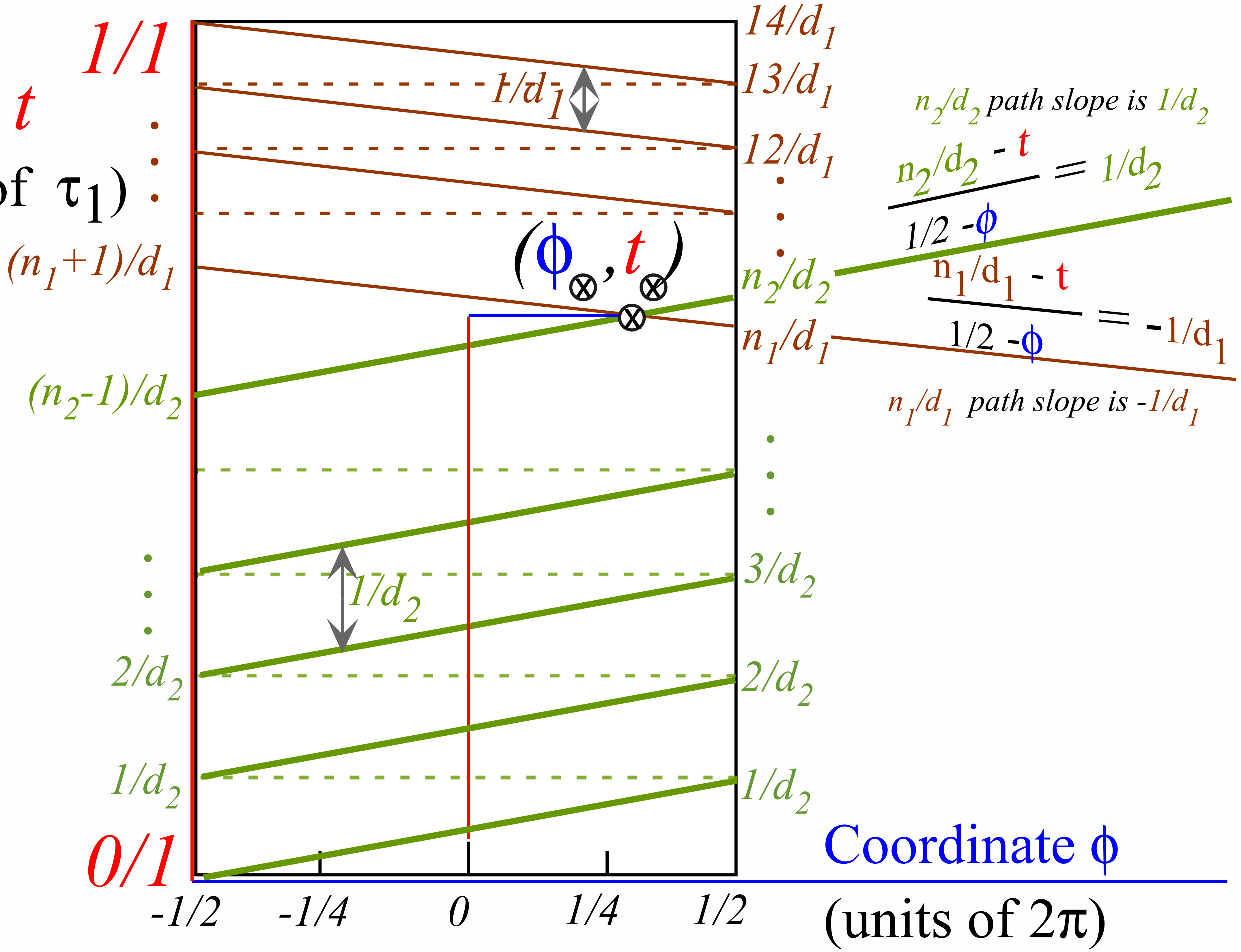
Farey Sum algebra of revival-beat wave dynamics

Label by *numerators N* and *denominators D* of rational fractions *N/D*

Solving: $\frac{\frac{n_2}{d_2}-t}{\frac{n_1}{d_1}-t} = -\frac{d_1}{d_2}$



n_2/d_2 path slope is $1/d_2$

$$\frac{n_2/d_2 - t}{1/2 - \phi} = 1/d_2$$

$$\frac{n_1/d_1 - t}{1/2 - \phi} = -1/d_1$$

n_1/d_1 path slope is $-1/d_1$

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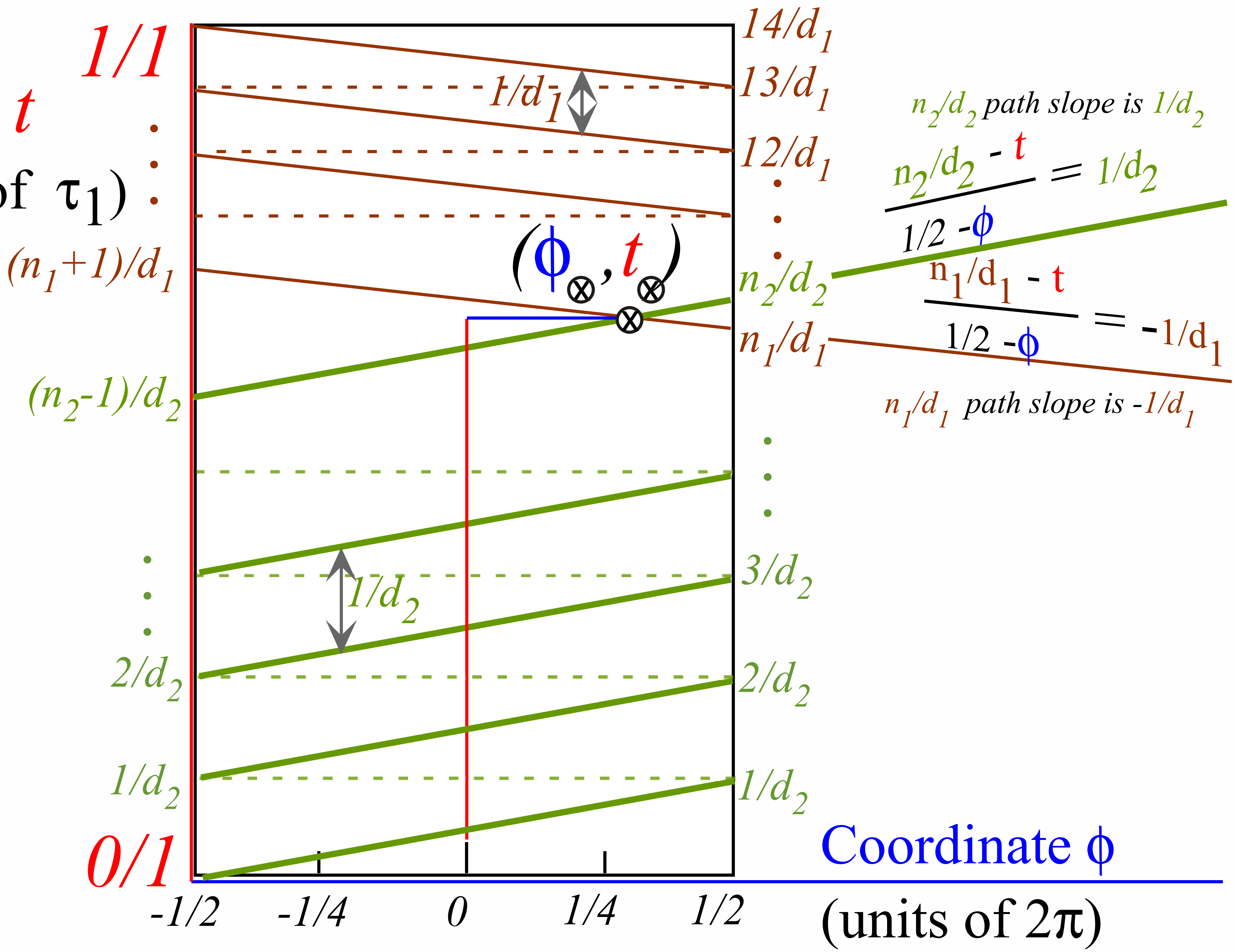
Farey Sum algebra of revival-beat wave dynamics

Label by *numerators N* and *denominators D* of rational fractions *N/D*

$$\text{Solving:}\ \frac{\frac{n_2}{d_2}-t}{\frac{n_1}{d_1}-t}=-\frac{d_1}{d_2}$$

$$\frac{n_2}{d_2}-t=-\frac{d_1}{d_2}\frac{n_1}{d_1}+\frac{d_1}{d_2}t$$



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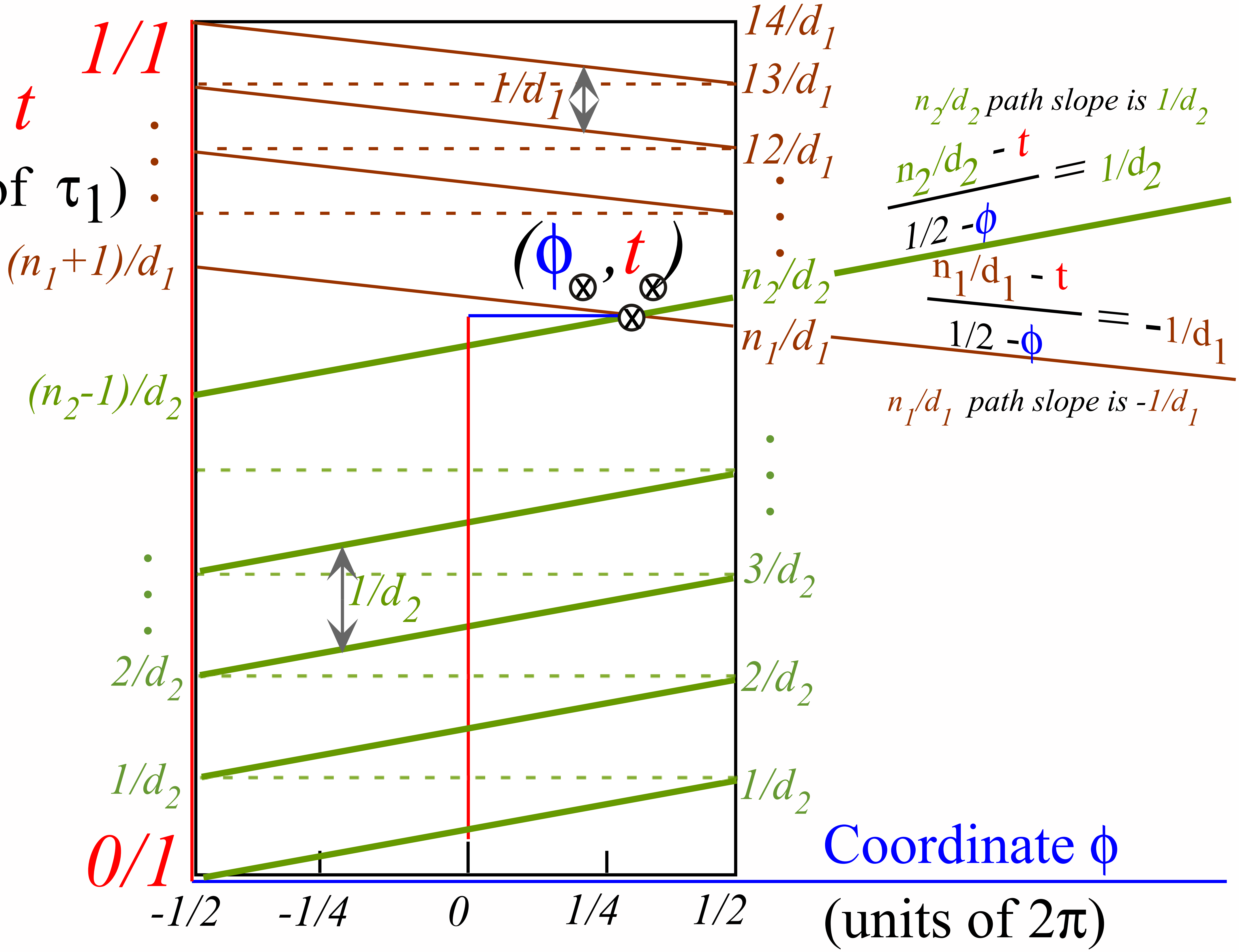
Farey Sum algebra of revival-beat wave dynamics

Label by *numerators N* and *denominators D* of rational fractions *N/D*

Time *t*

(units of τ_1)



Solving: $\frac{\frac{n_2}{d_2}-t}{\frac{n_1}{d_1}-t} = -\frac{d_1}{d_2}$

$$\frac{n_2}{d_2} - t = -\frac{d_1}{d_2}\frac{n_1}{d_1} + \frac{d_1}{d_2}t$$

$$= -\frac{n_1}{d_2} + \frac{d_1}{d_2}t$$

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Farey Sum algebra of revival-beat wave dynamics

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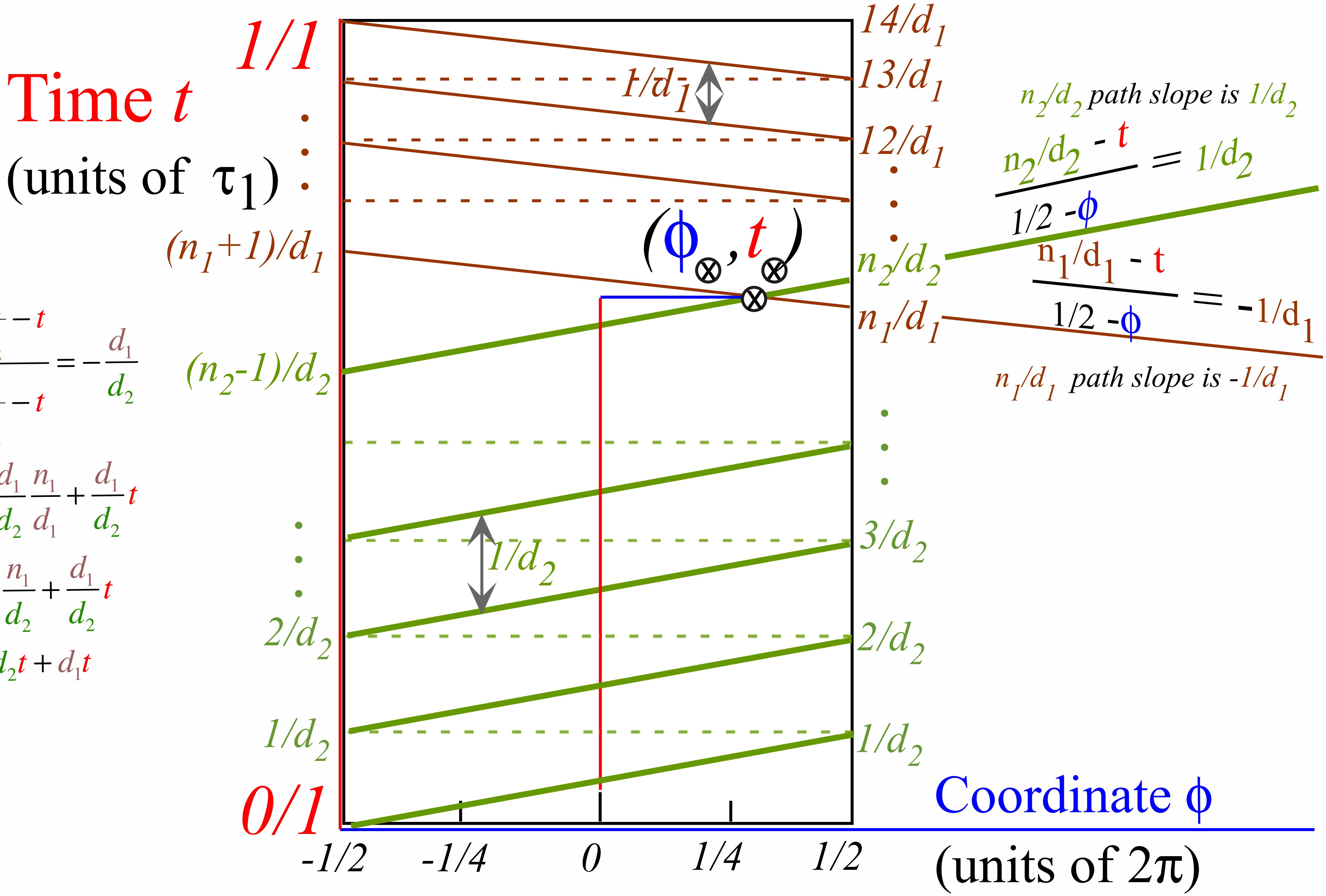

n_2/d_2 path slope is $1/d_2$

$$\frac{n_2/d_2 - t}{1/2 - \phi} = 1/d_2$$

$$\frac{n_1/d_1 - t}{1/2 - \phi} = -1/d_1$$

n_1/d_1 path slope is $-1/d_1$

Solving: $\frac{\frac{n_2}{d_2}-t}{\frac{n_1}{d_1}-t} = -\frac{d_1}{d_2}$

$$\frac{n_2}{d_2} - t = -\frac{d_1}{d_2}\frac{n_1}{d_1} + \frac{d_1}{d_2}t$$

$$= -\frac{n_1}{d_2} + \frac{d_1}{d_2}t$$

$$n_2 + n_1 = d_2 t + d_1 t$$

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Farey Sum algebra of revival-beat wave dynamics

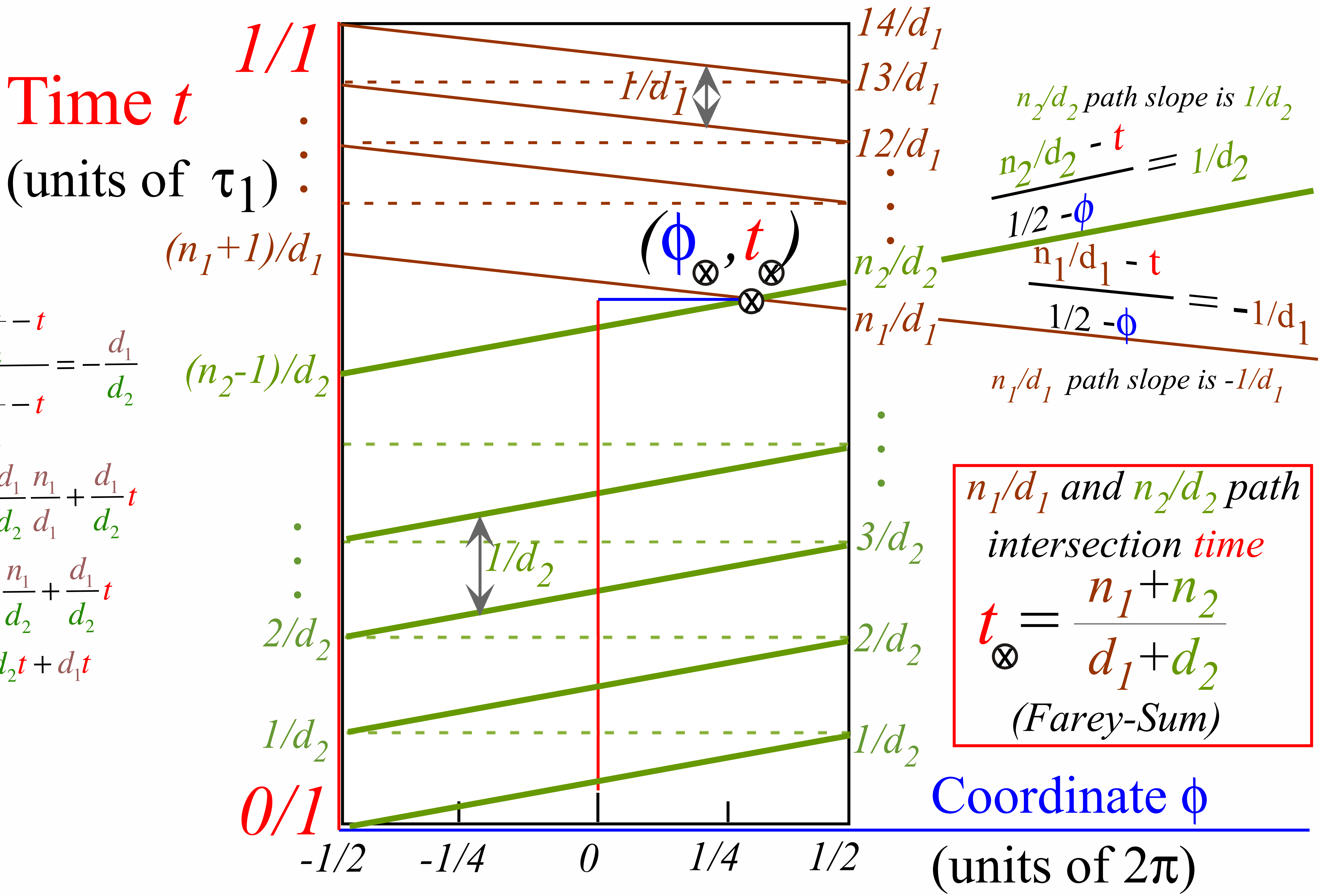
Label by *numerators N* and *denominators D* of rational fractions *N/D*

Solving:
$$\frac{\frac{n_2}{d_2}-t}{\frac{n_1}{d_1}-t}=-\frac{d_1}{d_2}$$

$$\frac{n_2}{d_2}-t=-\frac{d_1}{d_2}\frac{n_1}{d_1}+\frac{d_1}{d_2}t$$

$$=-\frac{n_1}{d_2}+\frac{d_1}{d_2}t$$

$$n_2+n_1=d_2t+d_1t$$



n_2/d_2 *path slope is* $1/d_2$

$$\frac{n_2/d_2-t}{1/2-\phi}=1/d_2$$

$$\frac{n_1/d_1-t}{1/2-\phi}=-1/d_1$$

n_1/d_1 *path slope is* $-1/d_1$

n_1/d_1 and n_2/d_2 path intersection time

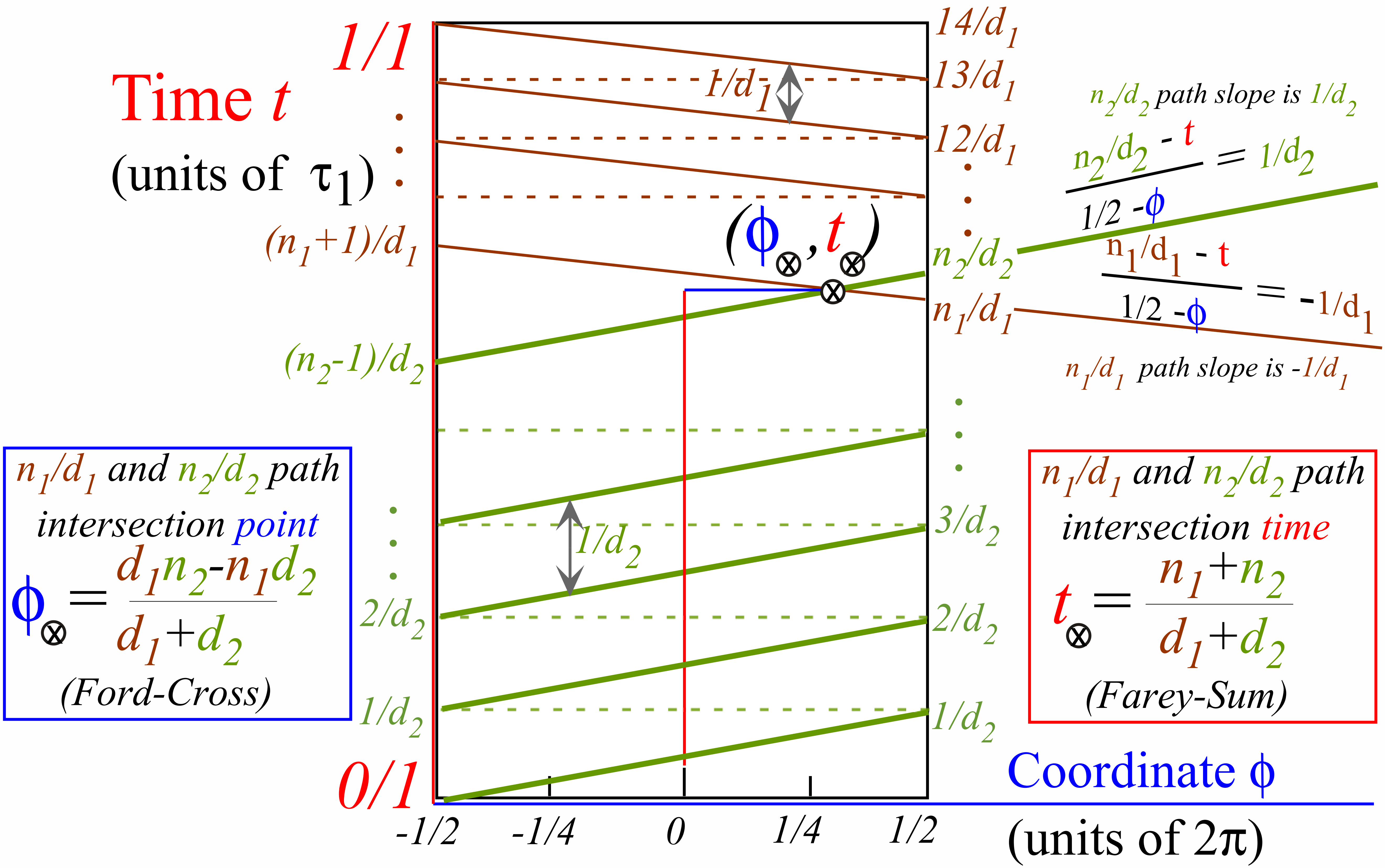
$$t_\otimes=\frac{n_1+n_2}{d_1+d_2}$$

(Farey-Sum)

[Lester. R. Ford, Am. Math. Monthly 45,586(1938)]   [John Farey, Phil. Mag.(1816) Wolfram]   [Harter, Li, UAF, (2013)]

Farey Sum algebra of revival-beat wave dynamics

Label by *numerators N* and *denominators D* of rational fractions *N/D*



n_2/d_2 path slope is $1/d_2$

$$\frac{n_2/d_2 - t}{1/2 - \phi} = 1/d_2$$

$$\frac{n_1/d_1 - t}{1/2 - \phi} = -1/d_1$$

n_1/d_1 path slope is $-1/d_1$

n_1/d_1 and n_2/d_2 path intersection point

$$\phi_\otimes = \frac{d_1 n_2 - n_1 d_2}{d_1 + d_2}$$

(Ford-Cross)

n_1/d_1 and n_2/d_2 path intersection time

$$t_\otimes = \frac{n_1 + n_2}{d_1 + d_2}$$

(Farey-Sum)

[Lester. R. Ford, Am. Math. Monthly 45,586(1938)] [John Farey, Phil. Mag.(1816) Wolfram] [Harter, Li, UAF, (2013)]

Bohr-rotor wave dynamics and group vs. phase velocity

- *Gaussian wave-packet bandwidth and uncertainty*
  - *Gaussian Bohr-rotor revivals and quantum fractals*

Understanding quantum fractals using geometry of fractions (Rationalizing rationals)

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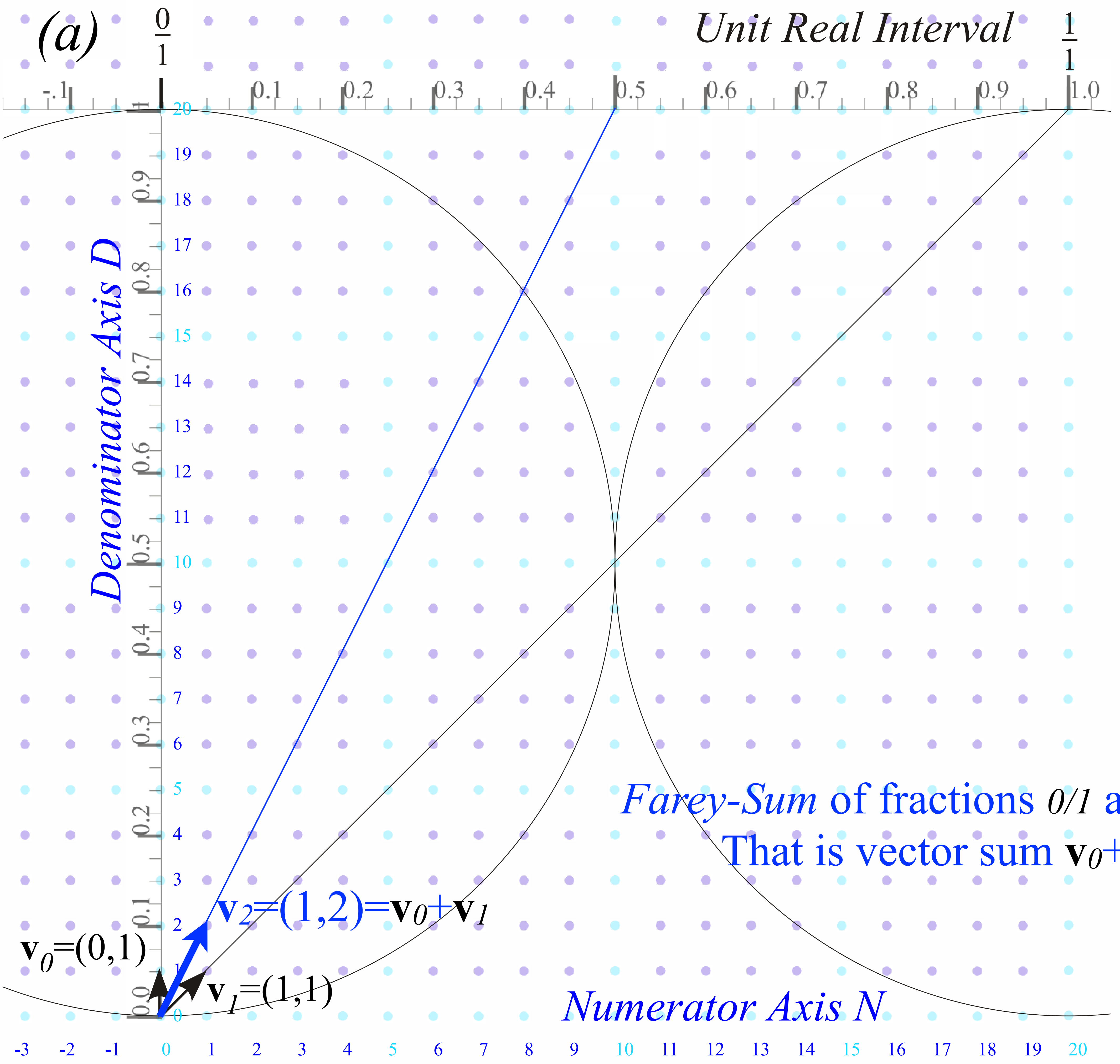
Farey Sum related to vector sum and *Ford Circles*

1/1-circle has diameter *1*



Farey-Sum of fractions *0/1* and *1/1* is *1/2*

That is vector sum $\mathbf{v}_0+\mathbf{v}_1 = (1,2) = \mathbf{v}_2$

Li, Harter, Chem.Phys.Letters **213**, *208-213 (2015)]*

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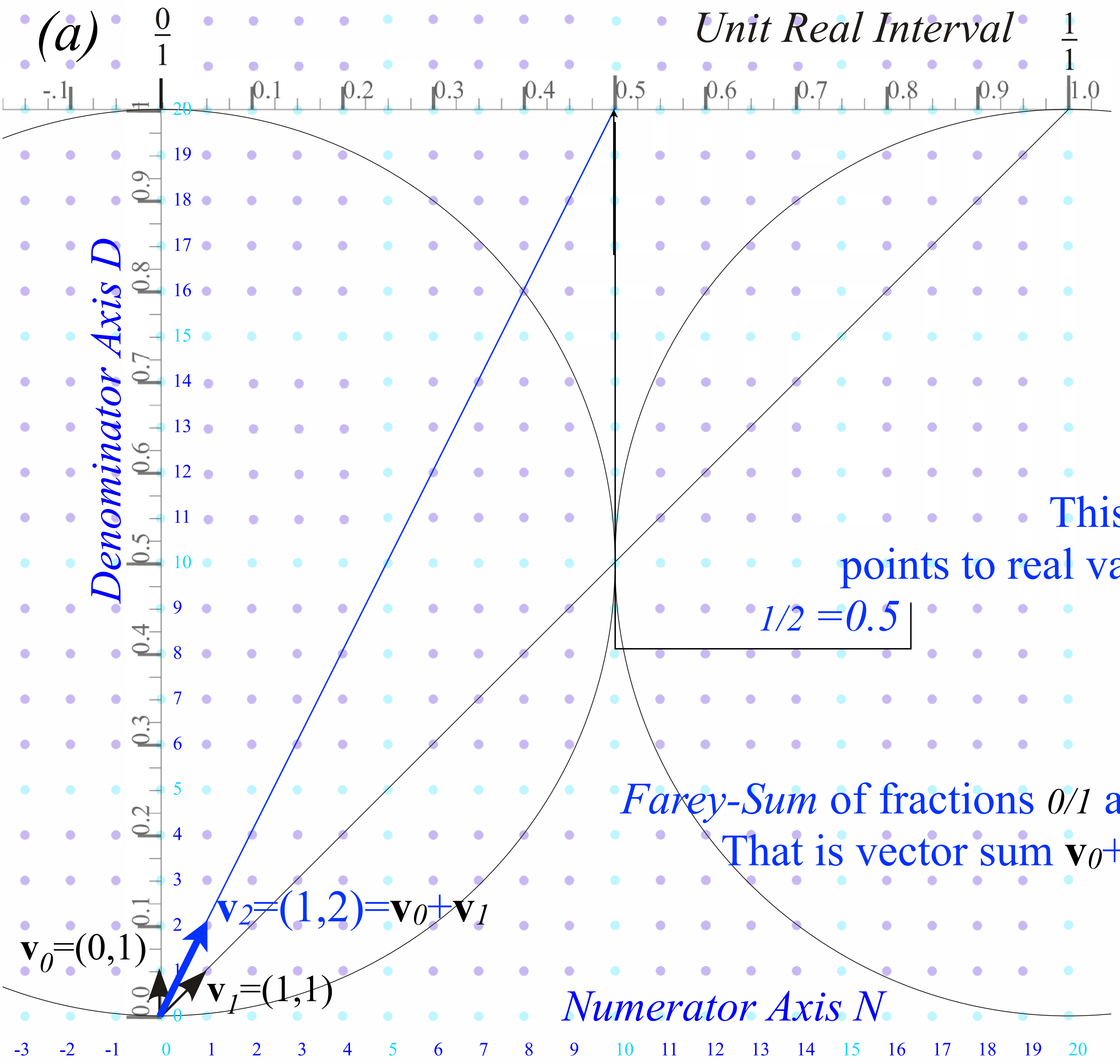

This vector $\mathbf{v}_2$ points to real value *1/2 =0.5*

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Li, Harter, Chem.Phys.Letters ***213**, 208-213 (2015)]*

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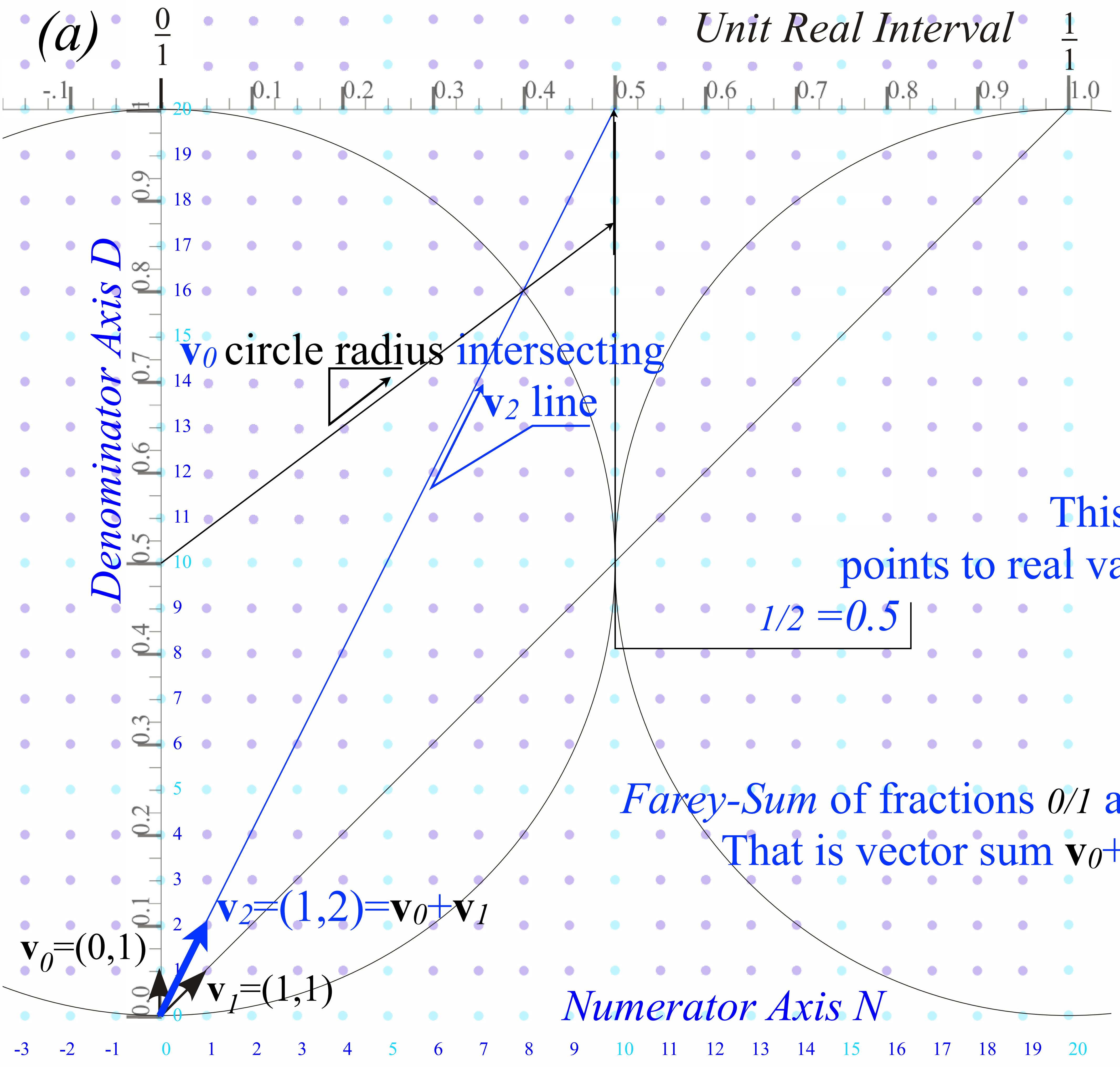

$\mathbf{v}_0$ circle radius intersecting $\mathbf{v}_2$ line

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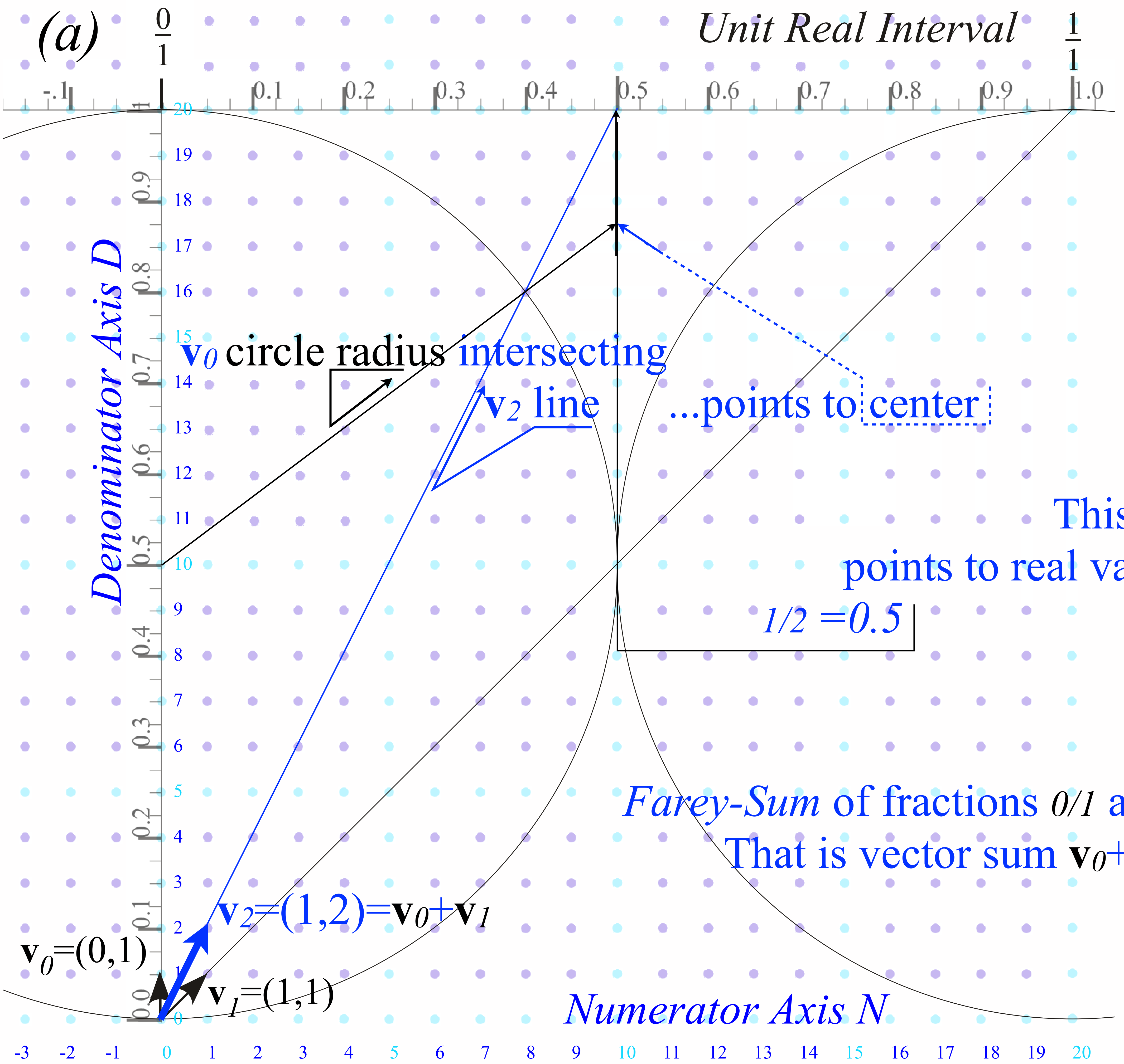

$\mathbf{v}_0$ circle radius intersecting $\mathbf{v}_2$ line

...points to center

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Li, Harter, Chem.Phys.Letters ***213**, 208-213 (2015)]*

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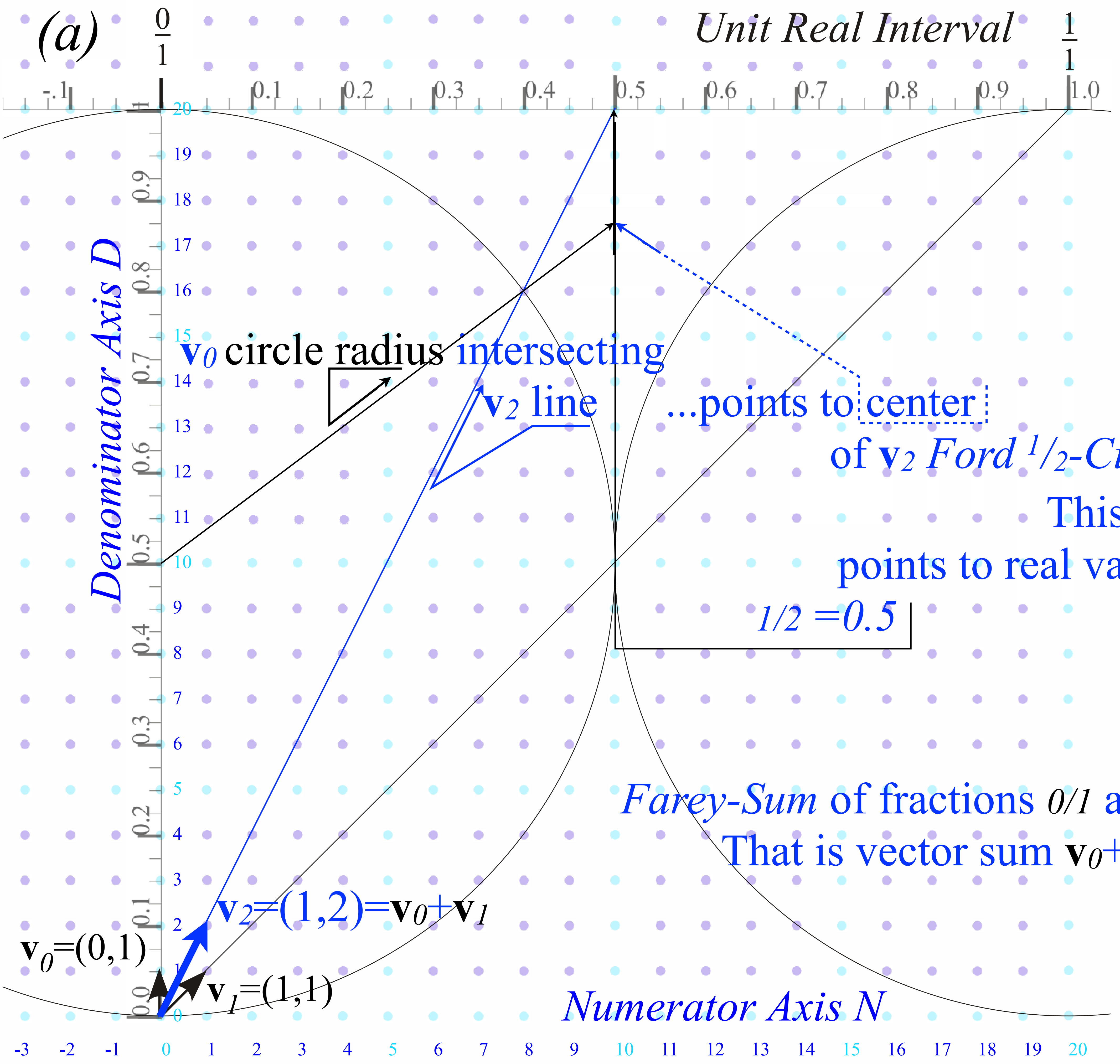

$\mathbf{v}_0$ circle radius intersecting $\mathbf{v}_2$ line

...points to center of $\mathbf{v}_2$ *Ford* $^1/_2$*-Circle*

This vector $\mathbf{v}_2$ points to real value *1/2 =0.5*

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That is vector sum $\mathbf{v}_0+\mathbf{v}_1 = (1,2) = \mathbf{v}_2$

$\mathbf{v}_2=(1,2)=\mathbf{v}_0+\mathbf{v}_1$

$\mathbf{v}_0=(0,1)$

$\mathbf{v}_1=(1,1)$

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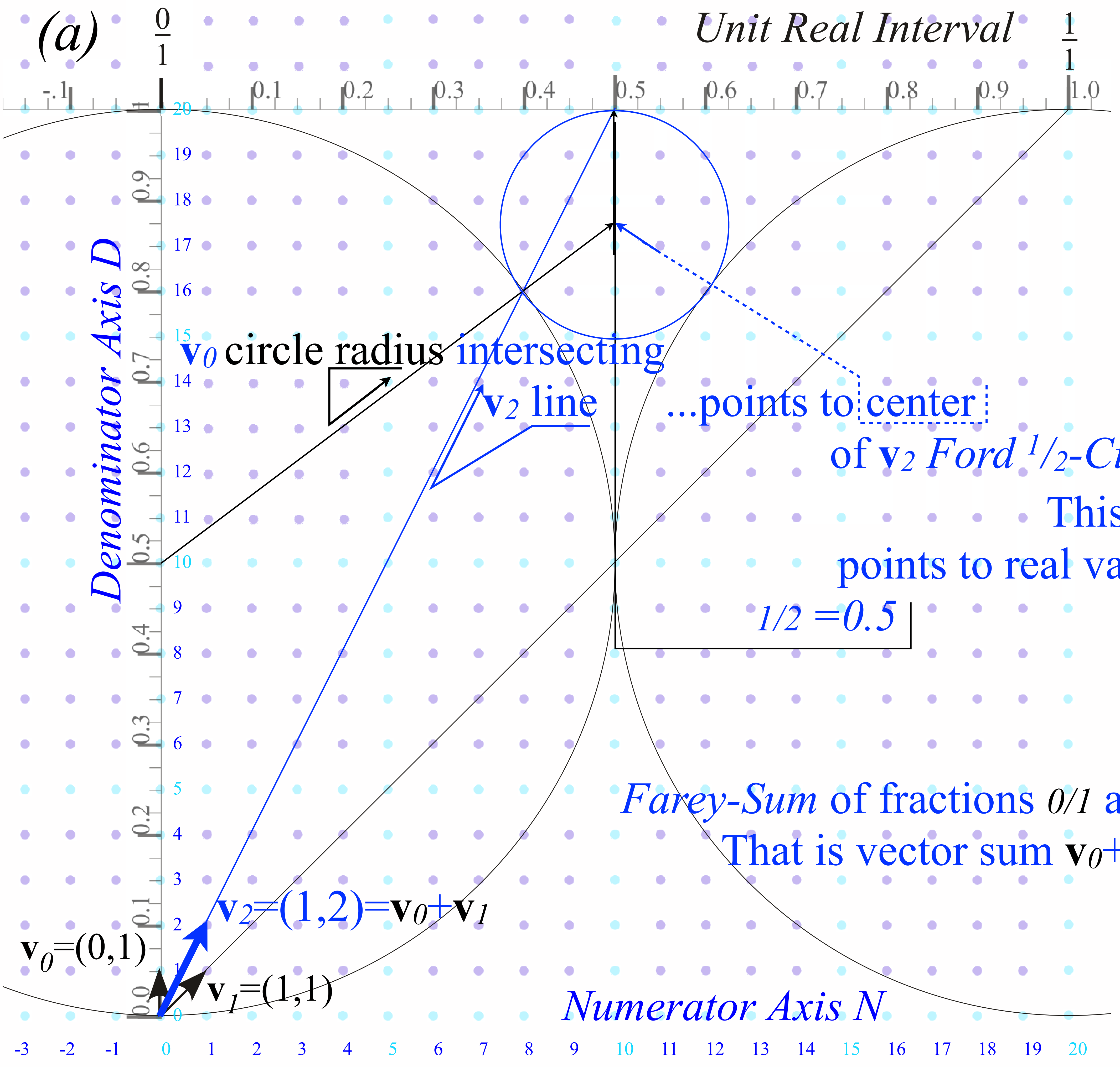
1/1-circle has diameter *1*



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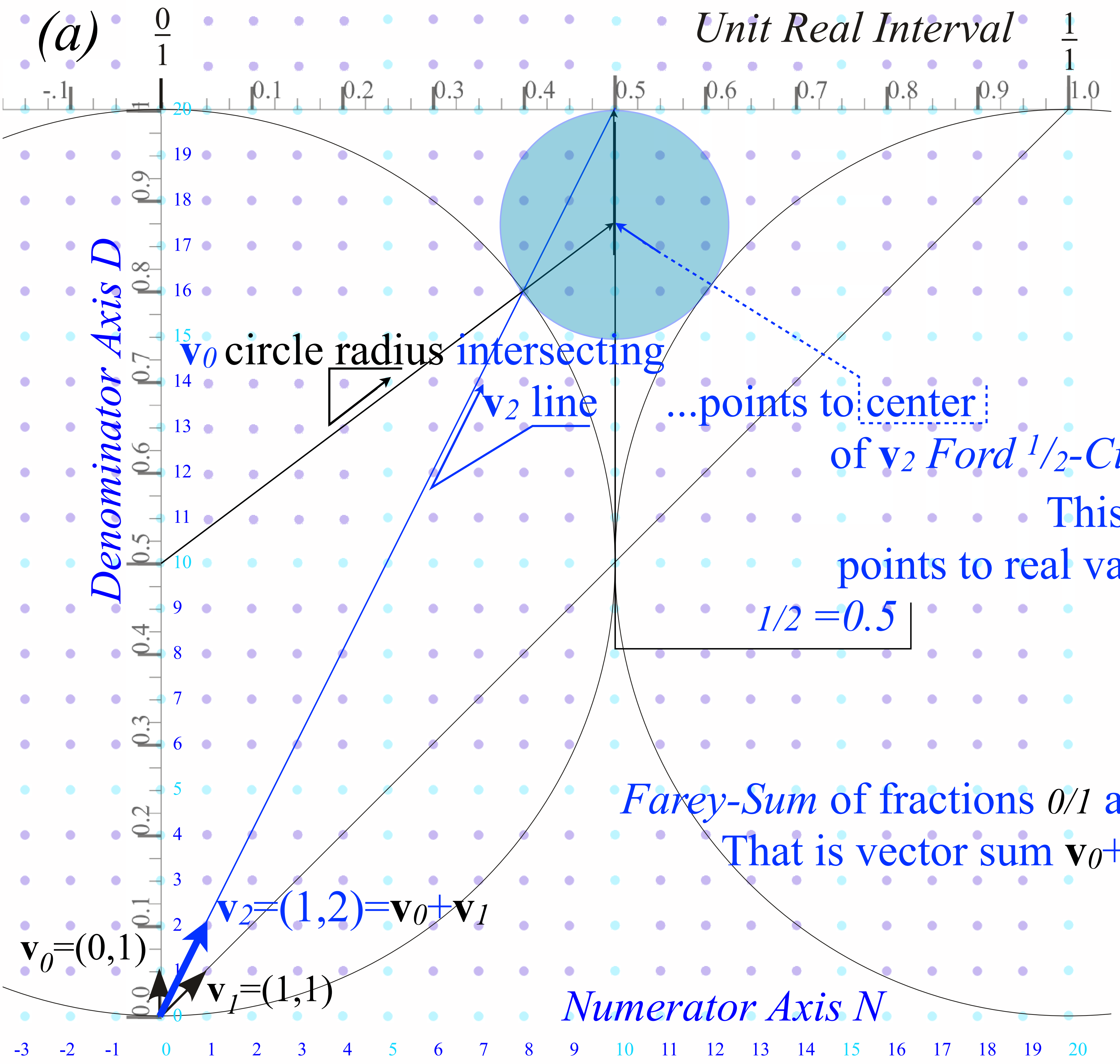

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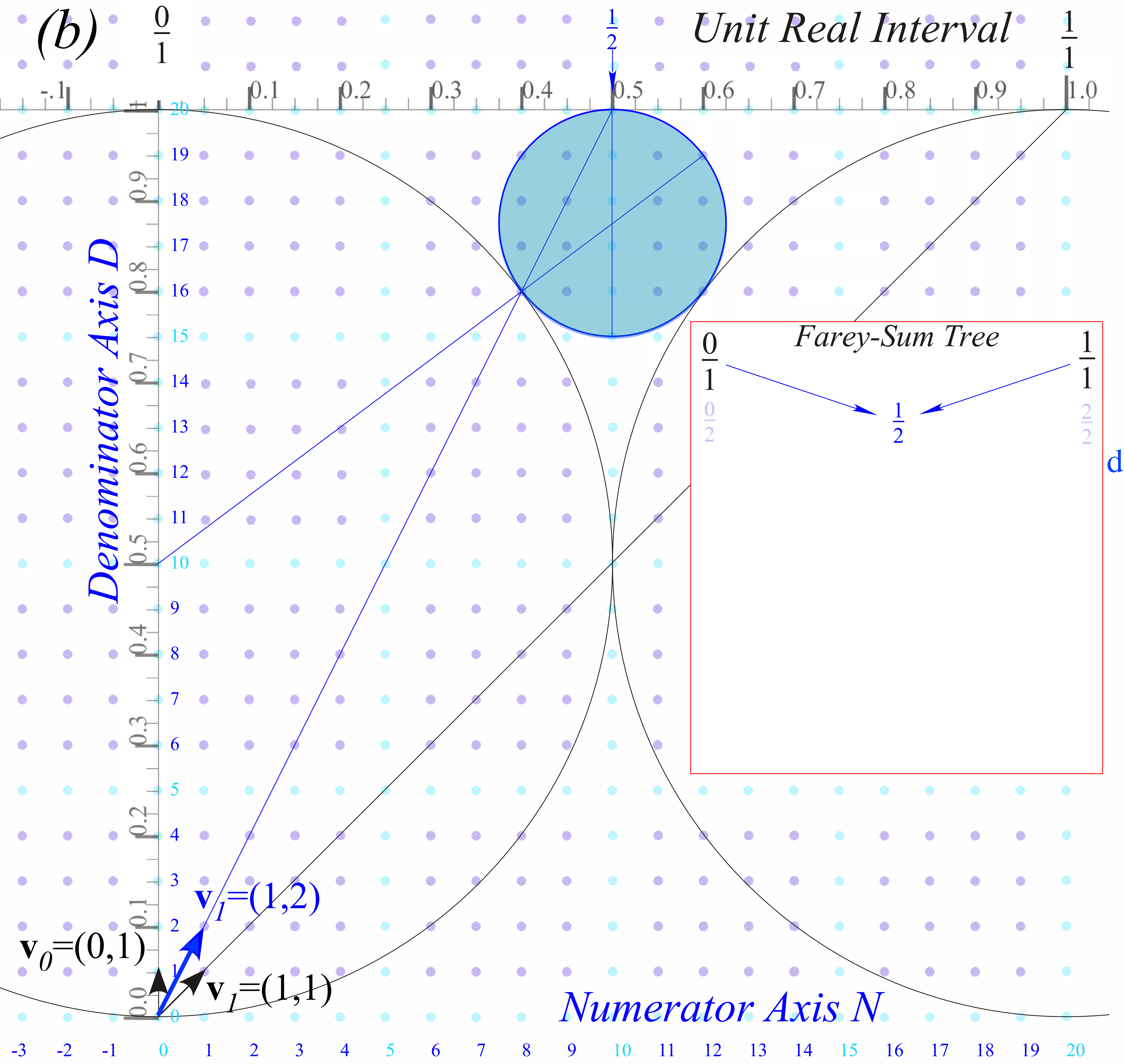
Li, Harter, Chem.Phys.Letters **213**, *208-213 (2015)]*

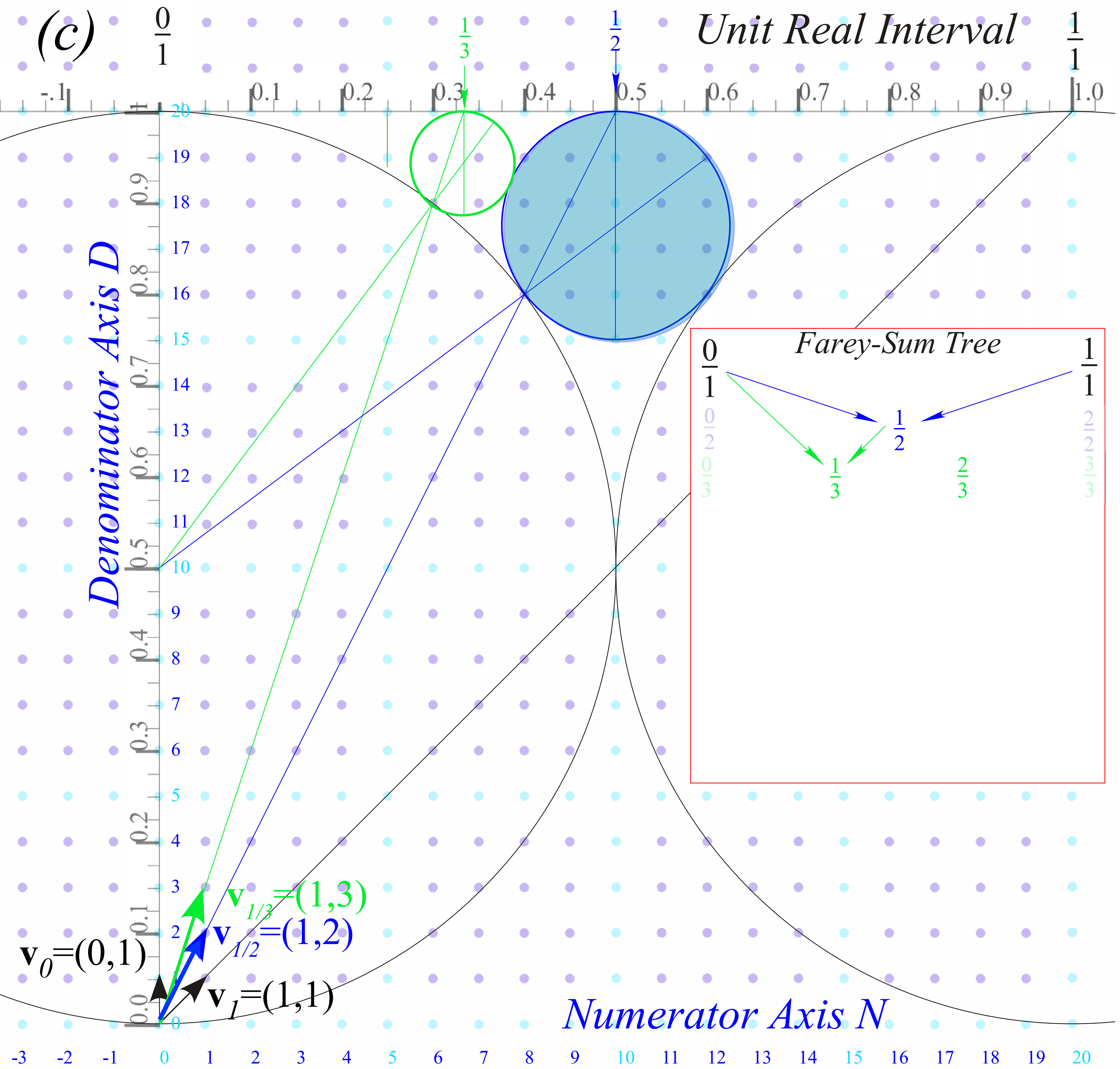


Farey Sum related to vector sum and *Ford Circles*

1/1-circle has diameter *1*

1/2-circle has diameter $1/2^2=1/4$

Li, Harter, Chem.Phys.Letters **213**, *208-213 (2015)*]

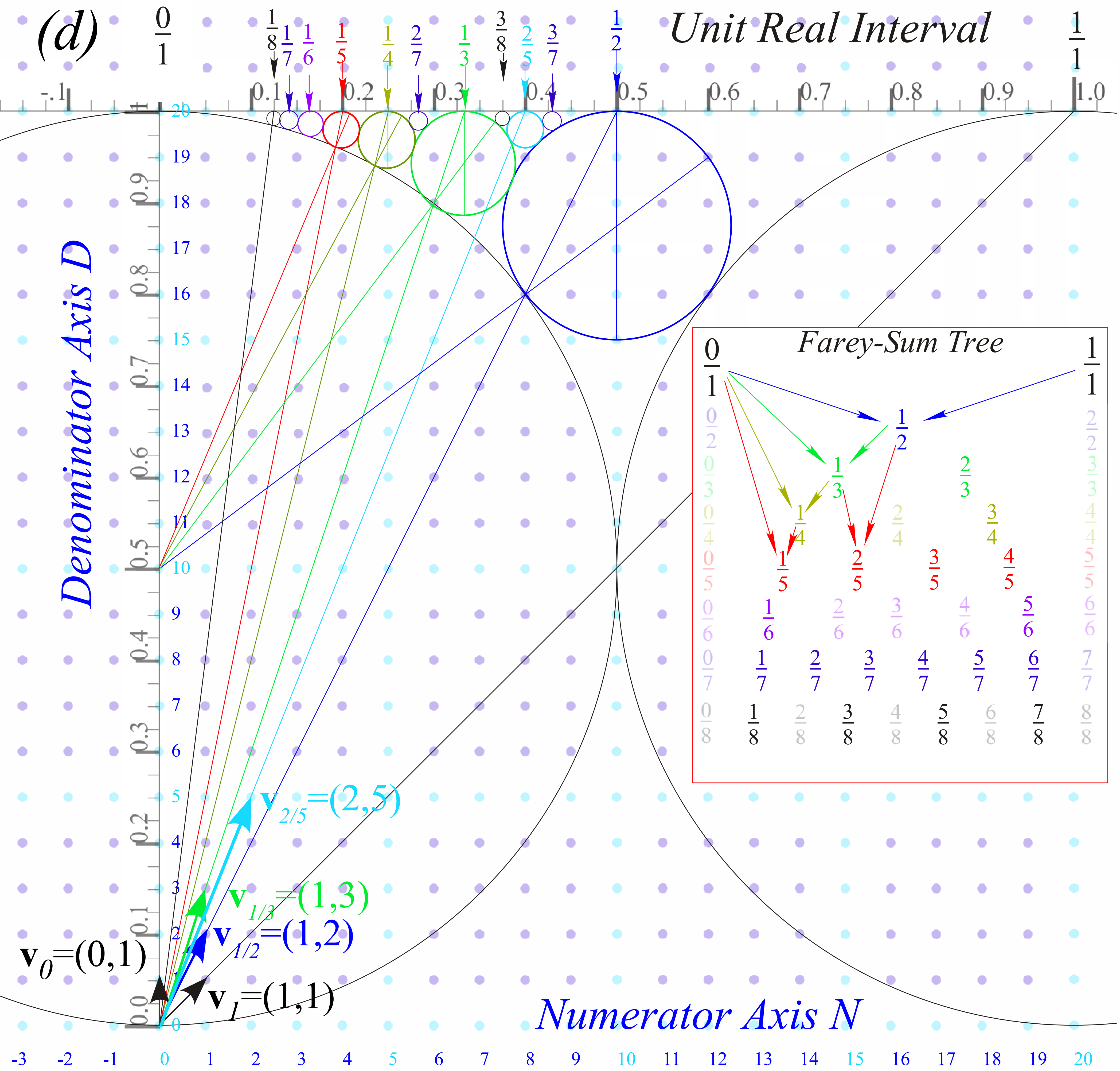


Farey Sum related to vector sum and *Ford Circles*

1/2-circle has diameter $1/2^2=1/4$

1/3-circles have diameter $1/3^2=1/9$

Li, Harter, Chem.Phys.Letters **213**, *208-213 (2015)]*



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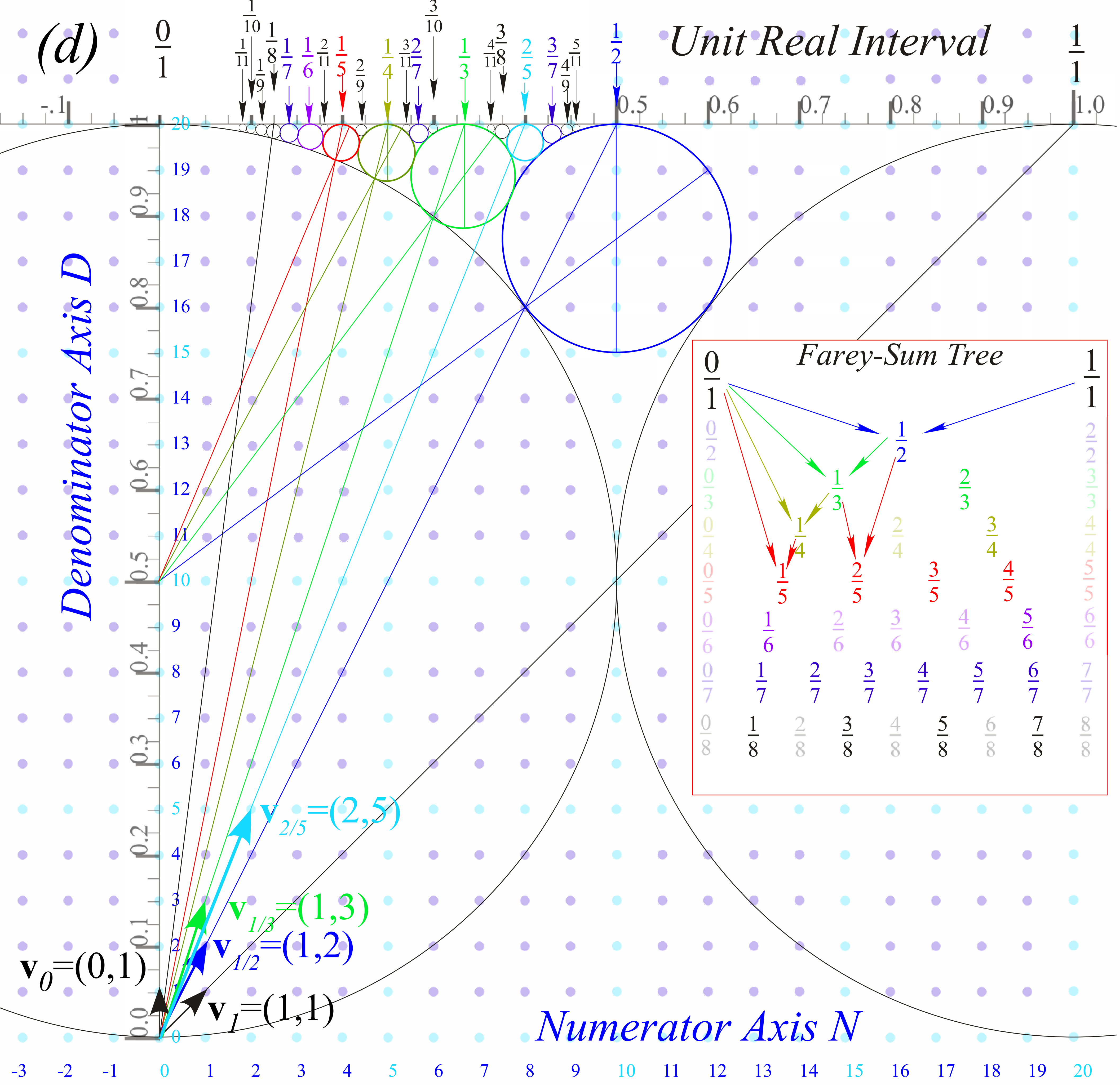
n/d-circles have diameter $1/d^2$

Li, Harter, Chem.Phys.Letters **213**, *208-213 (2015)]*



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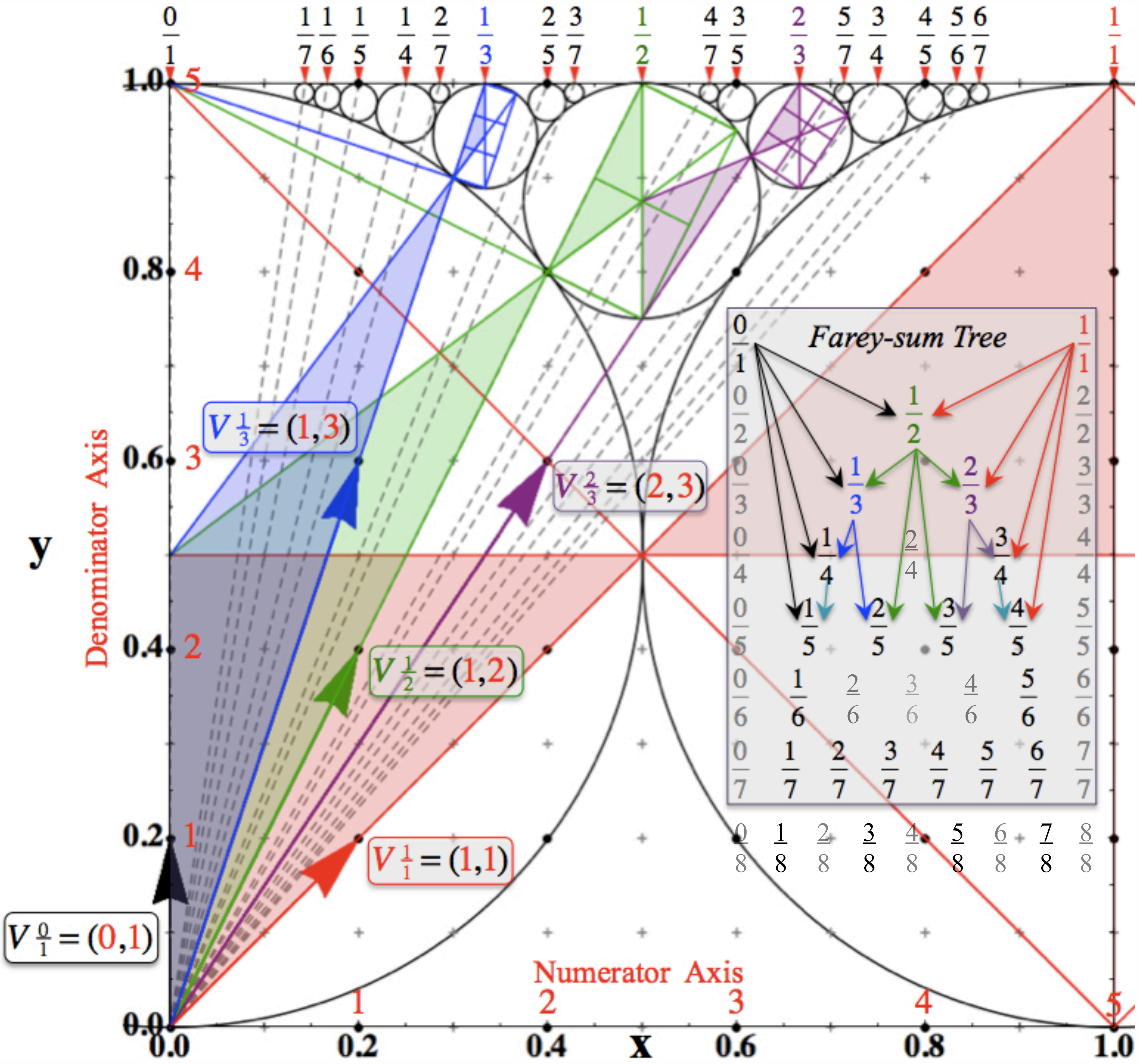
Li, Harter, Chem.Phys.Letters ***213**, 208-213 (2015)]*



Thales Rectangles

provide
analytic geometry
of
fractal structure

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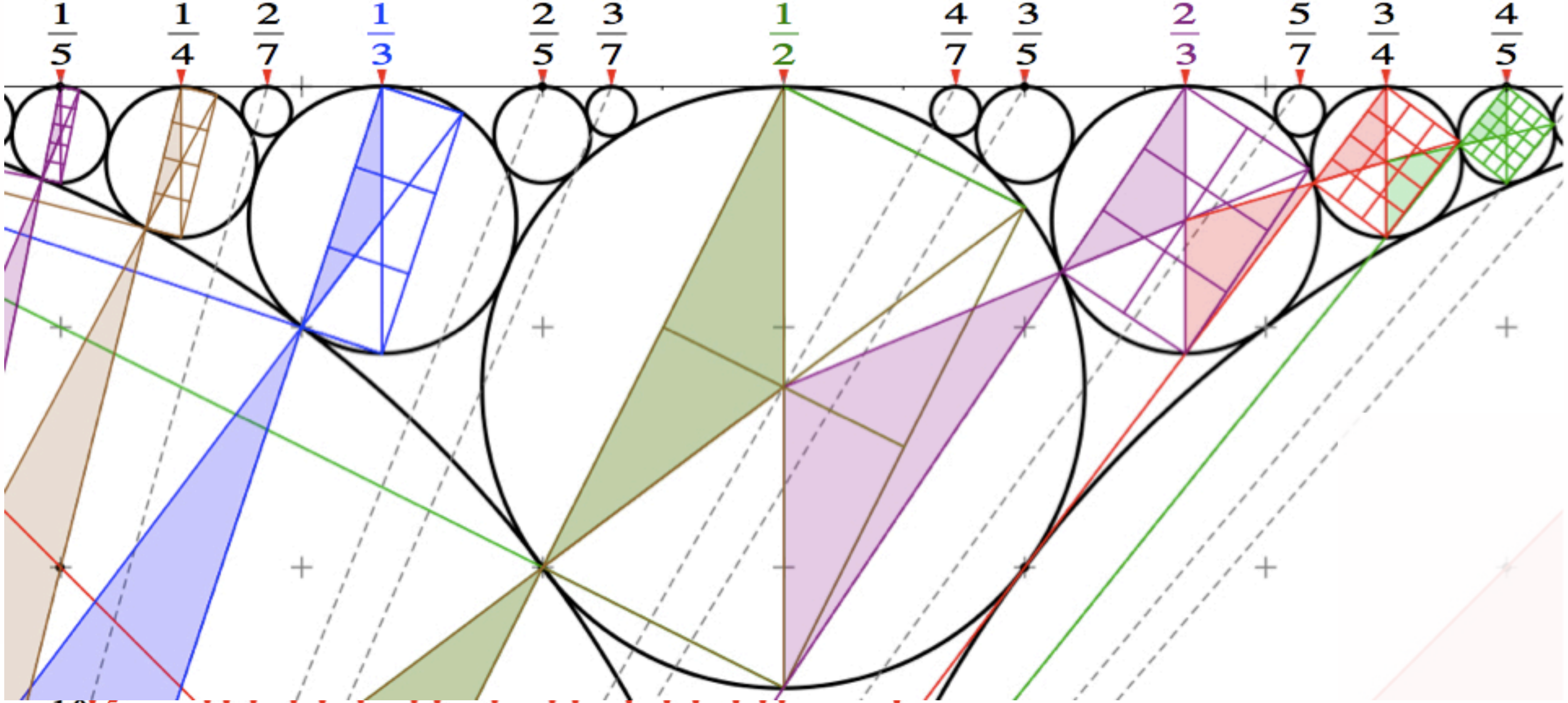
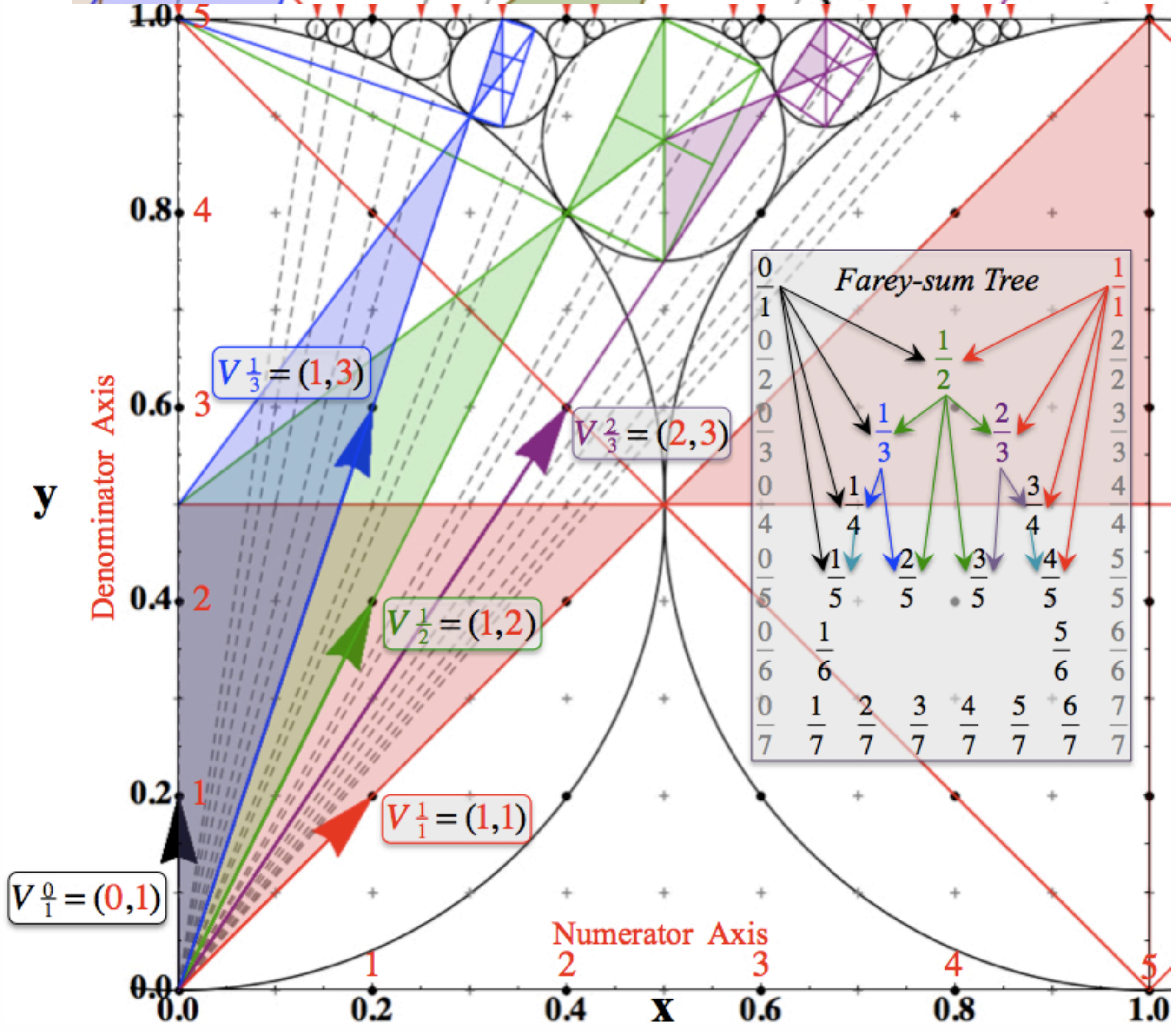


"Quantized" Thales Rectangles

provide
analytic geometry
of
fractal structure

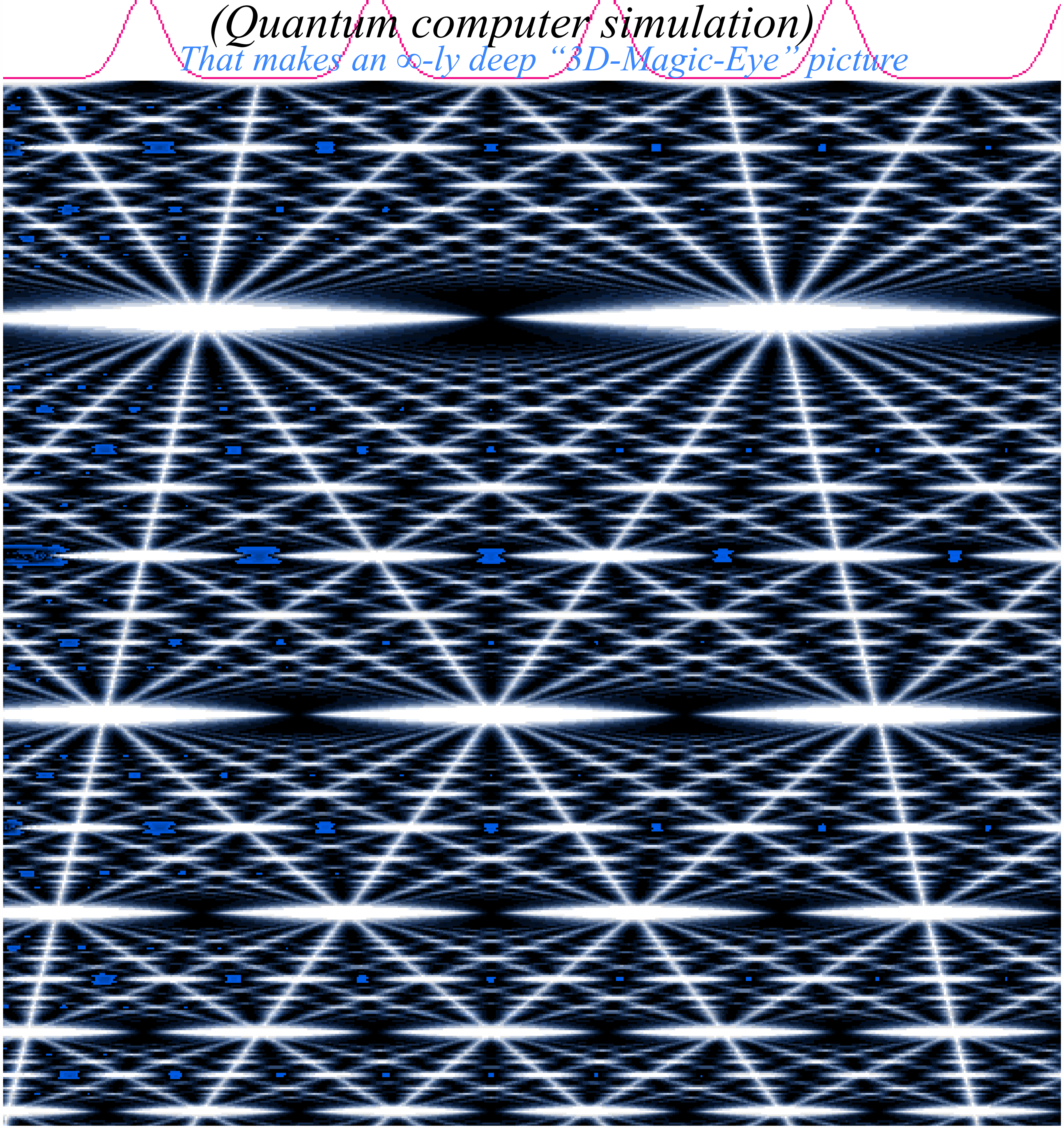


Li, Harter, Chem.Phys.Letters
213, *208-213 (2015)*]

$D \le 1$	$\boldsymbol{\frac{0}{1}}$																						$\boldsymbol{\frac{1}{1}}$
$D \le 2$	$\frac{0}{1}$											$\boldsymbol{\frac{1}{2}}$											$\frac{1}{1}$
$D \le 3$	$\frac{0}{1}$							$\boldsymbol{\frac{1}{3}}$				$\frac{1}{2}$				$\boldsymbol{\frac{2}{3}}$							$\frac{1}{1}$
$D \le 4$	$\frac{0}{1}$					$\boldsymbol{\frac{1}{4}}$		$\frac{1}{3}$				$\frac{1}{2}$				$\frac{2}{3}$		$\boldsymbol{\frac{3}{4}}$					$\frac{1}{1}$
$D \le 5$	$\frac{0}{1}$				$\boldsymbol{\frac{1}{5}}$	$\frac{1}{4}$		$\frac{1}{3}$		$\boldsymbol{\frac{2}{5}}$		$\frac{1}{2}$		$\boldsymbol{\frac{3}{5}}$		$\frac{2}{3}$		$\frac{3}{4}$	$\boldsymbol{\frac{4}{5}}$				$\frac{1}{1}$
$D \le 6$	$\frac{0}{1}$			$\boldsymbol{\frac{1}{6}}$	$\frac{1}{5}$	$\frac{1}{4}$		$\frac{1}{3}$		$\frac{2}{5}$		$\frac{1}{2}$		$\frac{3}{5}$		$\frac{2}{3}$		$\frac{3}{4}$	$\frac{4}{5}$	$\boldsymbol{\frac{5}{6}}$			$\frac{1}{1}$
$D \le 7$	$\frac{0}{1}$		$\boldsymbol{\frac{1}{7}}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\boldsymbol{\frac{2}{7}}$	$\frac{1}{3}$		$\frac{2}{5}$	$\boldsymbol{\frac{3}{7}}$	$\frac{1}{2}$	$\boldsymbol{\frac{4}{7}}$	$\frac{3}{5}$		$\frac{2}{3}$	$\boldsymbol{\frac{5}{7}}$	$\frac{3}{4}$	$\frac{4}{5}$	$\frac{5}{6}$	$\boldsymbol{\frac{6}{7}}$		$\frac{1}{1}$
$D \le 8$	$\frac{0}{1}$	$\boldsymbol{\frac{1}{8}}$	$\frac{1}{7}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{2}{7}$	$\frac{1}{3}$	$\boldsymbol{\frac{3}{8}}$	$\frac{2}{5}$	$\frac{3}{7}$	$\frac{1}{2}$	$\frac{4}{7}$	$\frac{3}{5}$	$\boldsymbol{\frac{5}{8}}$	$\frac{2}{3}$	$\frac{5}{7}$	$\frac{3}{4}$	$\frac{4}{5}$	$\frac{5}{6}$	$\frac{6}{7}$	$\boldsymbol{\frac{7}{8}}$	$\frac{1}{1}$

(Quantum computer simulation)

That makes an ∞-ly deep "3D-Magic-Eye" picture



Bohr-rotor wave dynamics and group vs. phase velocity
    Gaussian wave-packet bandwidth and uncertainty
        Gaussian Bohr-rotor revivals and quantum fractals
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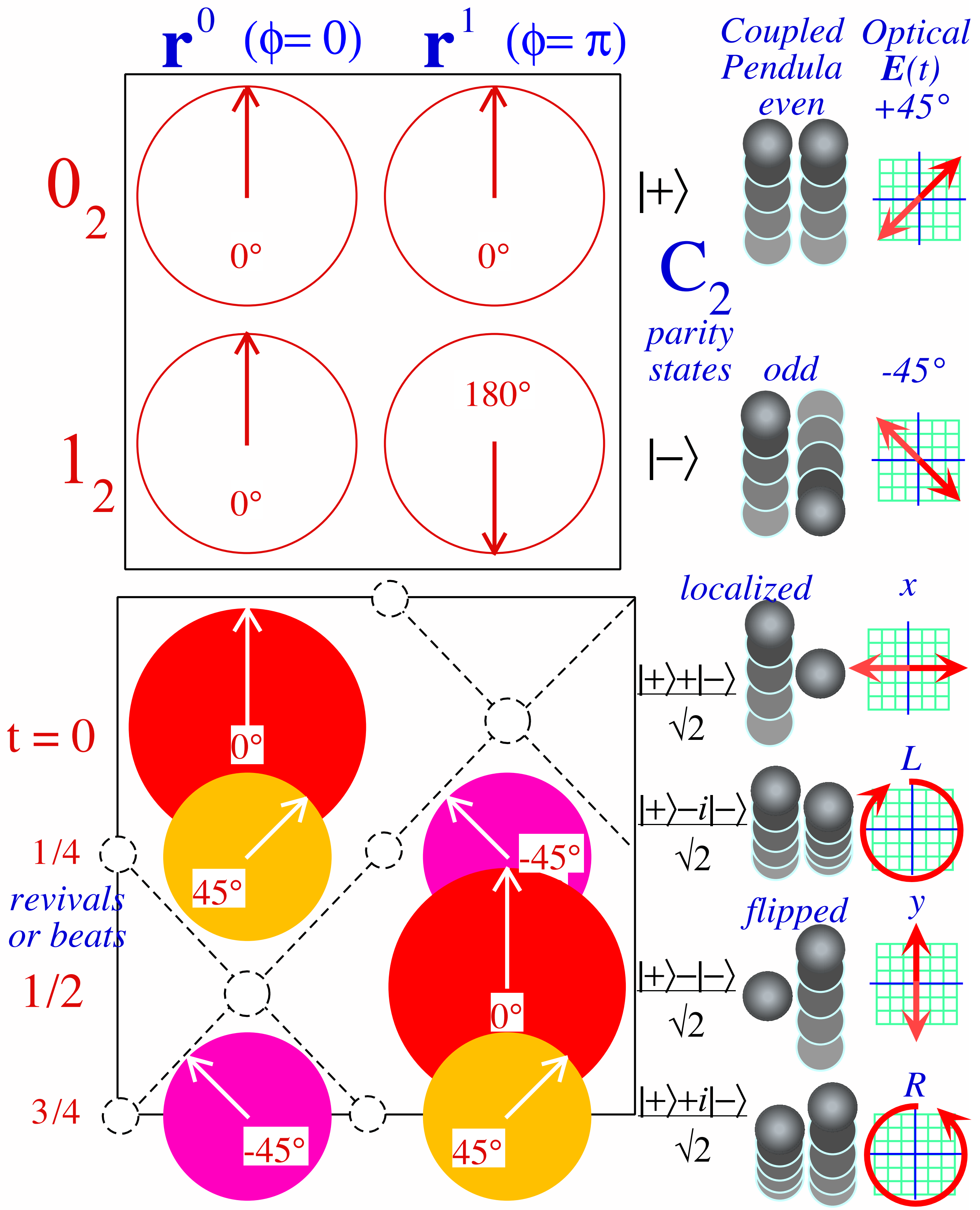
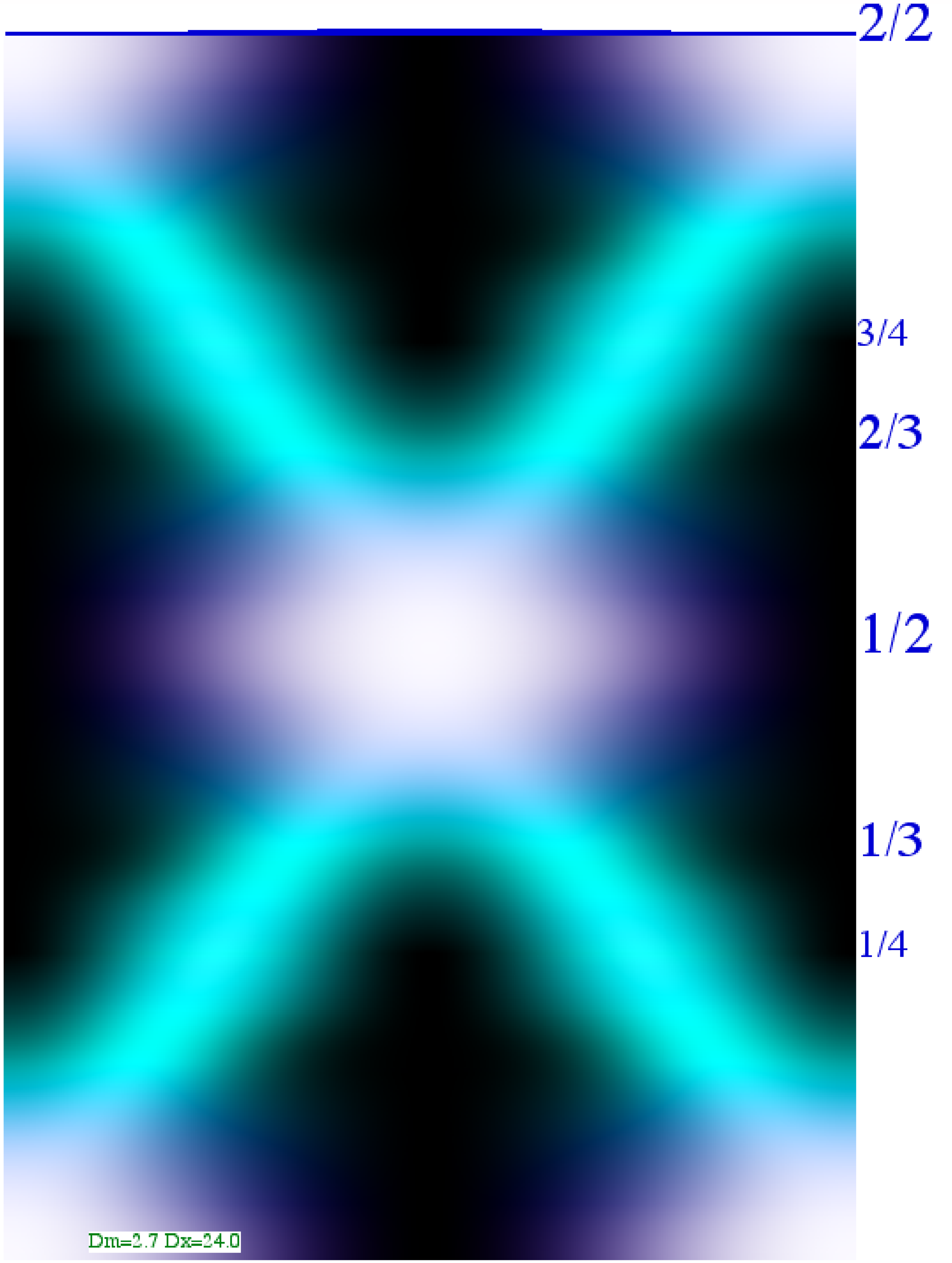
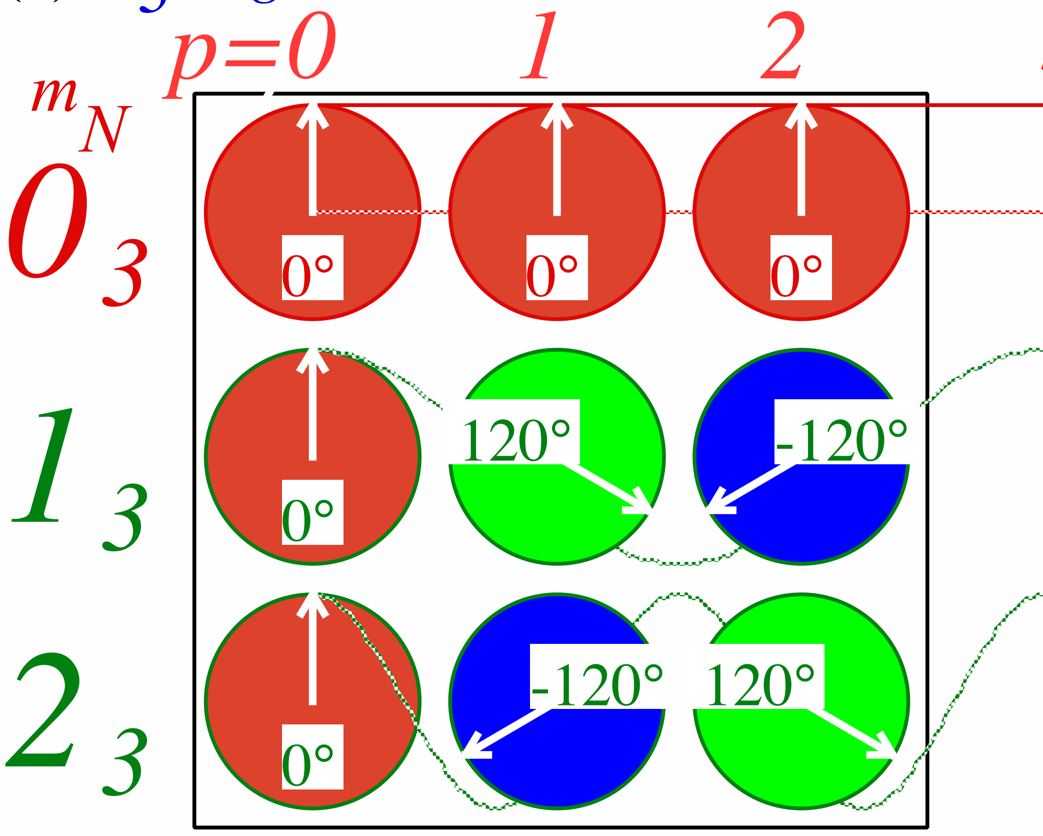
Fundamental Beats and 2-Level Transitions: The “Mother of all symmetry” is C_2

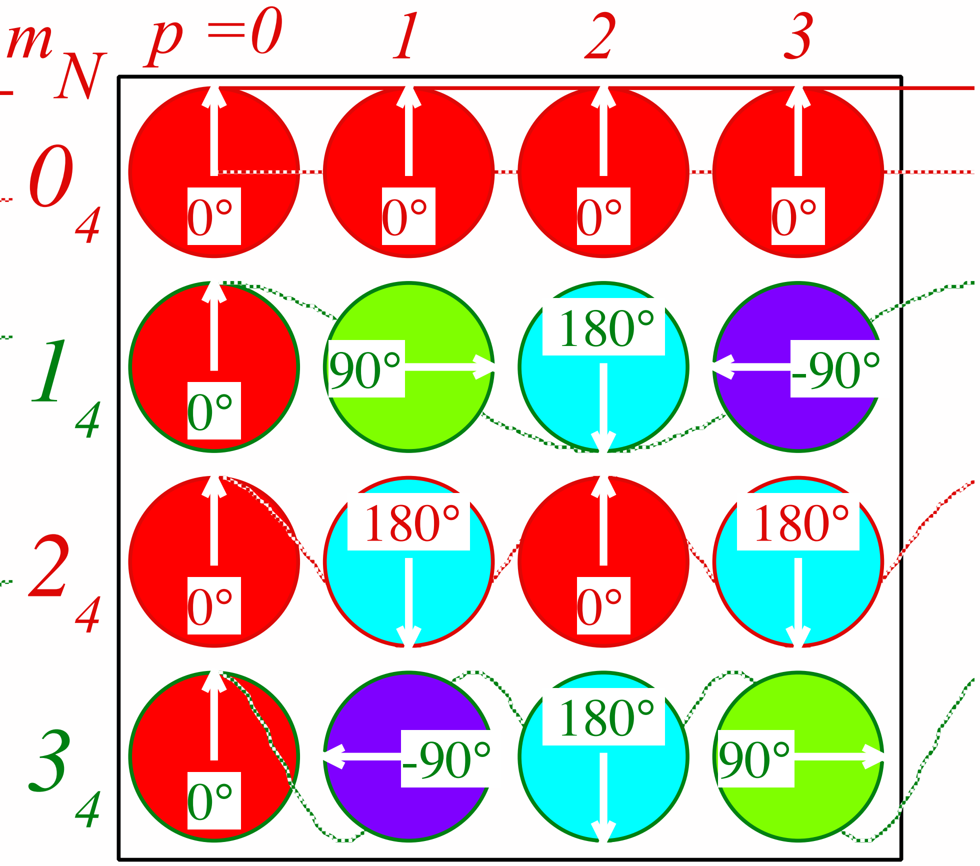




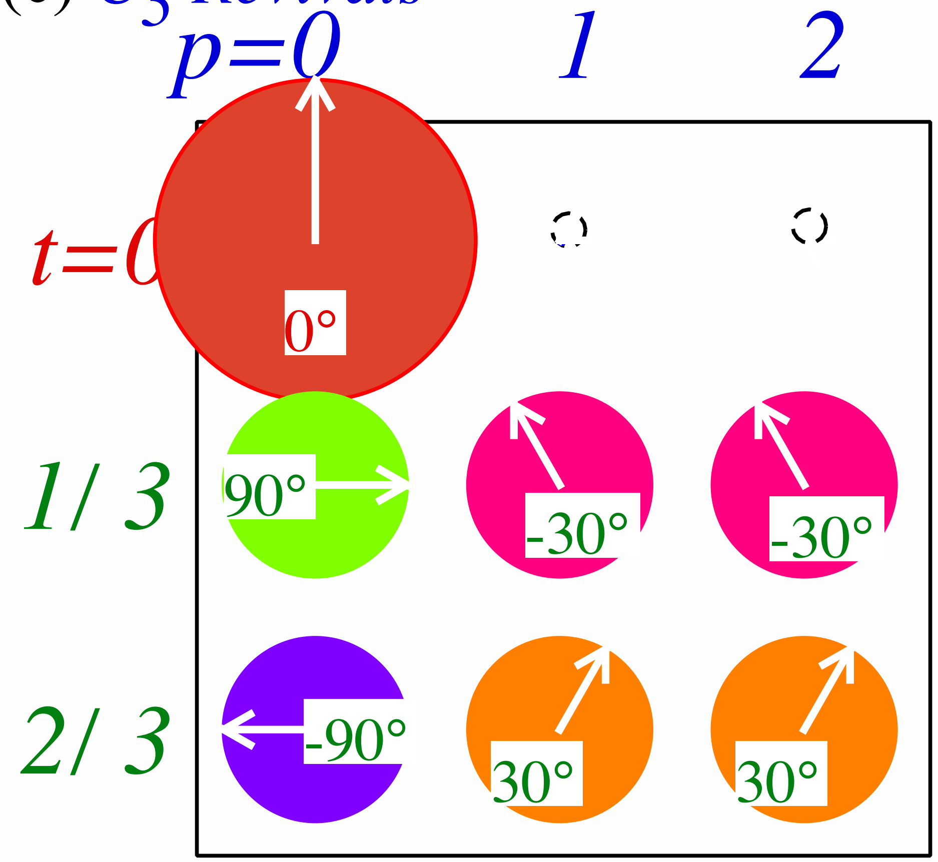
(a) C_3 Eigenstate Characters



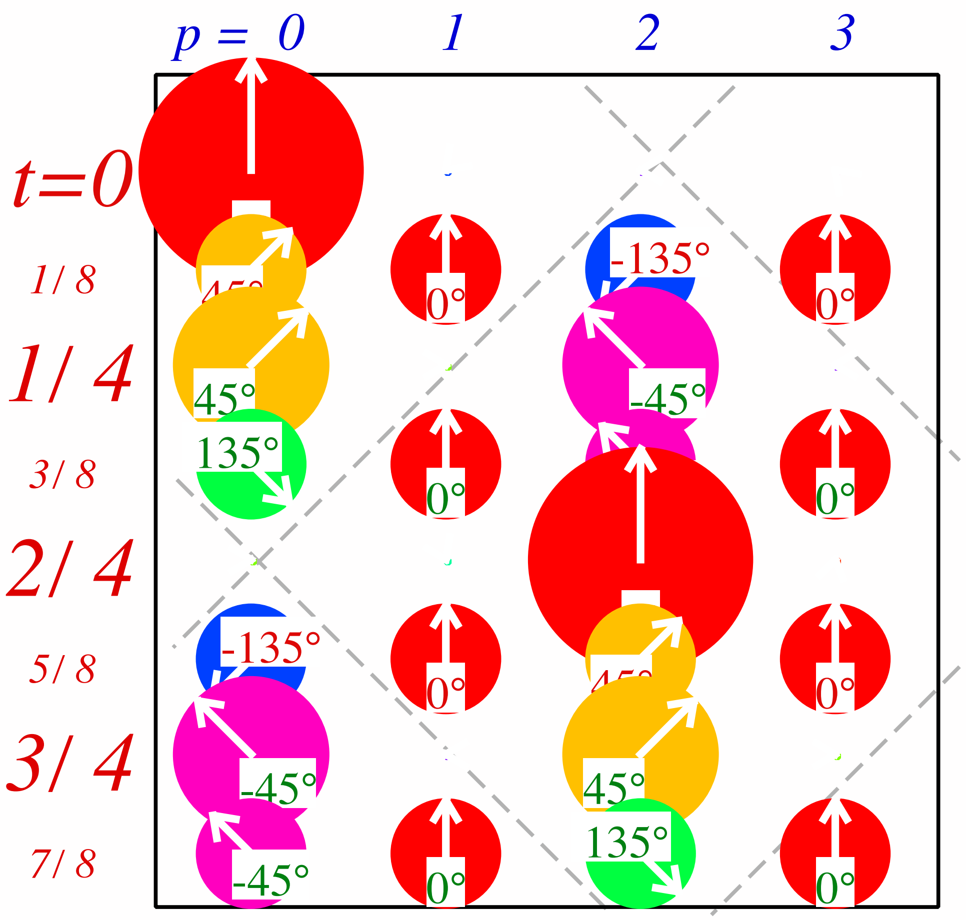
(b) C_4 Eigenstate Characters



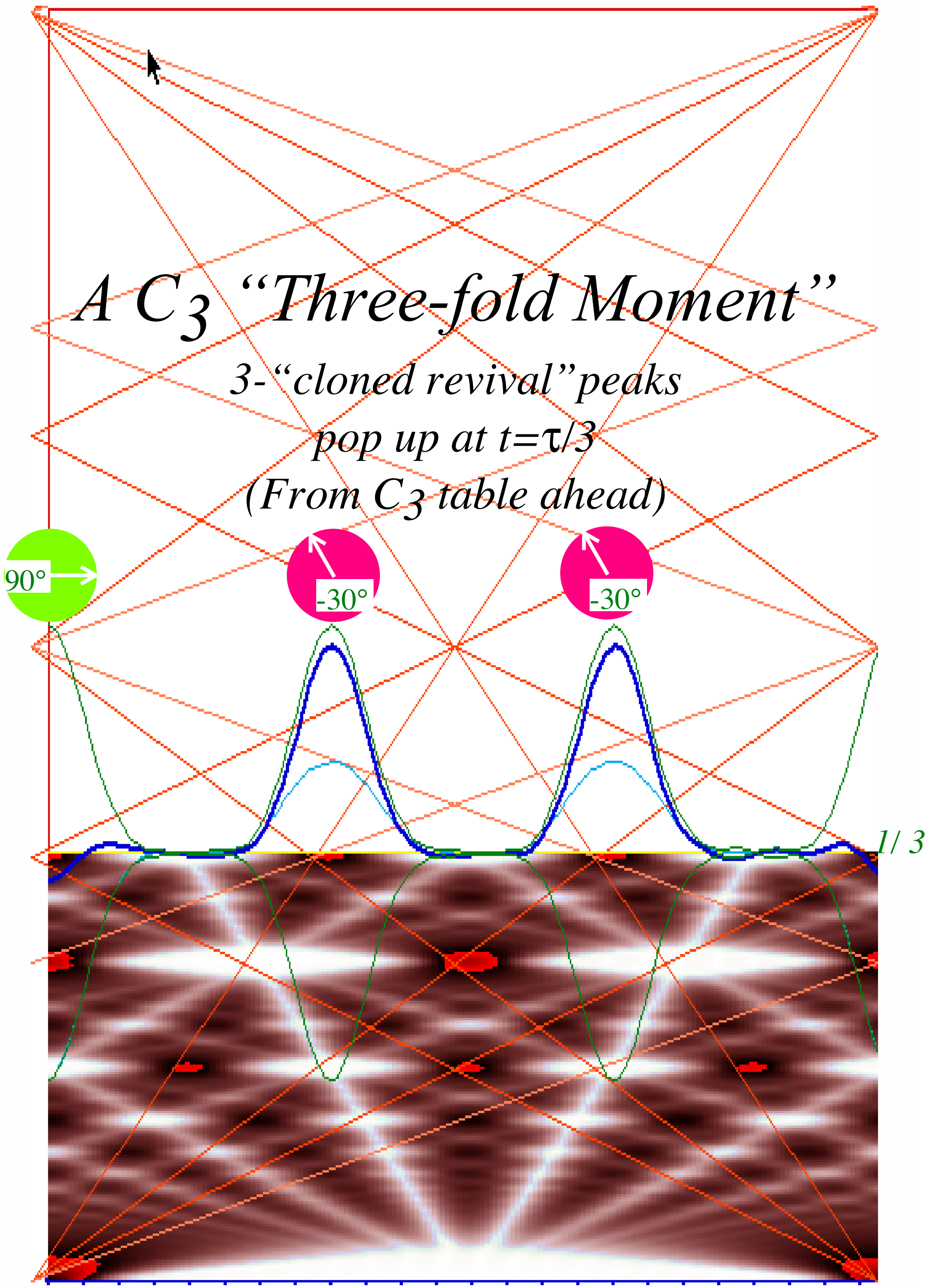
(c) C_3 Revivals



(d) C_4 Revivals

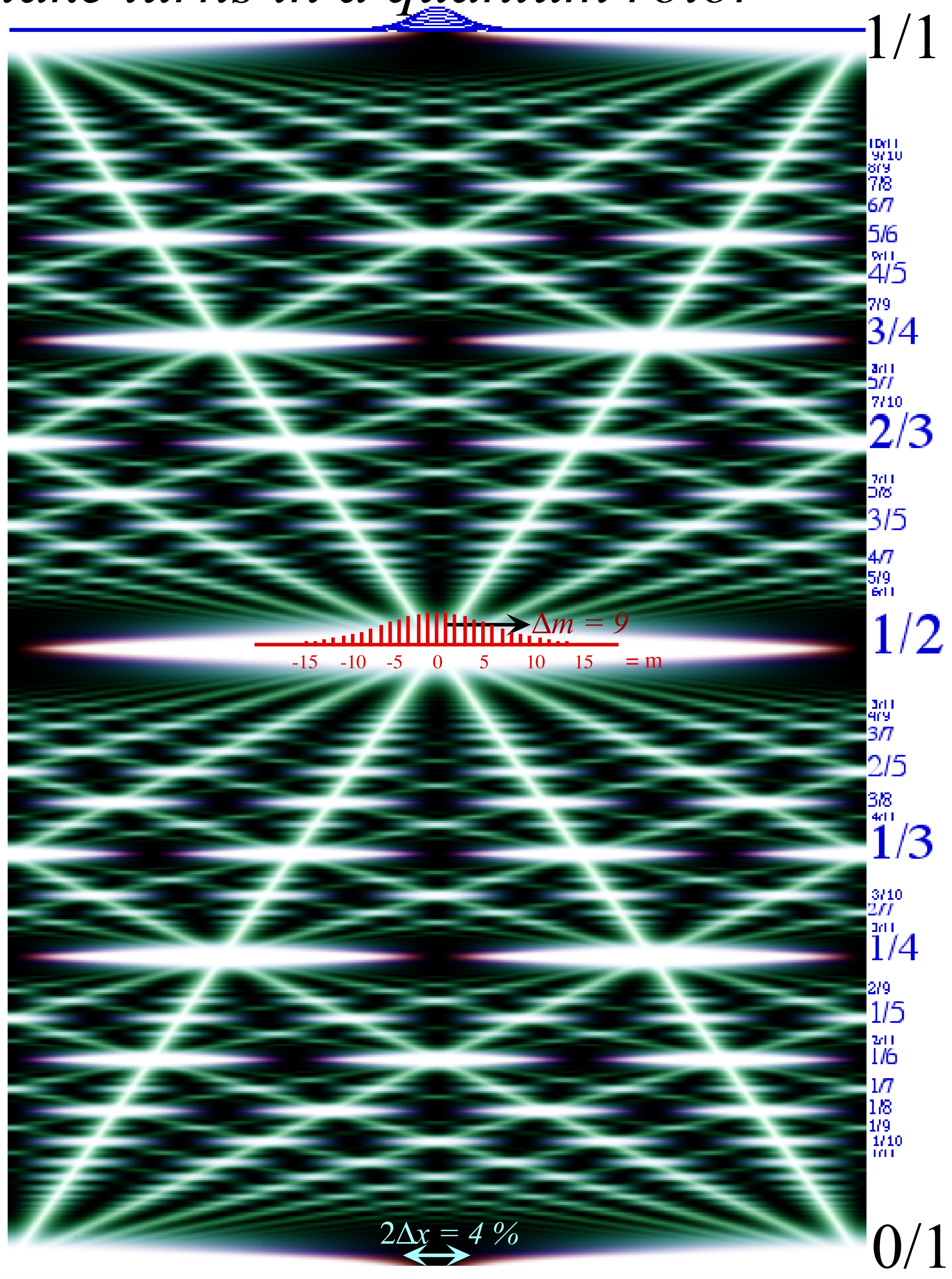


Revivals: All excited transitions take turns in a quantum rotor



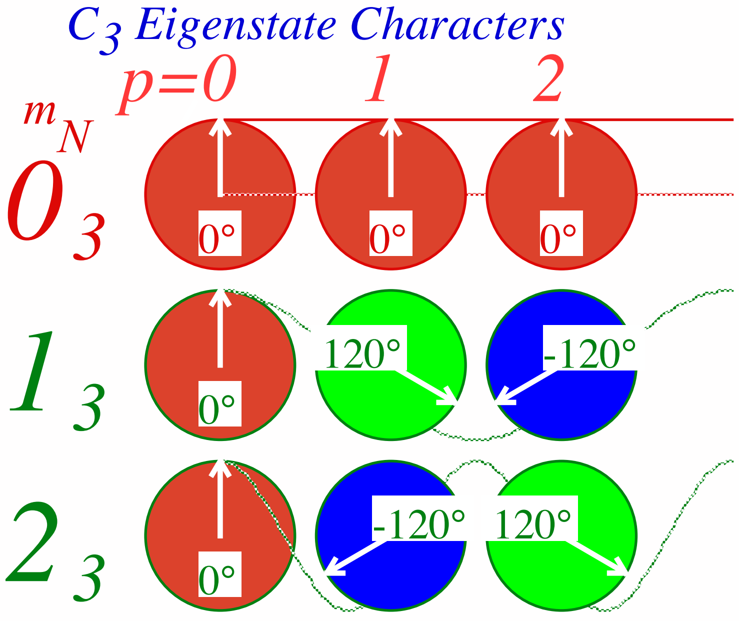
A C_3 "Three-fold Moment"

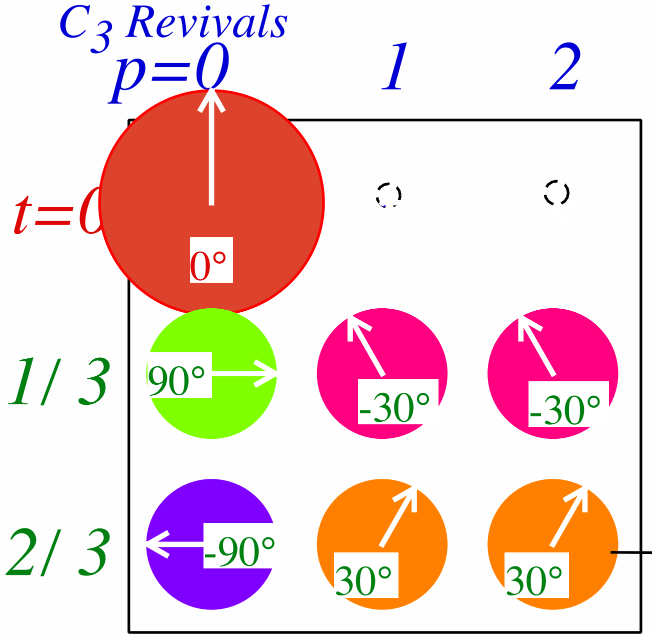
3-"cloned revival" peaks pop up at $t=\tau/3$ (From C_3 table ahead)



Simulating Complex Systems With Simpler Ones

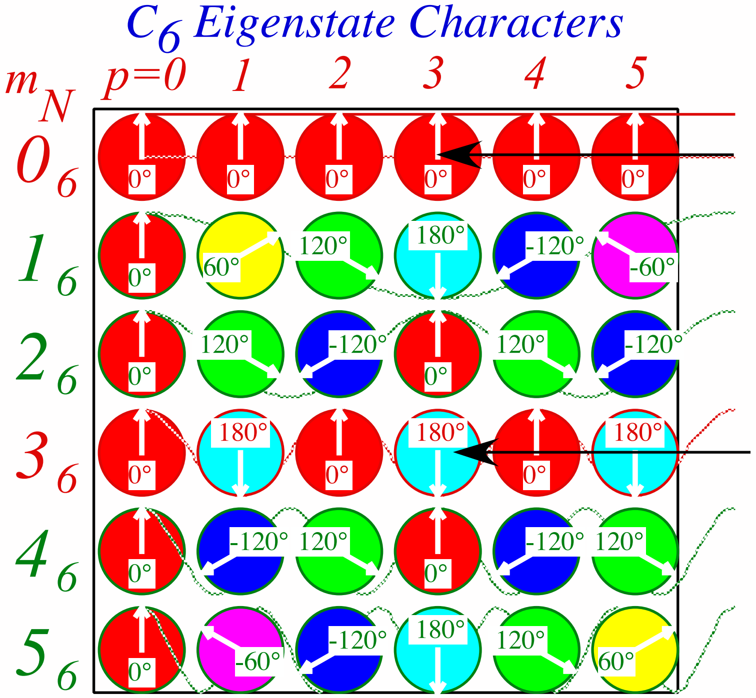
Discrete 3-State or Trigonal System
(Tesla's 3-Phase AC)





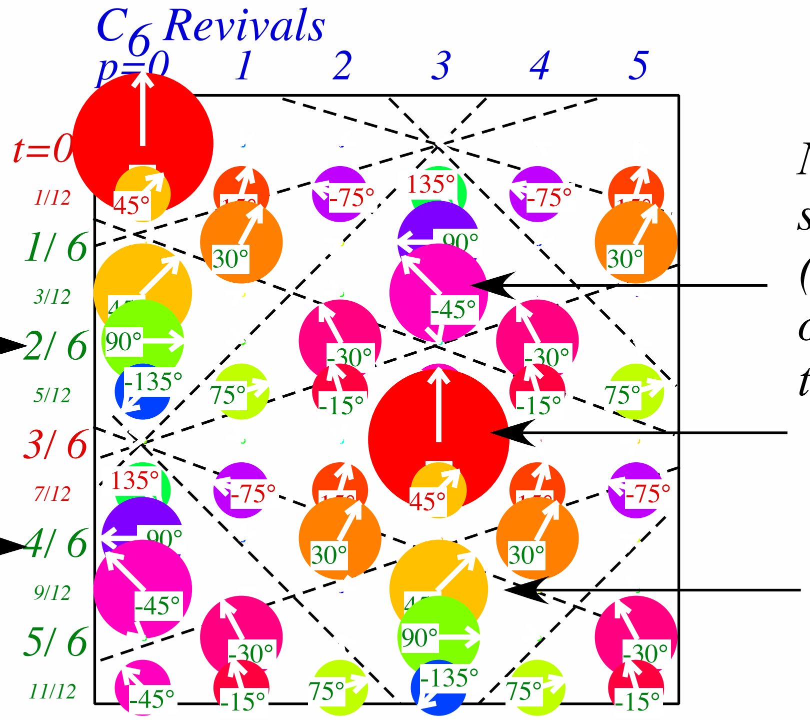
Note 3-phase sub-symmetry

Discrete 6-State or Hexagonal System
(6-Phase AC)



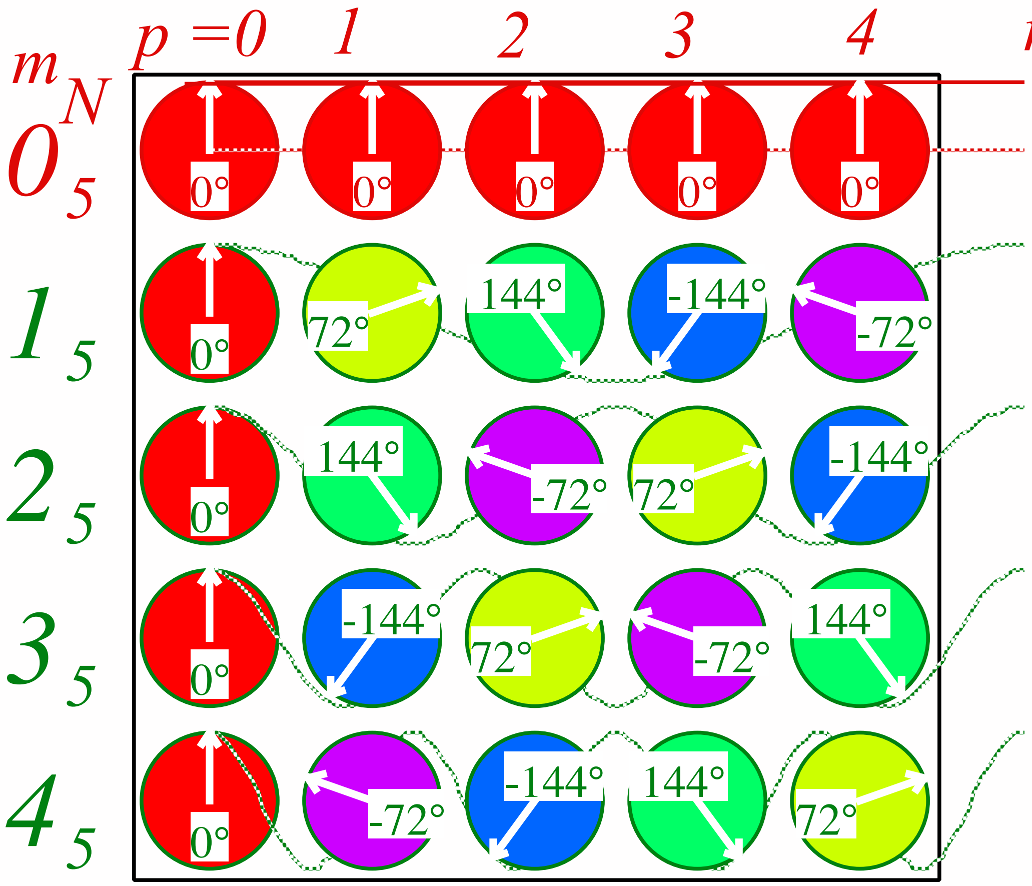
Note
2-phase
AC

C_2

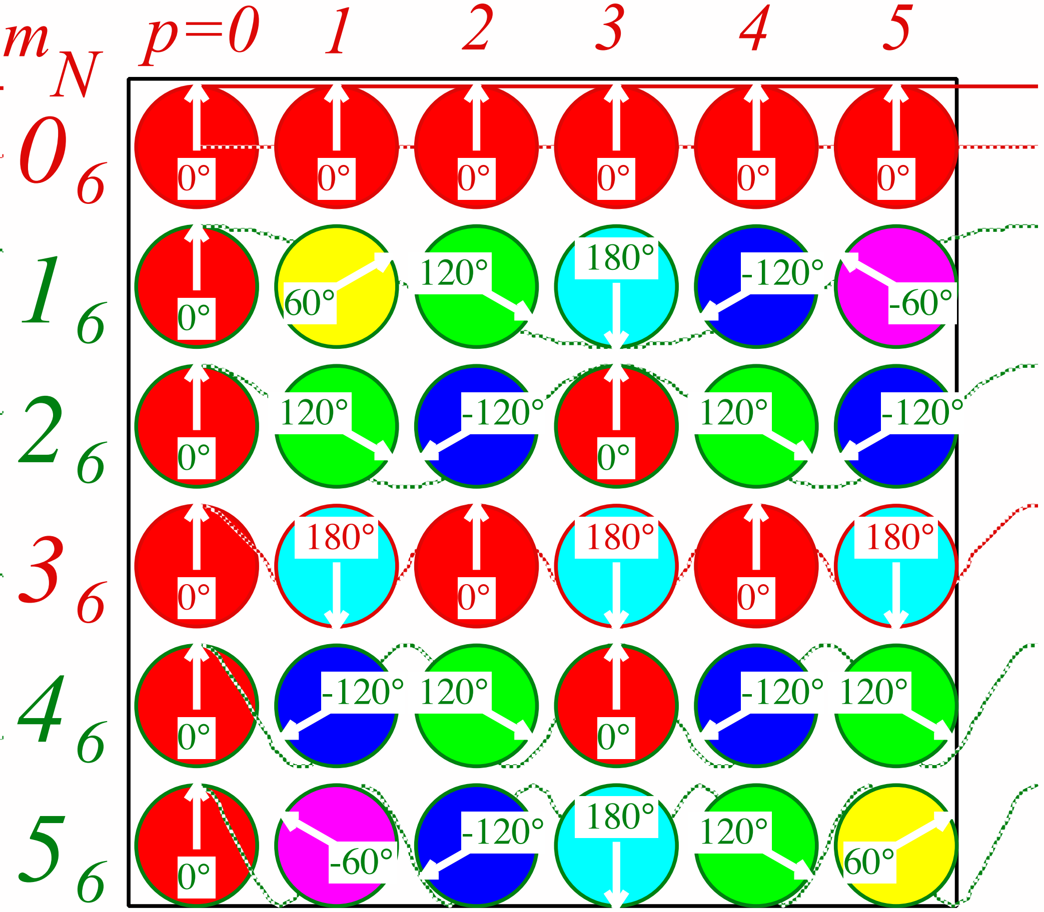


Note 2-phase sub-symmetry (The "Mother of all symmetry" is C_2)

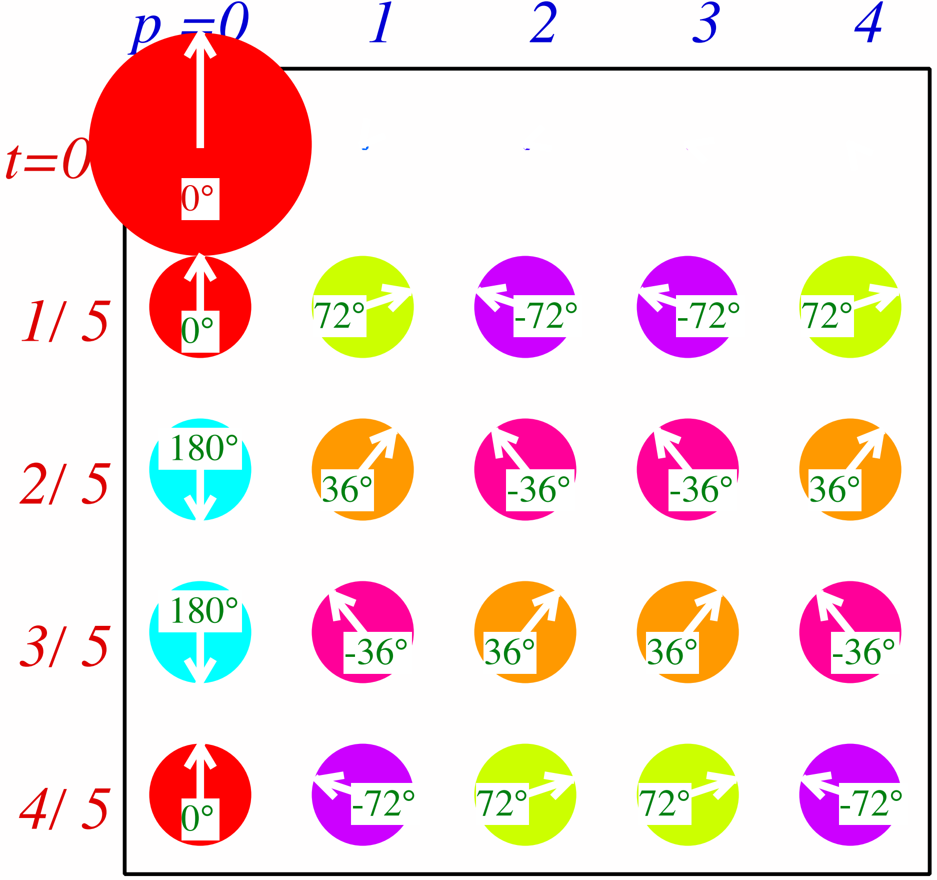
(a) C_5 *Eigenstate Characters*



(b) C_6 *Eigenstate Characters*



(c) C_5 *Revivals*



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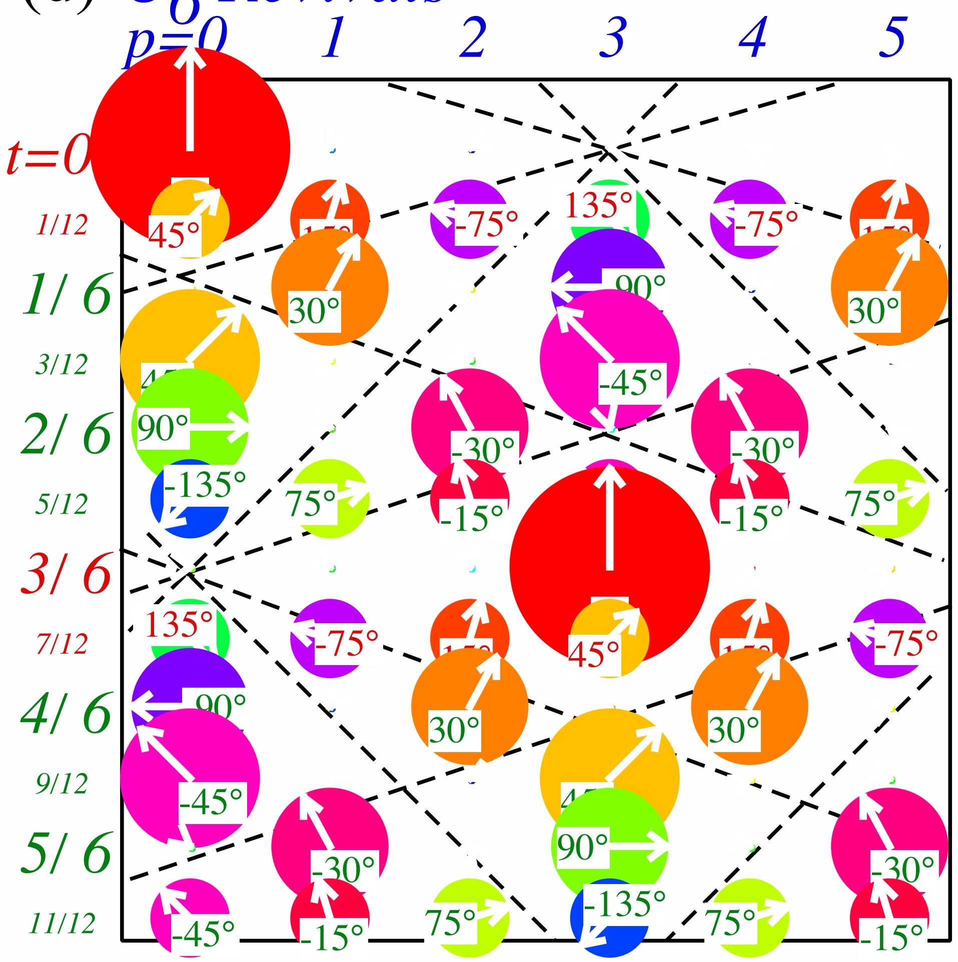


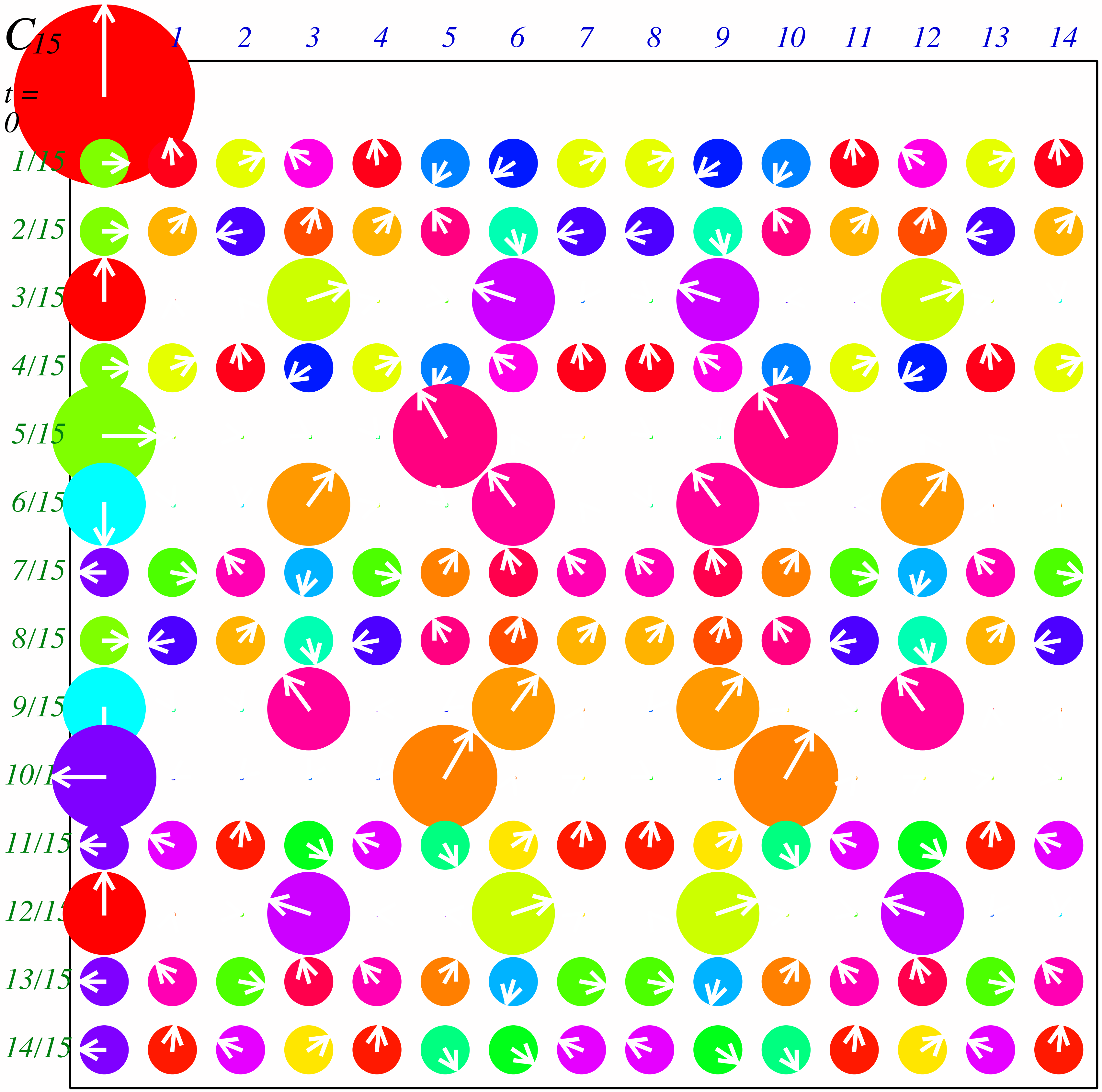
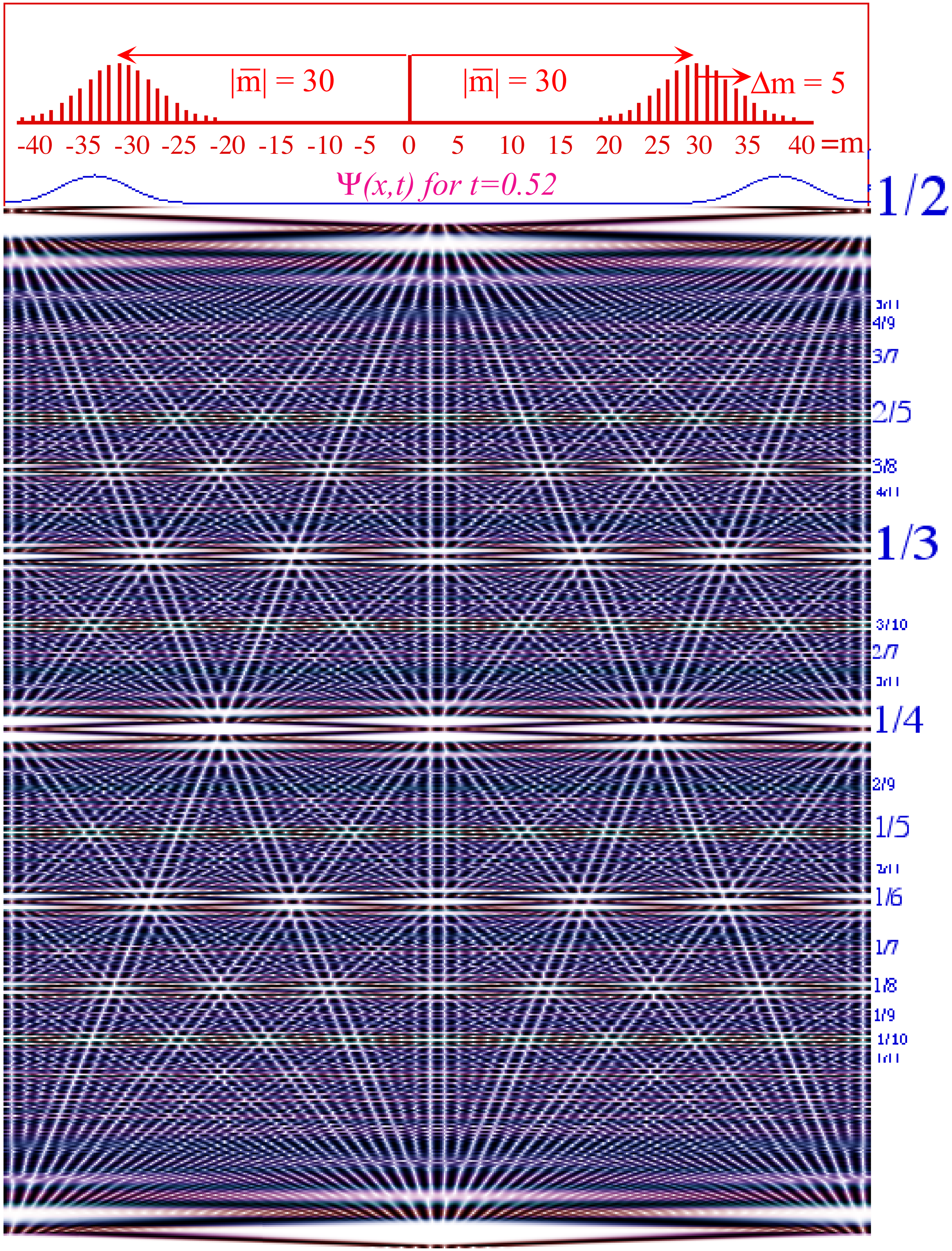


Fig. 9.4.4 Bohr space-time revival pattern for C_{15} Bohr system.


|m̄| = 30
|m̄| = 30
Δm = 5
-40 -35 -30 -25 -20 -15 -10 -5 0 5 10 15 20 25 30 35 40 =m
Ψ(x,t) for t=0.52
1/2
3/11
4/9
3/7
2/5
3/8
4/11
1/3
3/10
2/7
3/11
1/4
2/9
1/5
2/11
1/6
1/7
1/8
1/9
1/10
1/11

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The Classical “Monster Mash”

Classical introduction to

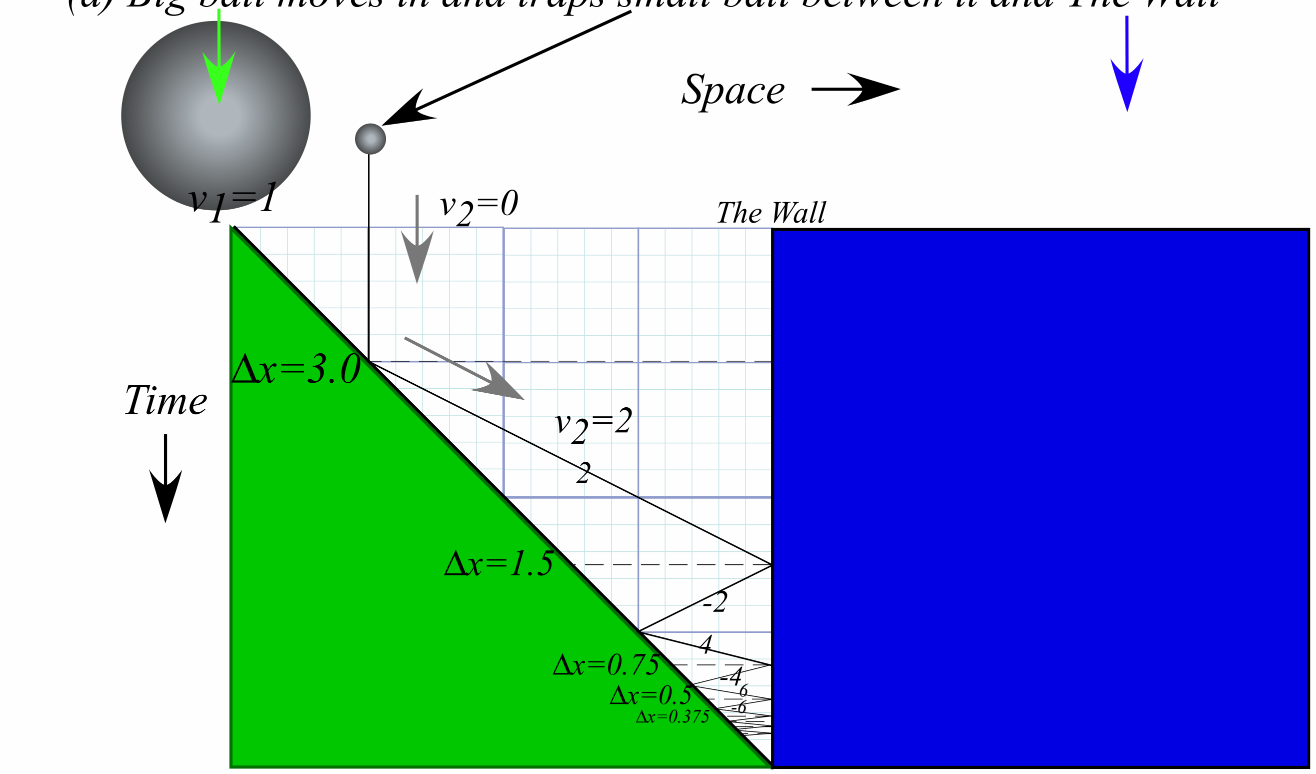
Heisenberg “Uncertainty” Relations

$$v_2 = \frac{const.}{Y} \quad \text{or:} \quad Y \cdot v_2 = const.$$

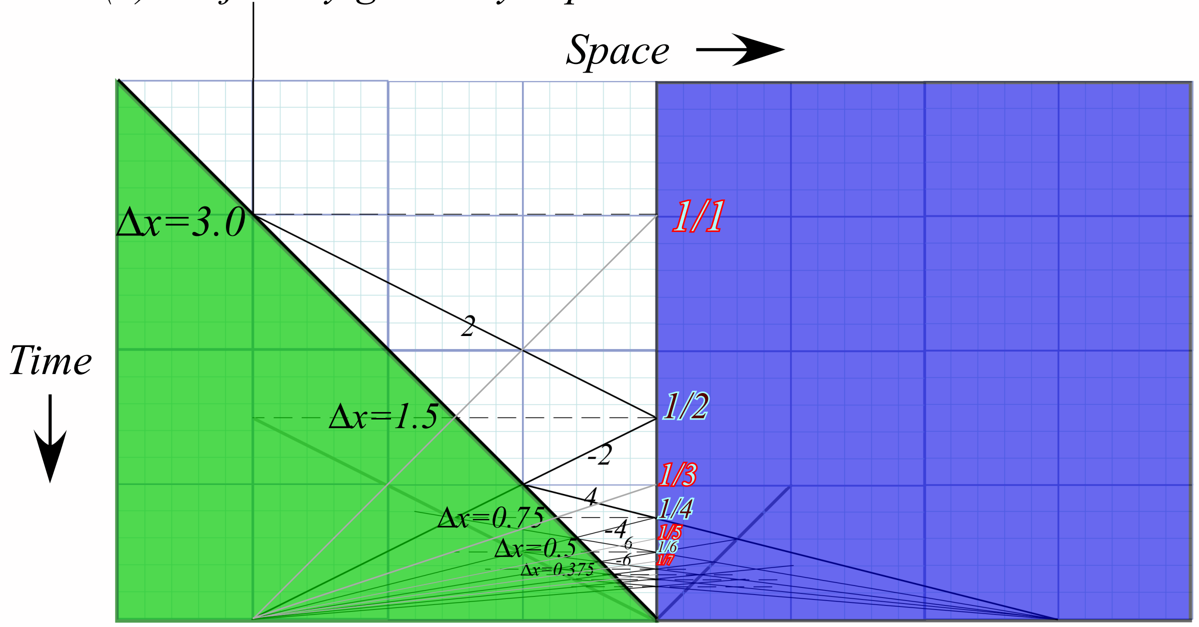
is analogous to: $\Delta x \cdot \Delta p = N \cdot \hbar$

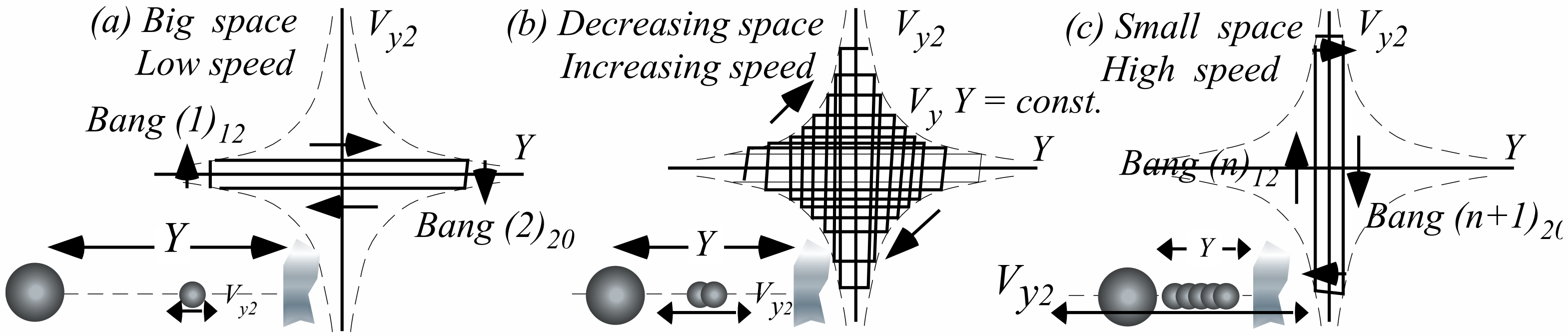
From CMwBang!
Unit 1
Fig. 6.4

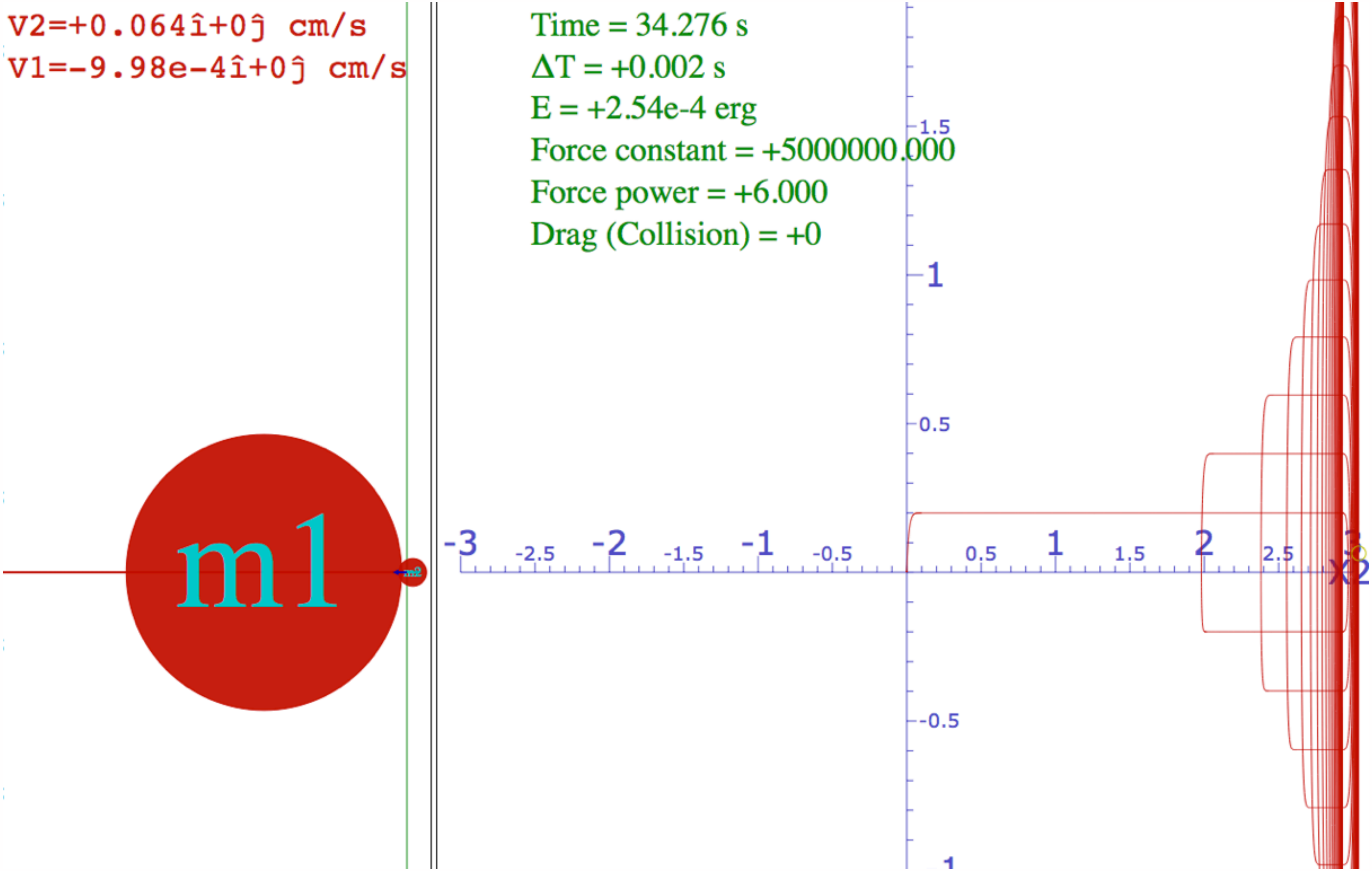
(a) Big ball moves in and traps small ball between it and The Wall



(b) Trajectory geometry exposed







V2=+0.064î+0ĵ cm/s

V1=-9.98e-4î+0ĵ cm/s

Time = 34.276 s

ΔT = +0.002 s

E = +2.54e-4 erg

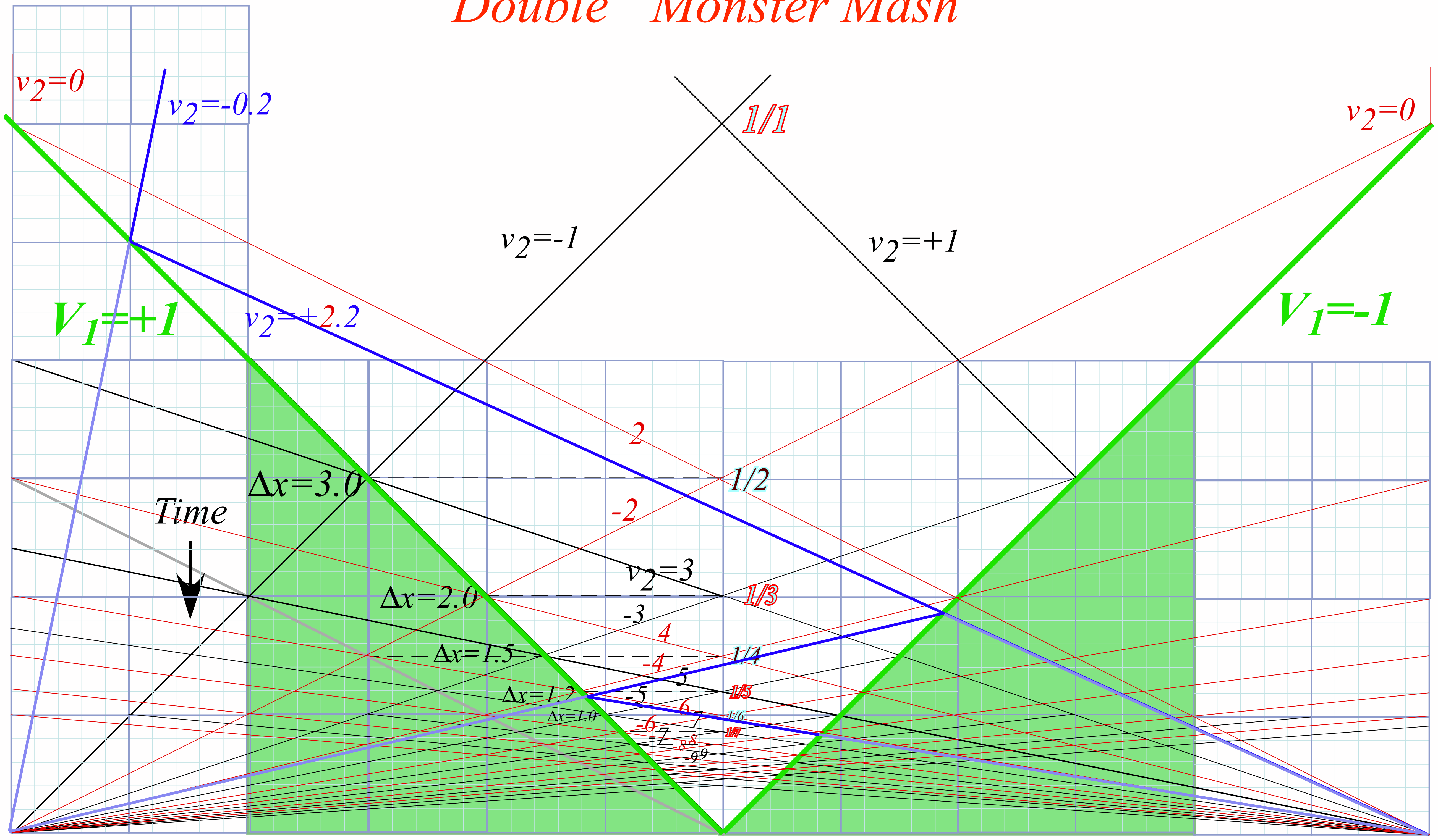
Force constant = +5000000.000

Force power = +6.000

Drag (Collision) = +0

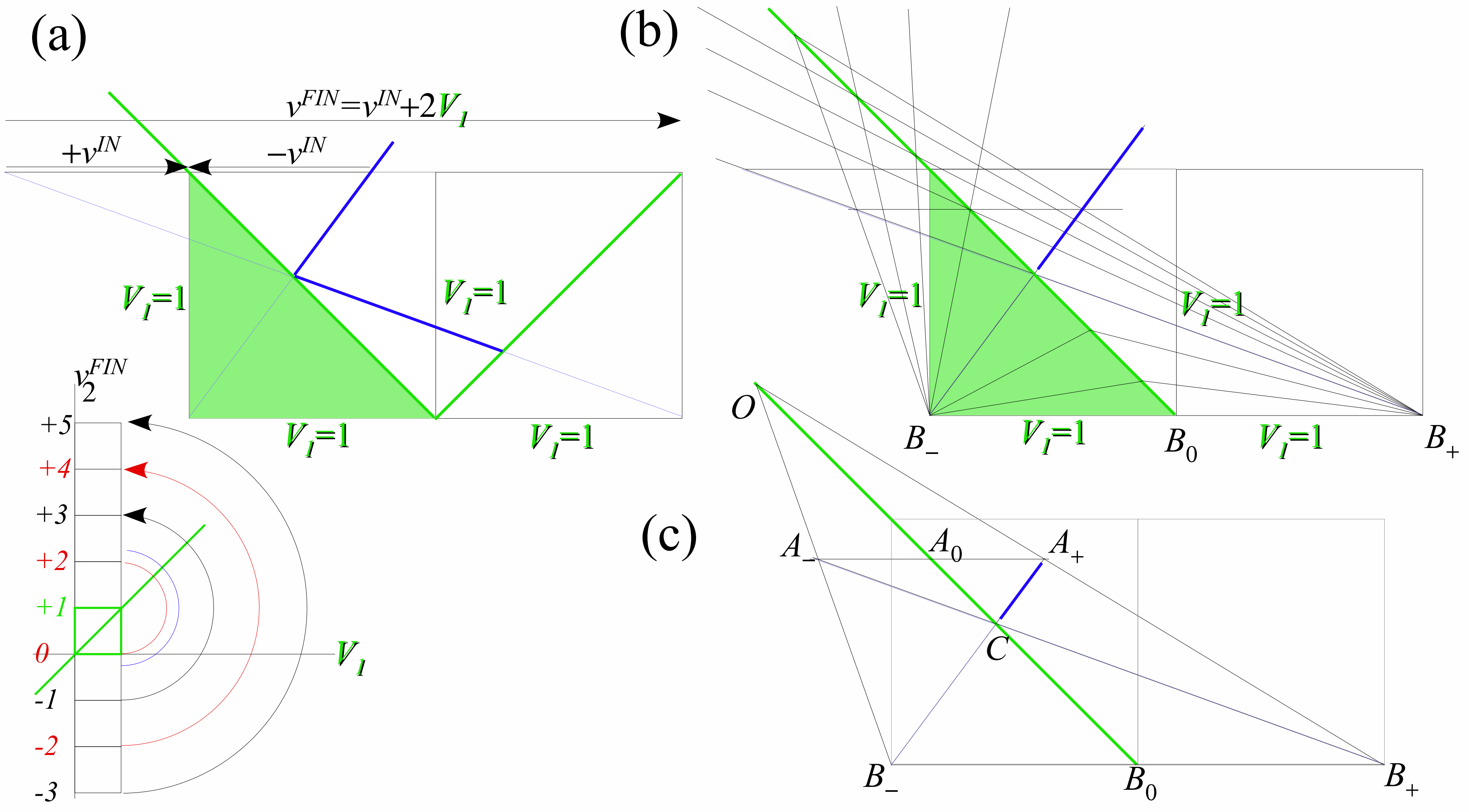
http://www.uark.edu/ua/modphys/markup/BounceItWeb.html?scenario=3000

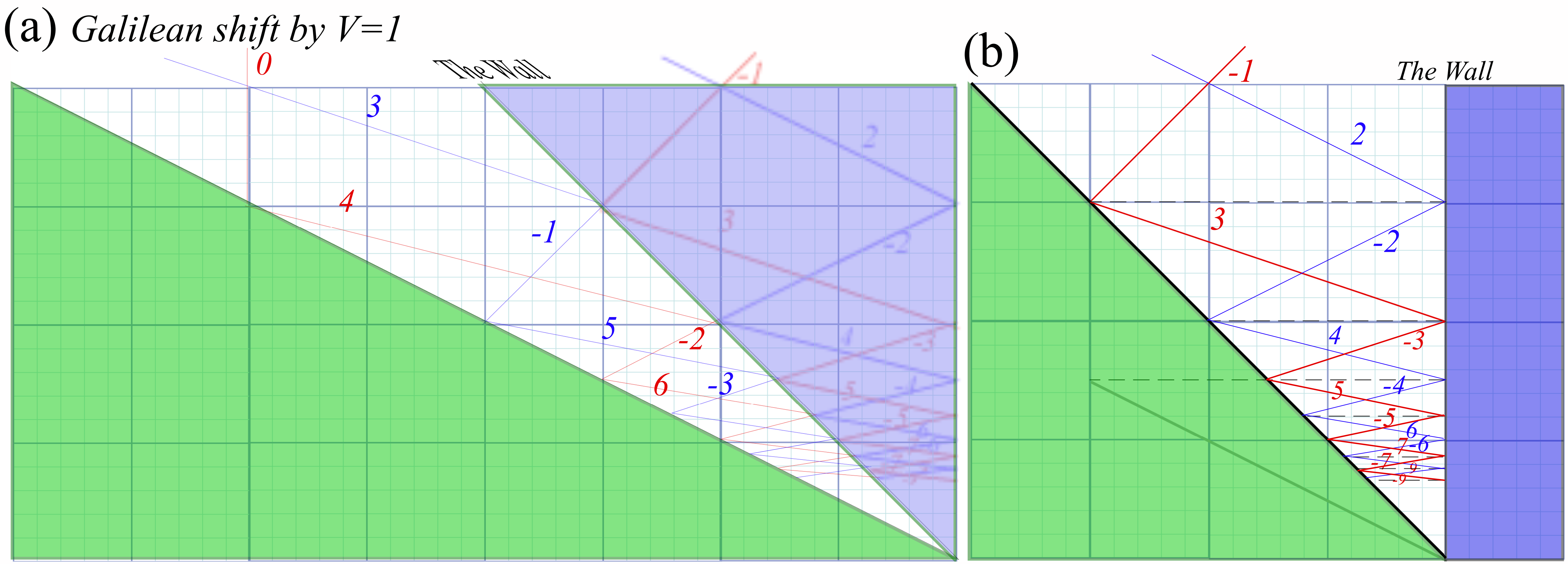
Double "Monster Mash"



From CMwBang! Unit 1
Fig. 6.5

From
CMwBang
Unit 1
Fig. 6.6
and
Fig. 6.7





Bohr-rotor wave dynamics and group vs. phase velocity
  - *Gaussian wave-packet bandwidth and uncertainty*
    - *Gaussian Bohr-rotor revivals and quantum fractals*

Understanding quantum fractals using geometry of fractions (Rationalizing rationals)
  - *Farey-Sums and Ford-products*
  - *Discrete C_N beat phase dynamics (Characters gone wild!)*
  - *The classical bouncing-ball Monster-Mash*

→ *Breaking C_N cyclic coupling into linear chains* ←
  - *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
    - *∞-Square well paths analyzed using Bohr rotor paths*
  - *Breaking C_{2N+2} to approximate linear N-chain*
    - *Band-It simulation: Intro to scattering approach to quantum symmetry*

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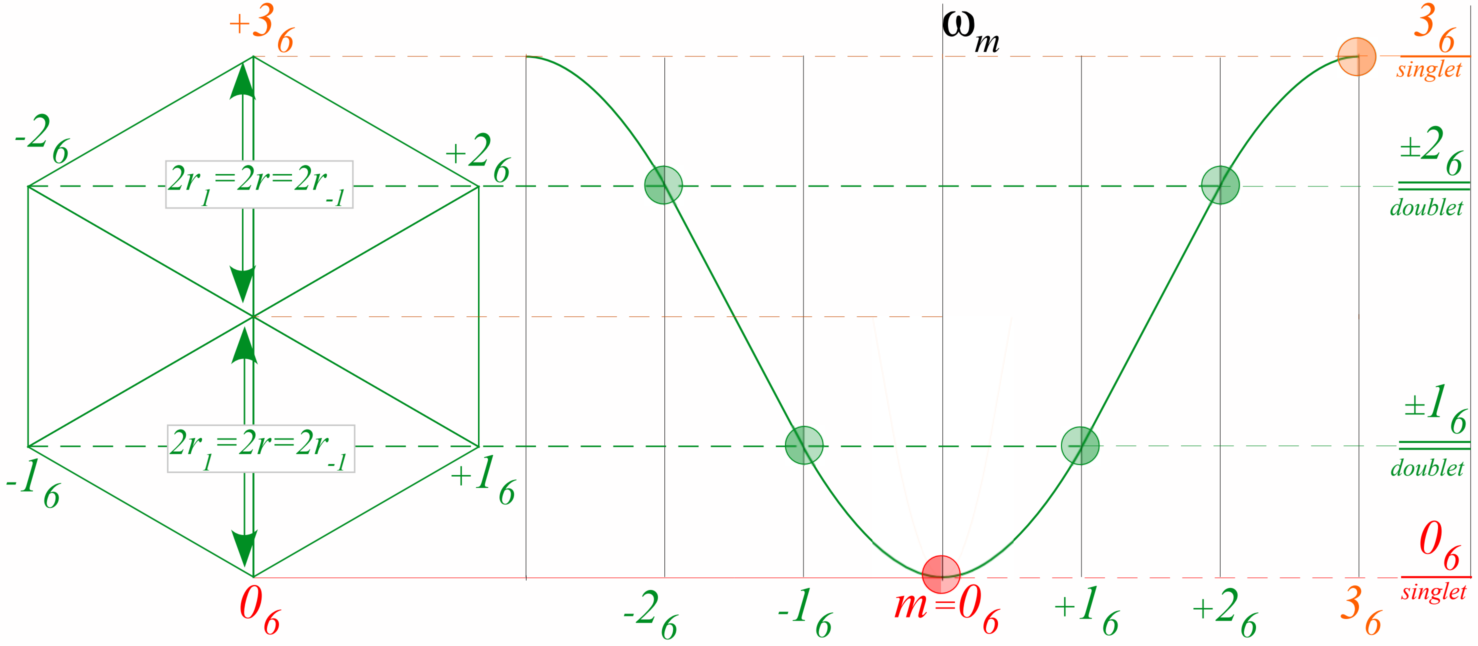
- *Breaking C_{2N} cyclic coupling down to C_N symmetry*
  - *Acoustical modes vs. Optical modes*
  - *Intro to other examples of band theory*
  - *Avoided crossing view of band-gaps*

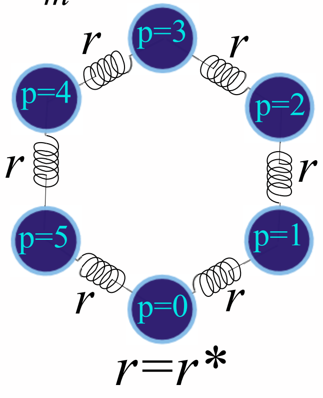
- *Finally! Symmetry groups that are not just C_N*
  - *The "4-Group(s)" D_2 and C_{2v}*
  - *Spectral decomposition of D_2*
    - *Some D_2 modes*
  - *Outer product properties and the Group Zoo*

C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1st neighbor coupling)

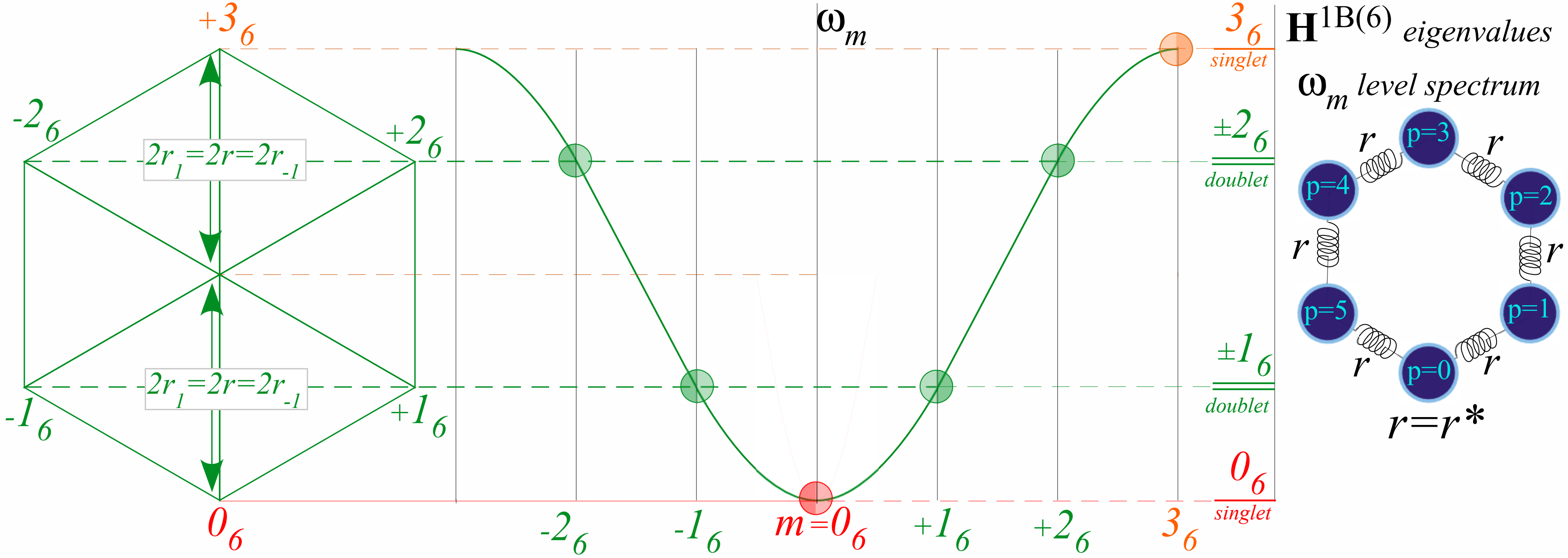


$\mathbf{H}^{1B(6)}$ *eigenvalues*

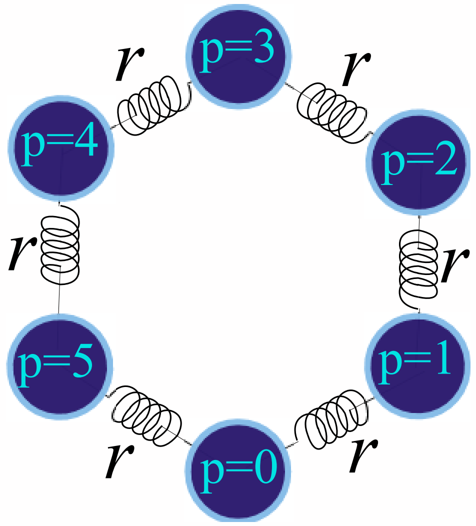
ω_m *level spectrum*



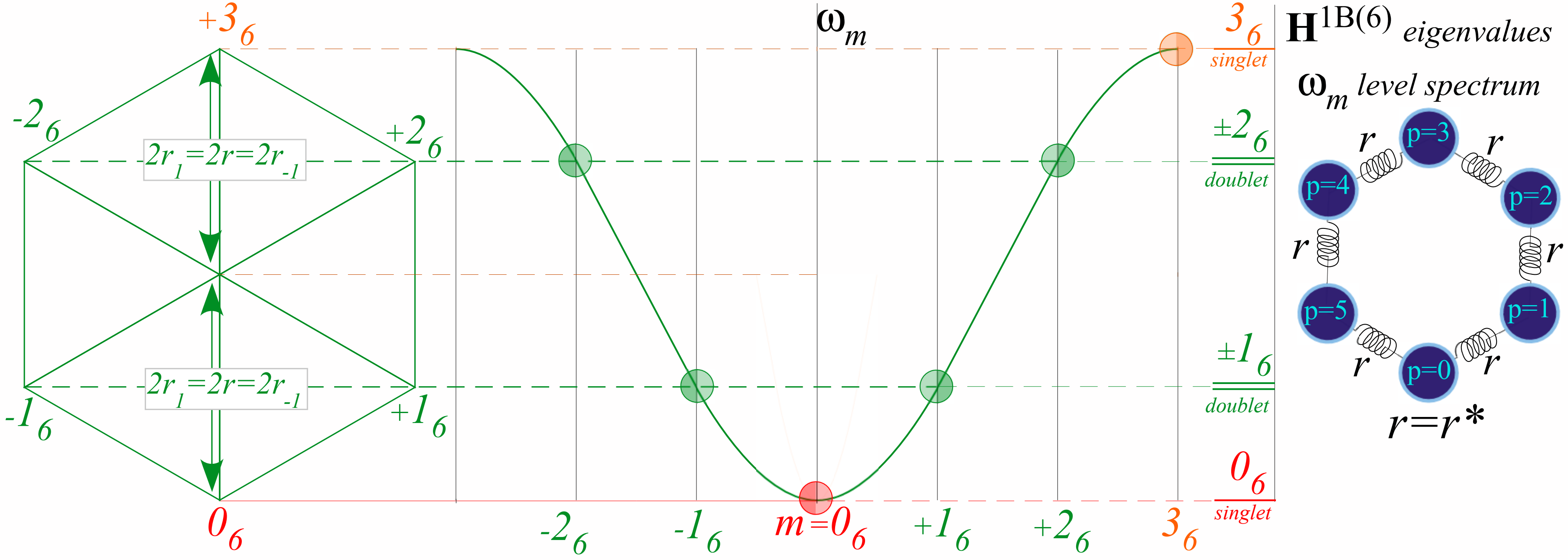
C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1^{st} neighbor coupling)



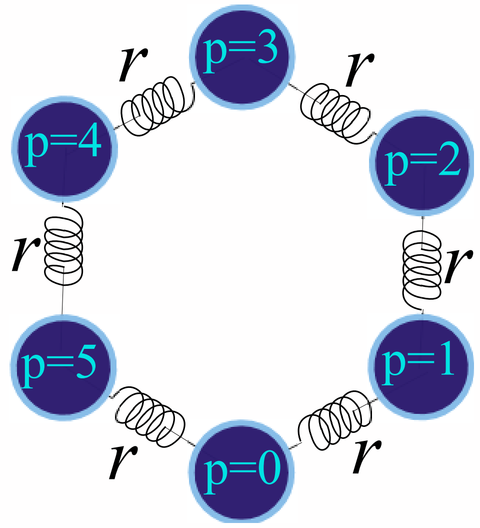
$$\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=\begin{array}{c}\begin{array}{cccccc} p=0 & 1 & 2 & 3 & 4 & 5\end{array}\\ \begin{pmatrix}2r & -r & \cdot & \cdot & \cdot & -r\\ -r & 2r & -r & \cdot & \cdot & \cdot\\ \cdot & -r & 2r & -r & \cdot & \cdot\\ \cdot & \cdot & -r & 2r & -r & \cdot\\ \cdot & \cdot & \cdot & -r & 2r & -r\\ -r & \cdot & \cdot & \cdot & -r & 2r\end{pmatrix}\end{array}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=2r\left(1-\cos\frac{2\pi m}{6}\right)\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}$$



C_6 symmetry: Elementary Bloch Hamiltonian $\mathbf{H}^{1B(6)}$ (1^{st} neighbor coupling)



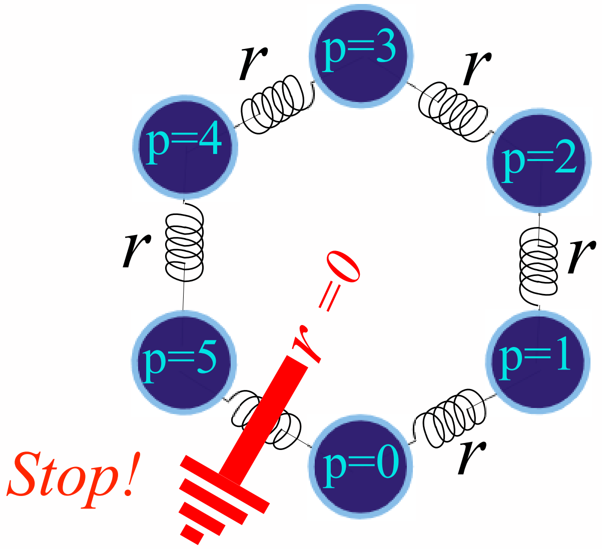
$$\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=\begin{array}{c}\begin{array}{cccccc}p=0 & 1 & 2 & 3 & 4 & 5\end{array}\\ \begin{pmatrix}2r & -r & \cdot & \cdot & \cdot & -r\\ -r & 2r & -r & \cdot & \cdot & \cdot\\ \cdot & -r & 2r & -r & \cdot & \cdot\\ \cdot & \cdot & -r & 2r & -r & \cdot\\ \cdot & \cdot & \cdot & -r & 2r & -r\\ -r & \cdot & \cdot & \cdot & -r & 2r\end{pmatrix}\end{array}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=2r\left(1-\cos\frac{2\pi m}{6}\right)\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}$$



$\mathbf{H}^{1B(6)}$ *eigensolutions are very sensitive to zeroing or constraining a coupling!*

$$\mathbf{H}^{1B(6)}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=\begin{array}{c}\begin{array}{cccccc}p=0 & 1 & 2 & 3 & 4 & 5\end{array}\\ \begin{pmatrix}2r & -r & \cdot & \cdot & \cdot & 0\\ -r & 2r & -r & \cdot & \cdot & \cdot\\ \cdot & -r & 2r & -r & \cdot & \cdot\\ \cdot & \cdot & -r & 2r & -r & \cdot\\ \cdot & \cdot & \cdot & -r & 2r & -r\\ 0 & \cdot & \cdot & \cdot & -r & 2r\end{pmatrix}\end{array}\begin{pmatrix}\psi_0^m\\ \psi_1^m\\ \psi_2^m\\ \psi_3^m\\ \psi_4^m\\ \psi_5^m\end{pmatrix}=?\begin{pmatrix}?\\ ?\\ ?\\ ?\\ ?\\ ?\end{pmatrix}$$

(Not eigenvectors)



Consider sine and cosine eigenvectors of a *14-by-14* elementary Bloch matrix $\mathbf{H}^{\text{EB}(14)}$

$$\langle cos^m| = \left(c_0^m{=}1 \;\middle|\; c_1^m \;\; c_2^m \;\; c_3^m \;\; c_4^m \;\; c_5^m \;\; c_6^m \;\middle|\; c_7^m{=}1 \;\middle|\; c_{-6}^m \;\; c_{-5}^m \;\; c_{-4}^m \;\; c_{-3}^m \;\; c_{-2}^m \;\; c_{-1}^m \right) \qquad c_p^m = \cos\left(m \cdot p \frac{\pi}{7}\right) = c_{-p}^m$$

$$\langle sin^m| = \left(s_0^m{=}0 \;\middle|\; s_1^m \;\; s_2^m \;\; s_3^m \;\; s_4^m \;\; s_5^m \;\; s_6^m \;\middle|\; s_7^m{=}0 \;\middle|\; s_{-6}^m \;\; s_{-5}^m \;\; s_{-4}^m \;\; s_{-3}^m \;\; s_{-2}^m \;\; s_{-1}^m \right) \qquad s_p^m = \sin\left(m \cdot p \frac{\pi}{7}\right) = -s_{-p}^m$$

$$\mathbf{H}^{\text{EB}(14)} |sin^m\rangle \quad = \omega^{m(14)} |sin^m\rangle$$

$$\begin{array}{c|c:cccccc:c:cccccc|}
{}^{p}/_{p'} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & -6 & -5 & -4 & -3 & -2 & -1 \\
\hline
0 & 2r & -r & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -r \\
\hdashline
1 & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot & & & & & & & \\
2 & \cdot & -r & 2r & -r & \cdot & \cdot & \cdot & & & & & & & \\
3 & \cdot & \cdot & -r & 2r & -r & \cdot & \cdot & & & & & & & \\
4 & \cdot & \cdot & \cdot & -r & 2r & -r & \cdot & & & & & & & \\
5 & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & & \\
6 & \cdot & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & \\
\hdashline
7 & \cdot & & & & & & -r & 2r & -r & & & & & \\
\hdashline
-6 & \cdot & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot \\
-5 & \cdot & & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot \\
-4 & \cdot & & & & & & & & \cdot & -r & 2r & -r & \cdot & \cdot \\
-3 & \cdot & & & & & & & & \cdot & \cdot & -r & 2r & -r & \cdot \\
-2 & \cdot & & & & & & & & \cdot & \cdot & \cdot & -r & 2r & -r \\
-1 & -r & & & & & & & & \cdot & \cdot & \cdot & \cdot & -r & 2r
\end{array}
\left(\begin{array}{c} \vdots \\ \hline 0 \\ \hdashline s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ \hdashline 0 \\ \hdashline s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{array}\right)
= \omega^{m(14)}
\left(\begin{array}{c} \vdots \\ \hline 0 \\ \hdashline s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ \hdashline 0 \\ \hdashline s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{array}\right)$$

where :

$$\omega^{m(14)} = 2r(1 - \cos\frac{2\pi m}{14})$$

Consider sine and cosine eigenvectors of a *14-by-14* elementary Bloch matrix $\mathbf{H}^{\mathrm{EB}(14)}$

$$\left\langle cos^m \right| = \left(c_0^m{=}1 \;\middle|\; c_1^m \;\; c_2^m \;\; c_3^m \;\; c_4^m \;\; c_5^m \;\; c_6^m \;\middle|\; c_7^m{=}1 \;\middle|\; c_{-6}^m \;\; c_{-5}^m \;\; c_{-4}^m \;\; c_{-3}^m \;\; c_{-2}^m \;\; c_{-1}^m \right) \qquad c_p^m = \cos\left(m \cdot p \frac{\pi}{7} \right) = c_{-p}^m$$

$$\left\langle sin^m \right| = \left(s_0^m{=}0 \;\middle|\; s_1^m \;\; s_2^m \;\; s_3^m \;\; s_4^m \;\; s_5^m \;\; s_6^m \;\middle|\; s_7^m{=}0 \;\middle|\; s_{-6}^m \;\; s_{-5}^m \;\; s_{-4}^m \;\; s_{-3}^m \;\; s_{-2}^m \;\; s_{-1}^m \right) \qquad s_p^m = \sin\left(m \cdot p \frac{\pi}{7} \right) = -s_{-p}^m$$

$$\mathbf{H}^{\mathrm{EB}(14)} \left| sin^m \right\rangle = \omega^{m(14)} \left| sin^m \right\rangle$$

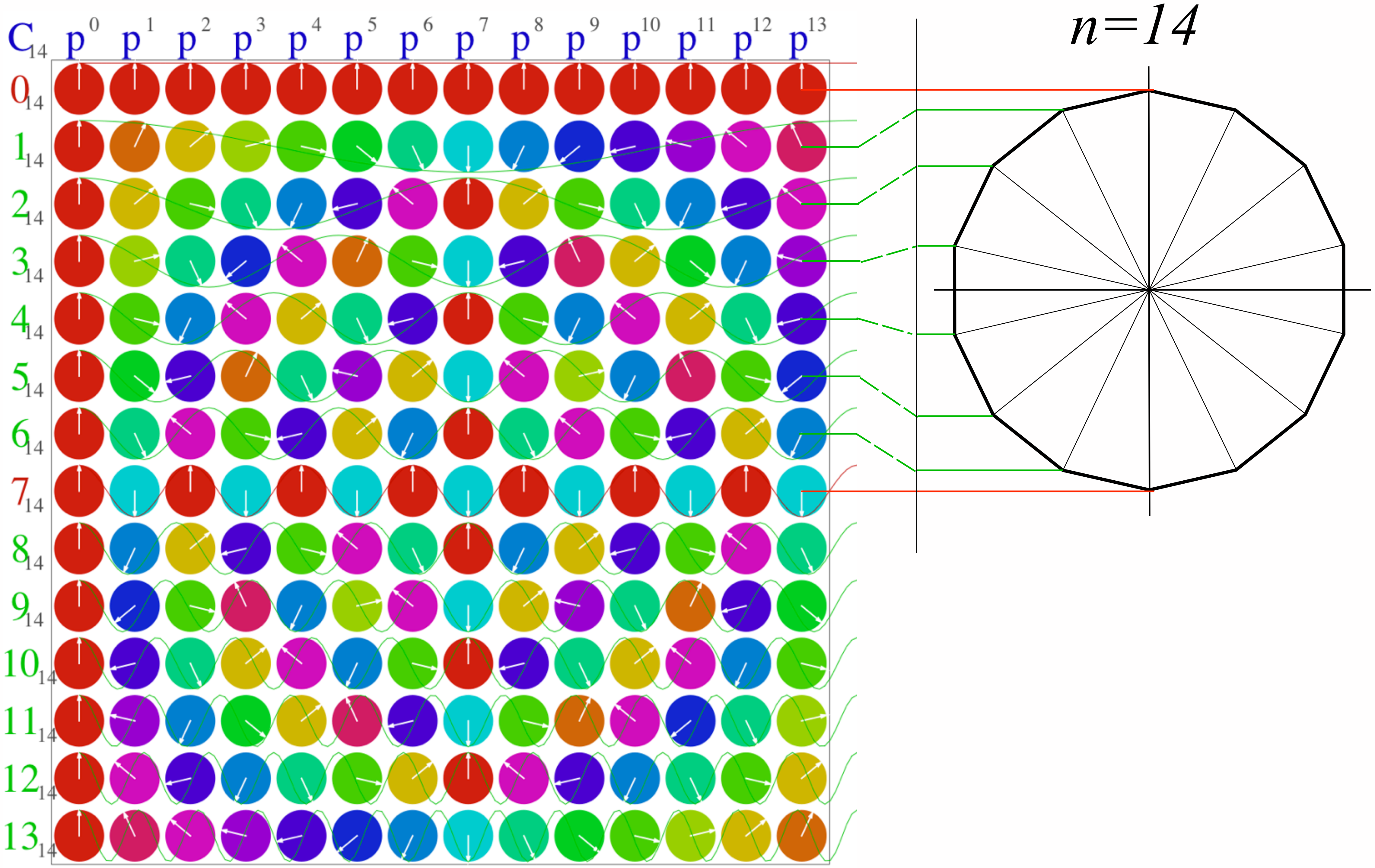
$\mathbf{H}^{\mathrm{EB}(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{\mathrm{CM}(6)}$

$$\begin{array}{c|c|cccccc|c|cccccc}
p \diagup p' & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & -6 & -5 & -4 & -3 & -2 & -1 \\
\hline
0 & 2r & -r & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -r \\
\hline
1 & -r & 2r & -r & \cdot & \cdot & \cdot & 0 & & & & & & & \\
2 & \cdot & -r & 2r & -r & \cdot & \cdot & \cdot & & & & & & & \\
3 & \cdot & \cdot & -r & 2r & -r & \cdot & \cdot & & & & & & & \\
4 & \cdot & \cdot & \cdot & -r & 2r & -r & \cdot & & & & & & & \\
5 & \cdot & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & & \\
6 & \cdot & 0 & \cdot & \cdot & \cdot & -r & 2r & -r & & & & & & \\
\hline
7 & \cdot & & & & & & -r & 2r & -r & & & & & \\
\hline
-6 & \cdot & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot & \cdot \\
-5 & \cdot & & & & & & & & -r & 2r & -r & \cdot & \cdot & \cdot \\
-4 & \cdot & & & & & & & & \cdot & -r & 2r & -r & \cdot & \cdot \\
-3 & \cdot & & & & & & & & \cdot & \cdot & -r & 2r & -r & \cdot \\
-2 & \cdot & & & & & & & & \cdot & \cdot & \cdot & -r & 2r & -r \\
-1 & -r & & & & & & & & \cdot & \cdot & \cdot & \cdot & -r & 2r
\end{array}
\begin{pmatrix} \vdots \\ 0 \\ s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ 0 \\ s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{pmatrix}
= \omega^{m(14)}
\begin{pmatrix} \vdots \\ 0 \\ s_1^m \\ s_2^m \\ s_3^m \\ s_4^m \\ s_5^m \\ s_6^m \\ 0 \\ s_{-6}^m \\ s_{-5}^m \\ s_{-4}^m \\ s_{-3}^m \\ s_{-2}^m \\ s_{-1}^m \end{pmatrix}$$

where:

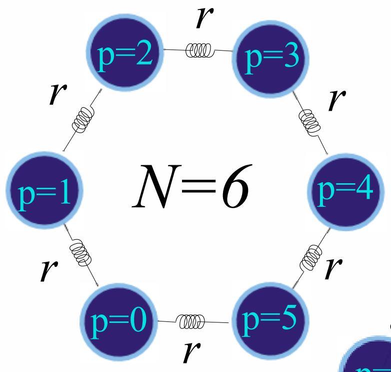
$$\omega^{m(14)} = 2r\left(1 - \cos\frac{2\pi m}{14}\right)$$

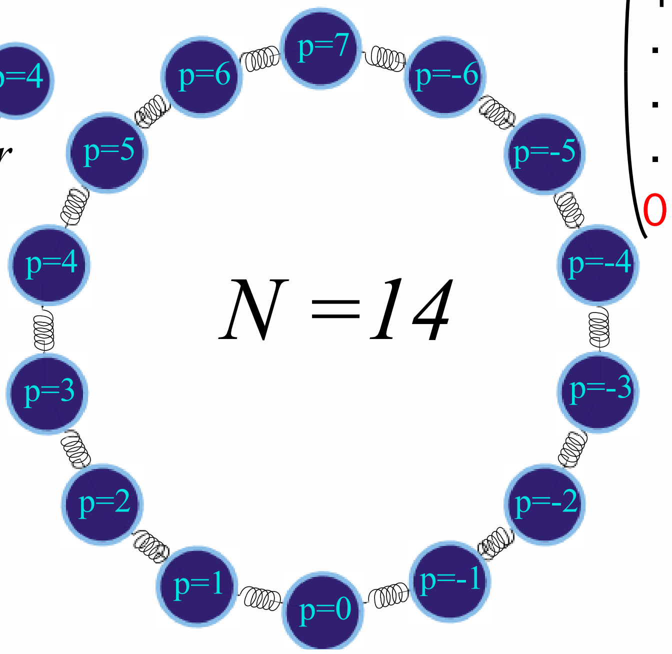
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only



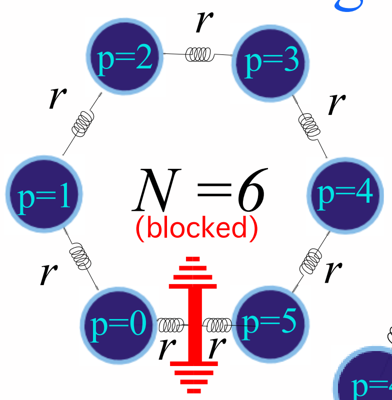
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

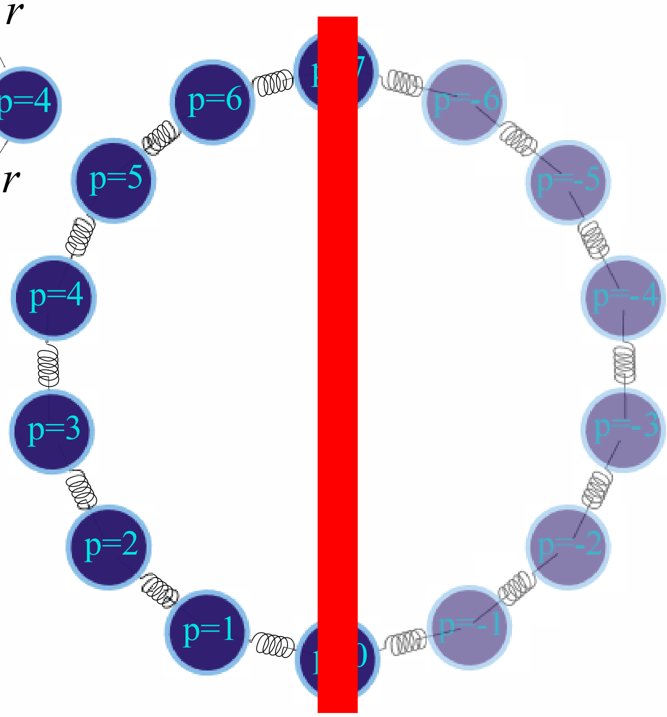
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$





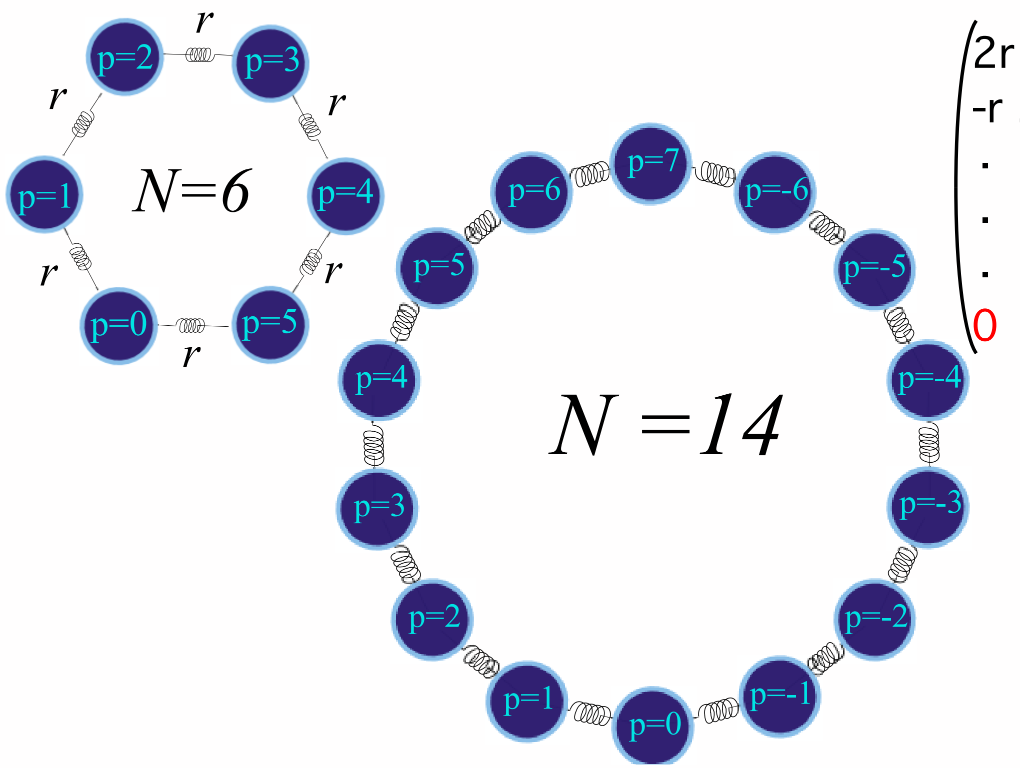
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



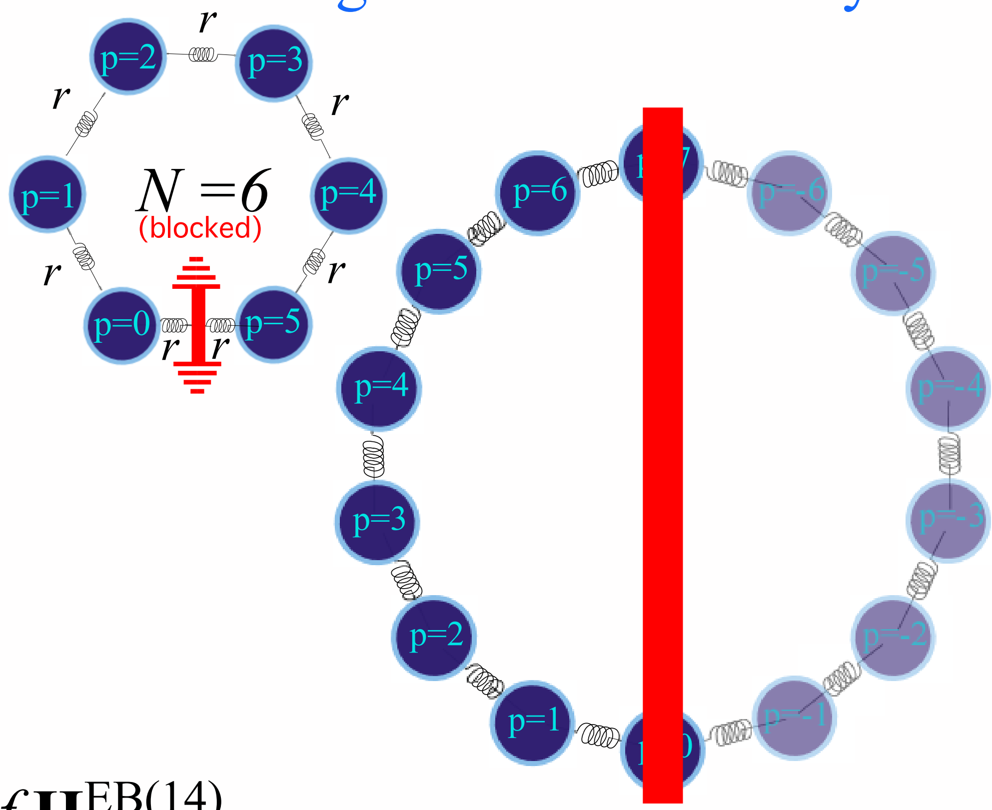


$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

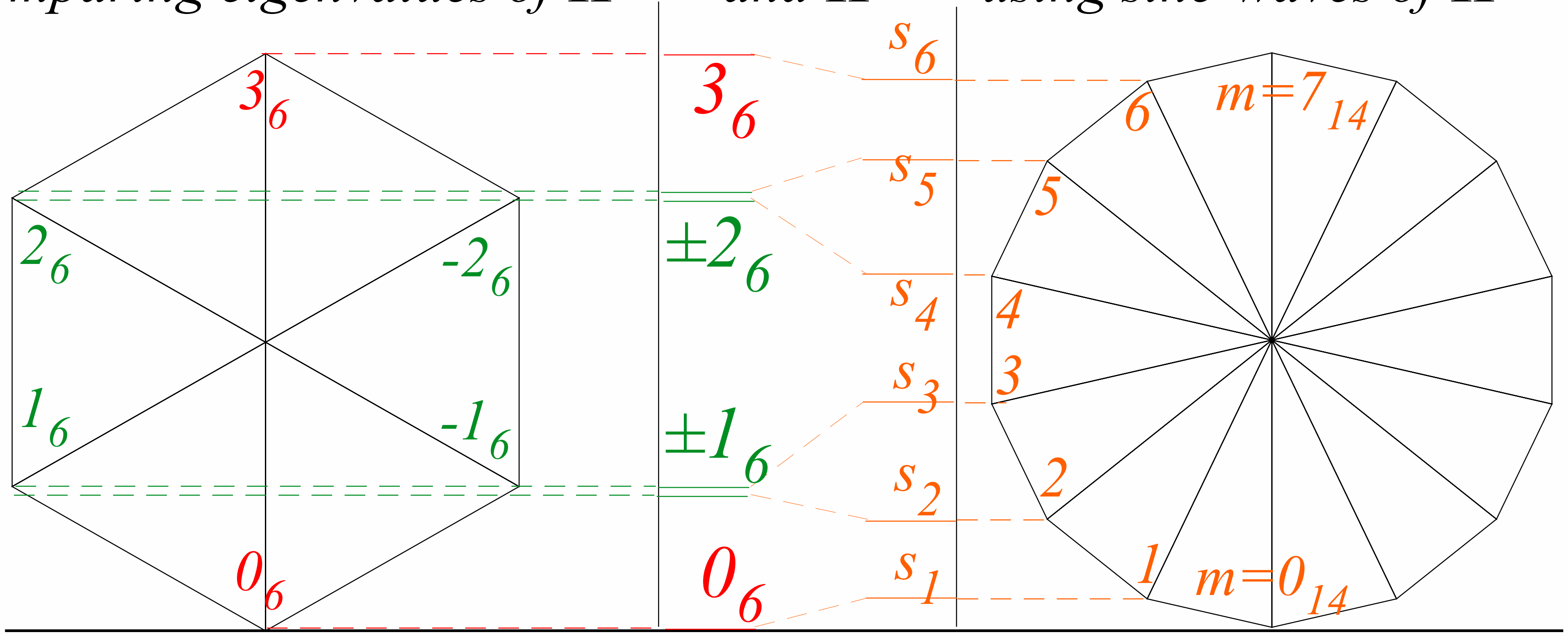
$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

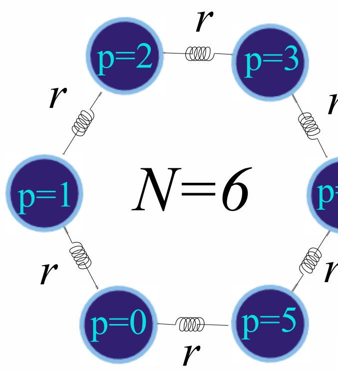


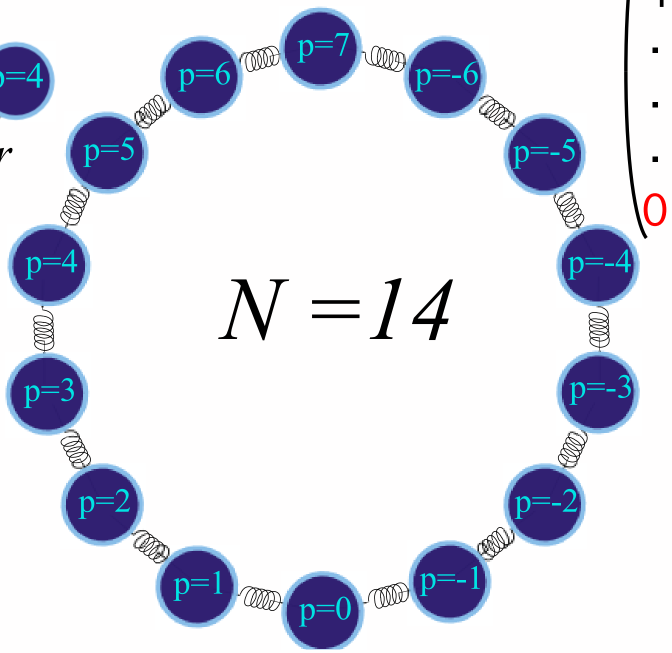
Comparing eigenvalues of $\mathbf{H}^{EB(6)}$ *and* $\mathbf{H}^{CM(6)}$ *using sine-waves of* $\mathbf{H}^{EB(14)}$



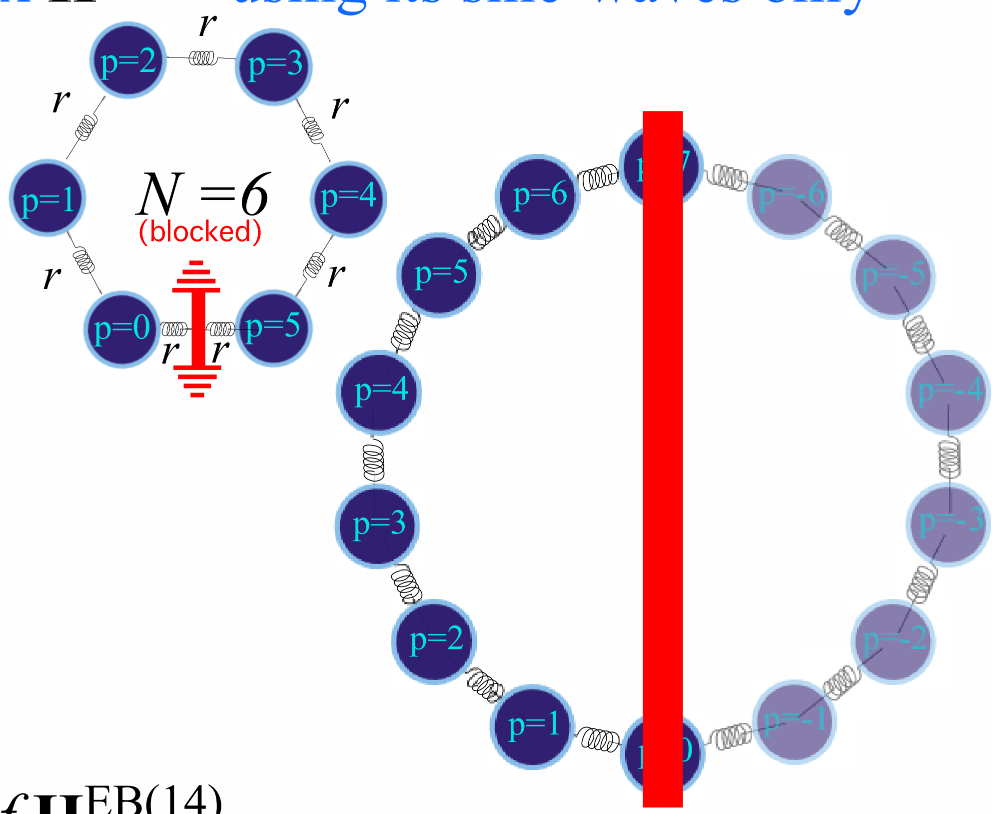
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only

$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & -r \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ -r & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$

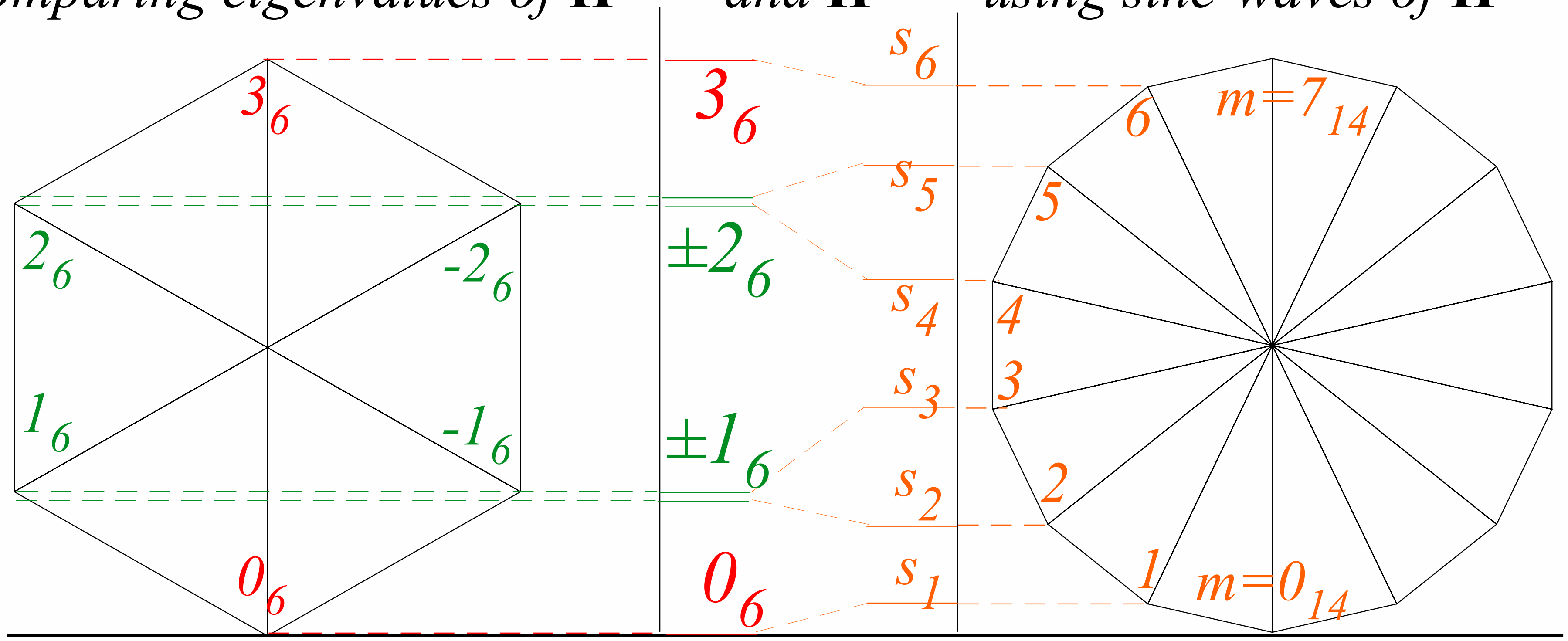


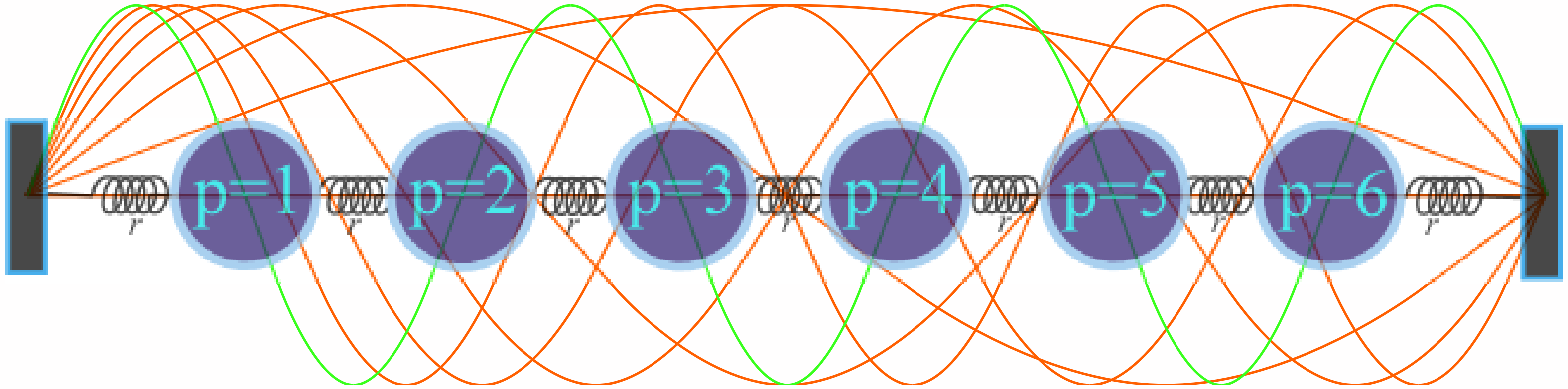


$$\begin{pmatrix} 2r & -r & \cdot & \cdot & \cdot & 0 \\ -r & 2r & -r & \cdot & \cdot & \cdot \\ \cdot & -r & 2r & -r & \cdot & \cdot \\ \cdot & \cdot & -r & 2r & -r & \cdot \\ \cdot & \cdot & \cdot & -r & 2r & -r \\ 0 & \cdot & \cdot & \cdot & -r & 2r \end{pmatrix}$$



Comparing eigenvalues of $\mathbf{H}^{EB(6)}$ and $\mathbf{H}^{CM(6)}$ using sine-waves of $\mathbf{H}^{EB(14)}$





Breaking C_N cyclic coupling into linear chains
  - *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
    - *∞-Square well paths analyzed using Bohr rotor paths*
  - *Breaking C_{2N+2} to approximate linear N-chain*
    - *Band-It simulation: Intro to scattering approach to quantum symmetry*

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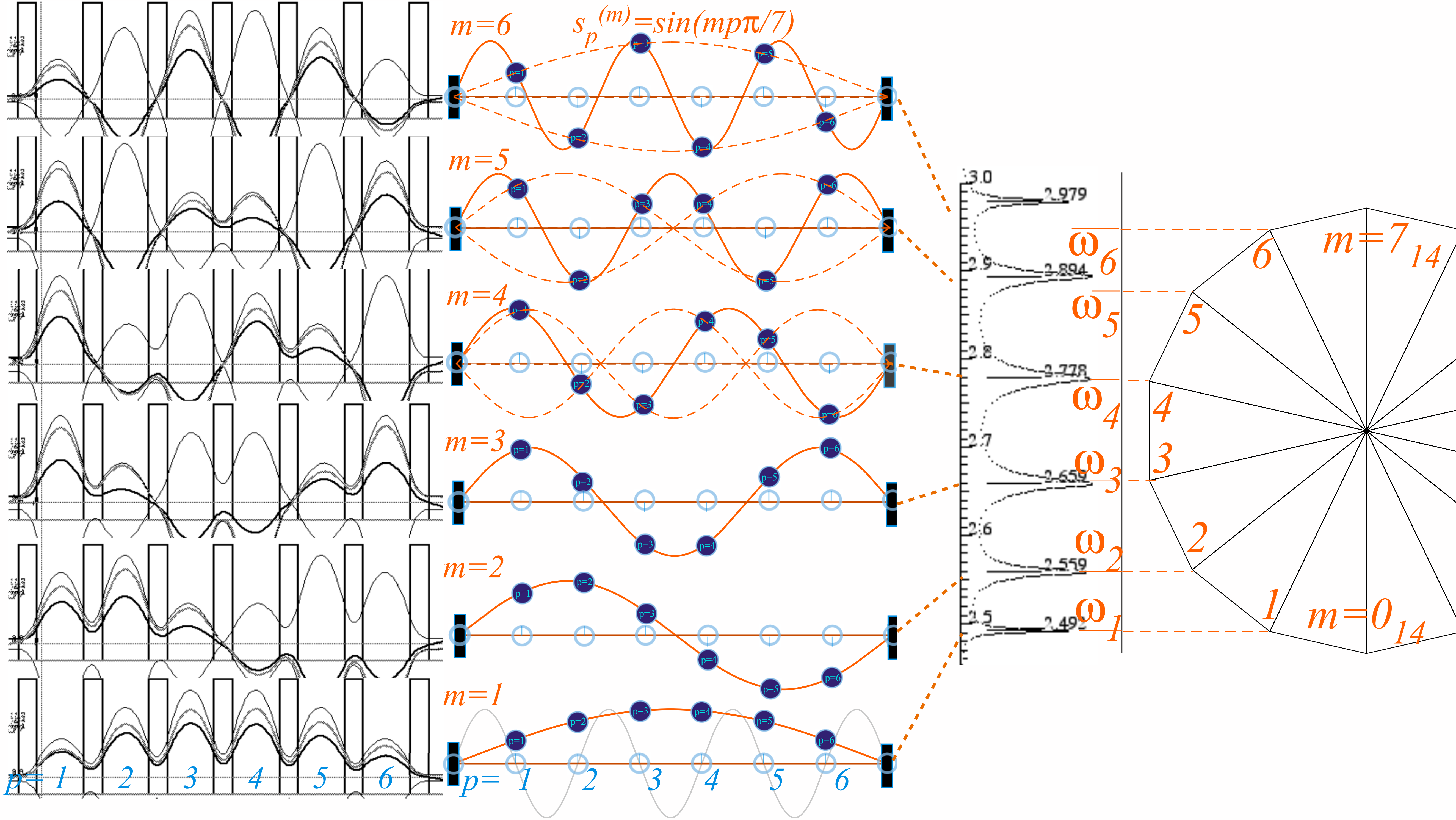
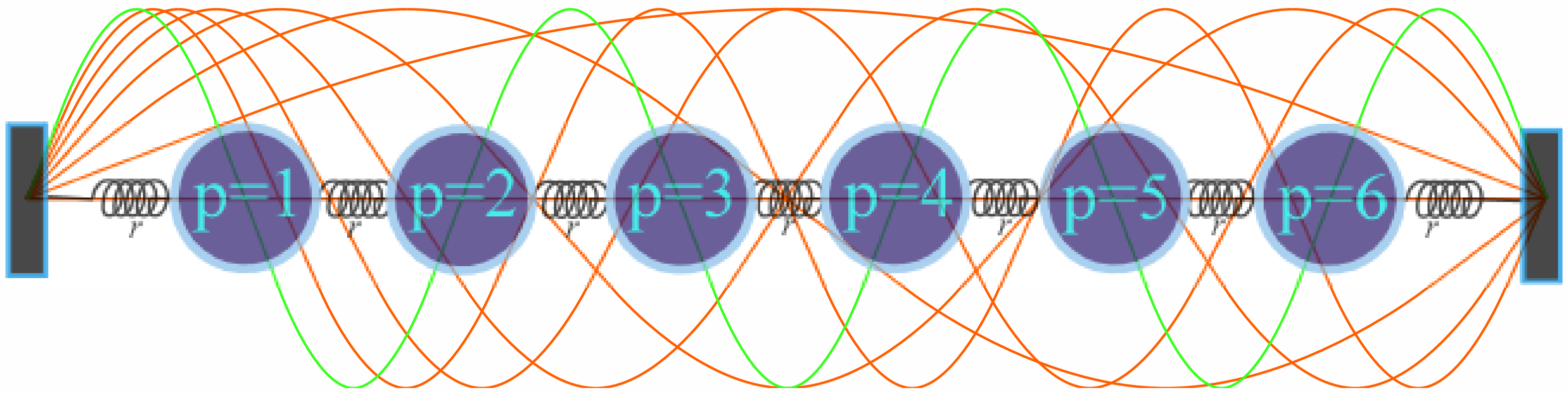
  - *Acoustical modes vs. Optical modes*
  - *Intro to other examples of band theory*
  - *Avoided crossing view of band-gaps*

Finally! Symmetry groups that are not just C_N
  - *The "4-Group(s)" D_2 and C_{2v}*
  - *Spectral decomposition of D_2*
    - *Some D_2 modes*
  - *Outer product properties and the Group Zoo*

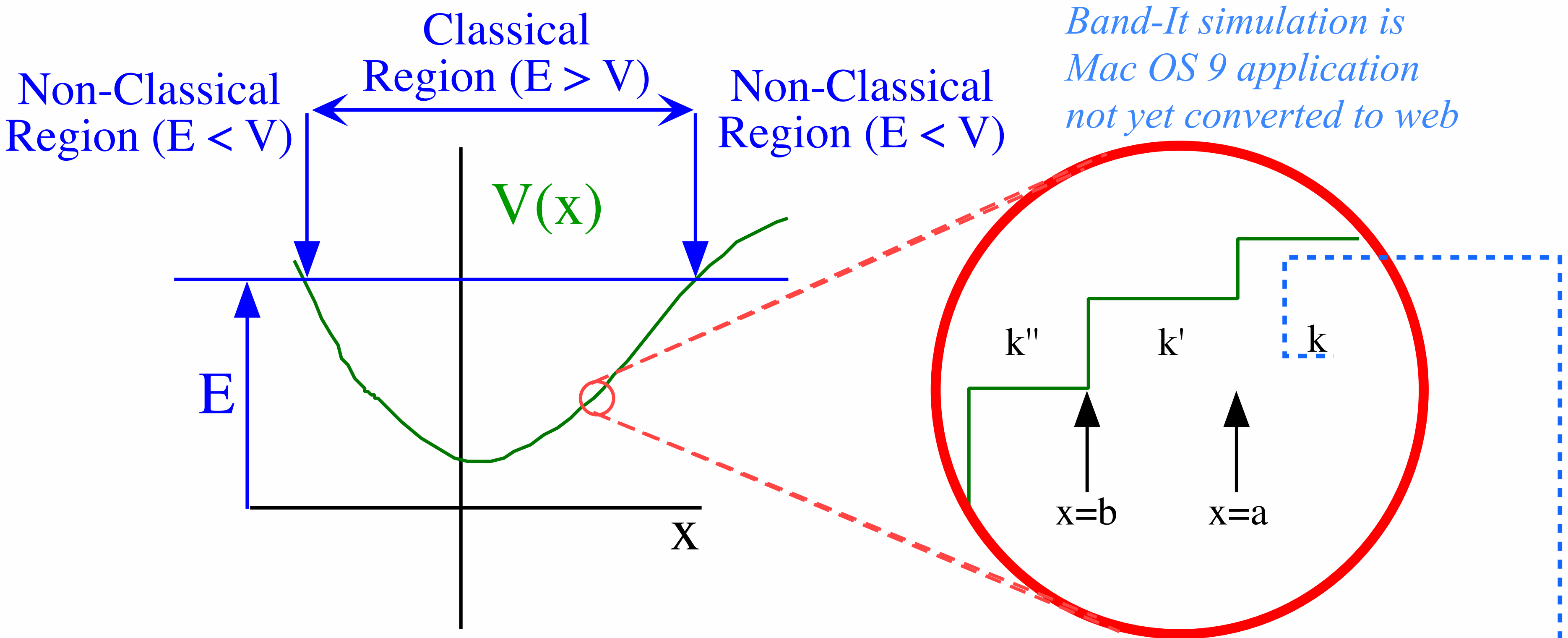
$\mathbf{H}^{EB(14)}$ gives eigensolution of a *6-by-6* constrained Bloch matrix $\mathbf{H}^{CM(6)}$ using its sine-waves only



Band-It simulation is
Mac OS 9 application
not yet converted to web



How Band-It simulation works (from QTfCA Unit 4 Chapter 13)



Band-It simulation is
Mac OS 9 application
not yet converted to web

Fig. 13.1.1 Non-constant potential V(x) approximated by a series of small constant-V steps.

Between each step potential, kinetic energy, and k are assumed constant.

$$\Psi_E(x,0) = Re^{ikx} + Le^{-ikx}$$

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

Band-It simulation is
Mac OS 9 application
not yet converted to web

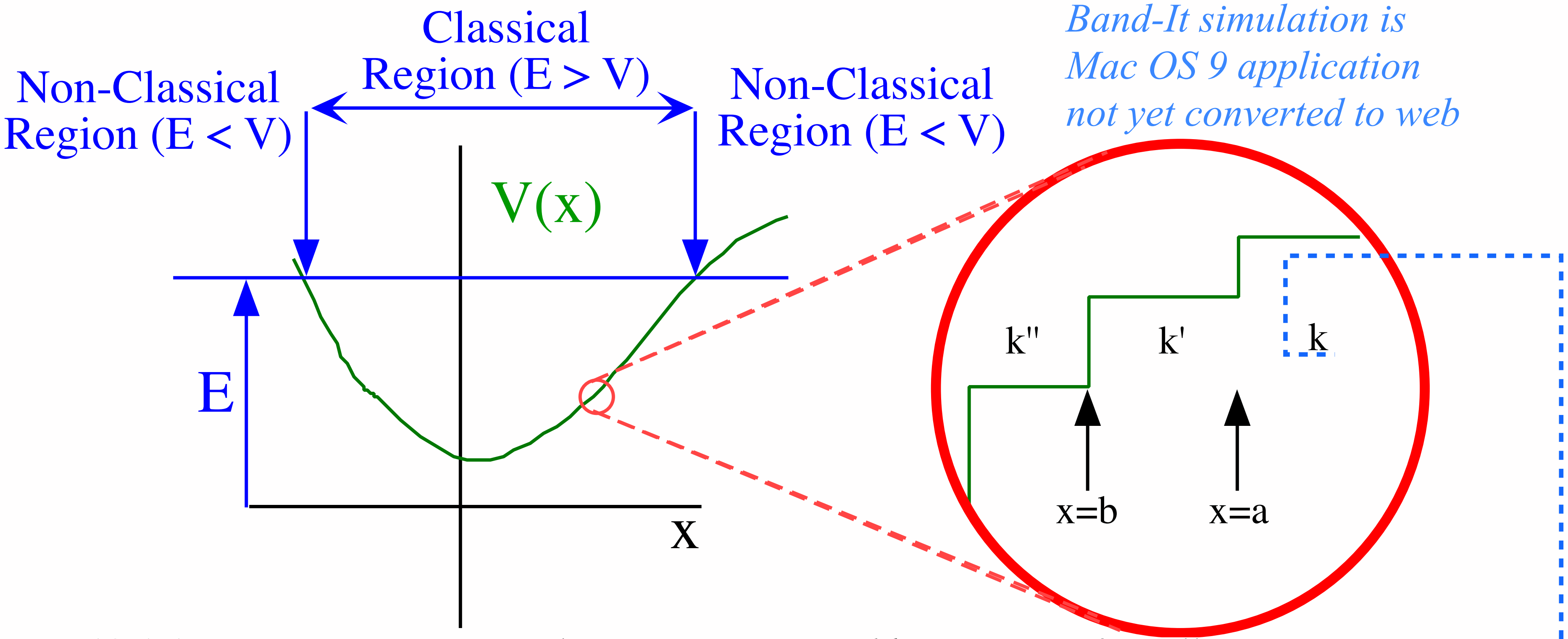


Fig. 13.1.1 Non-constant potential V(x) approximated by a series of small constant-V steps.

Between each step potential, kinetic energy, and *k* are assumed constant. *x*-derivative is denoted by $D\Psi$

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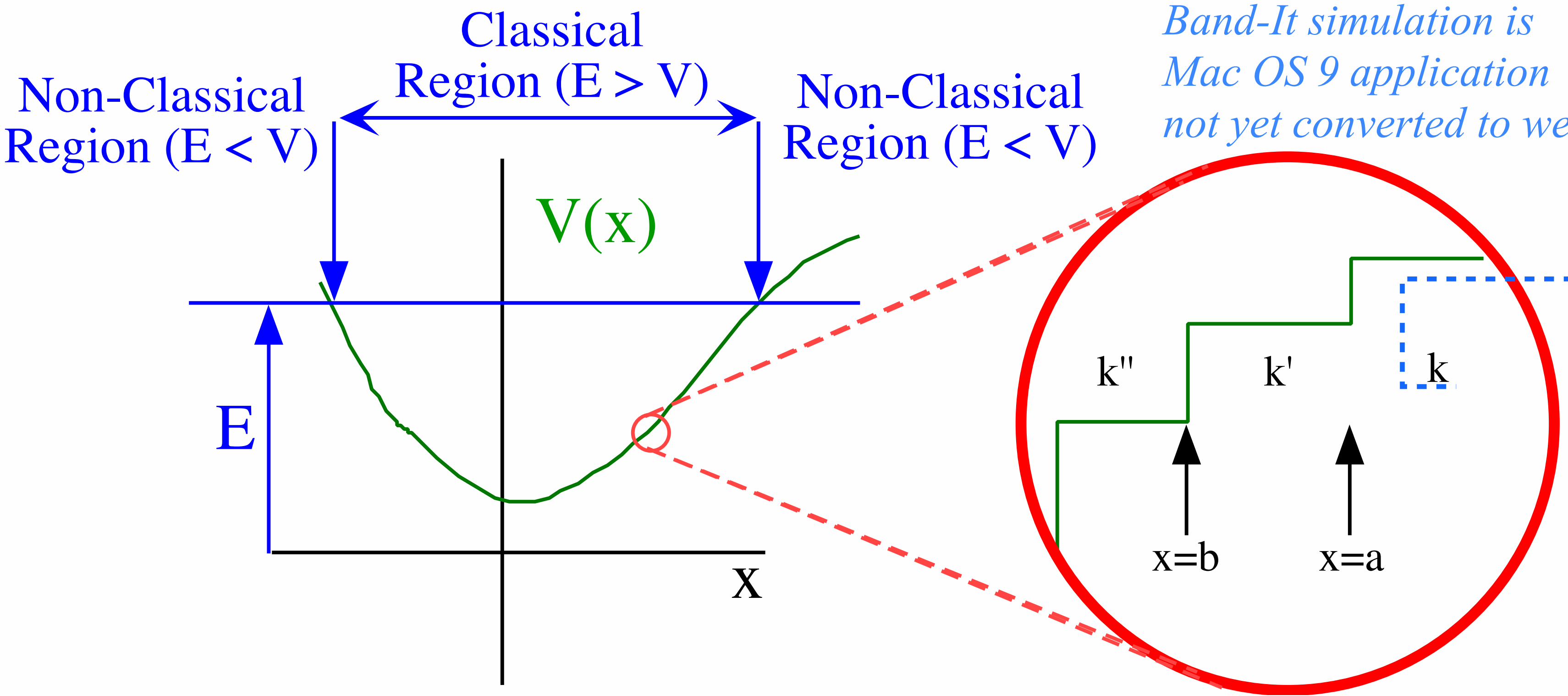

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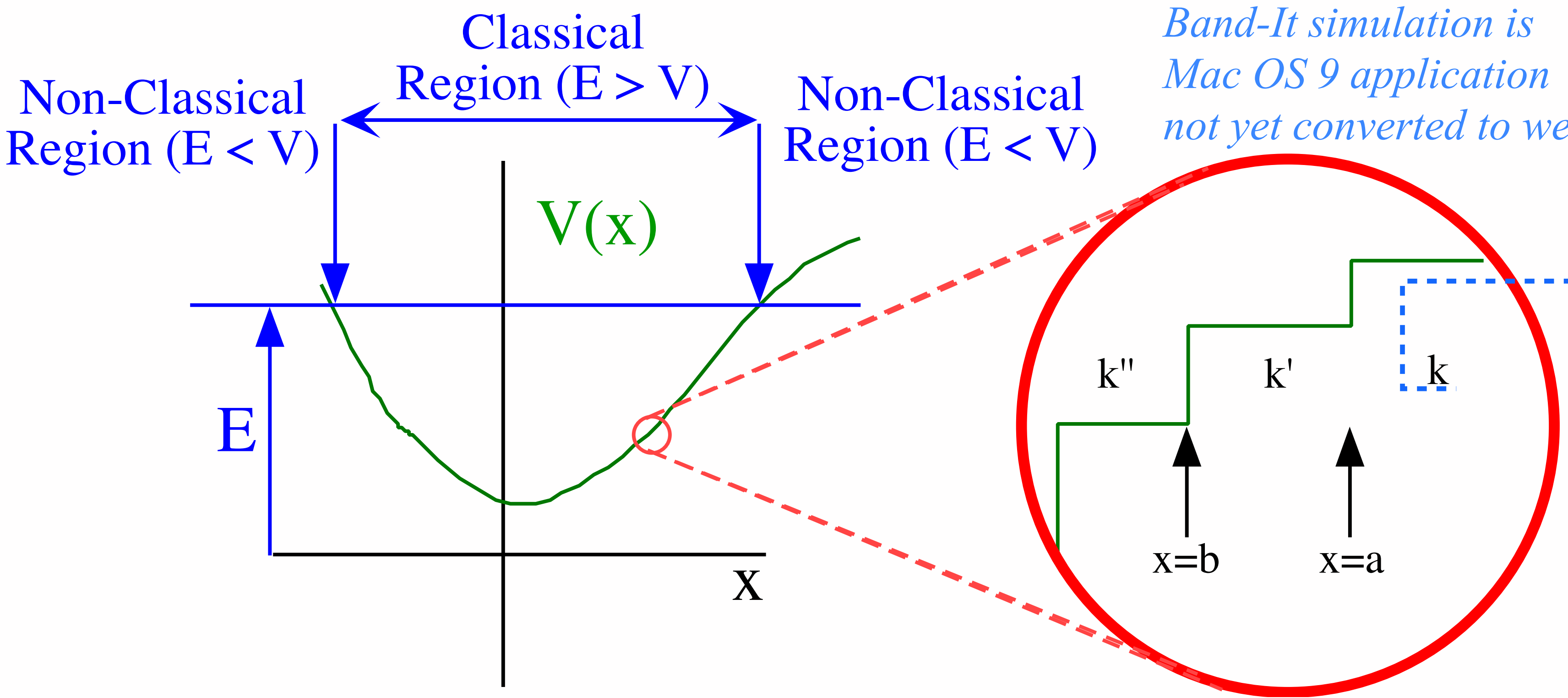
Relations between the pair (Ψ, $D\Psi$) and amplitudes (R, L) just above x=a.

$$\begin{pmatrix} \Psi \\ D\Psi \end{pmatrix} = \begin{pmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{pmatrix} \begin{pmatrix} R \\ L \end{pmatrix}$$

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)



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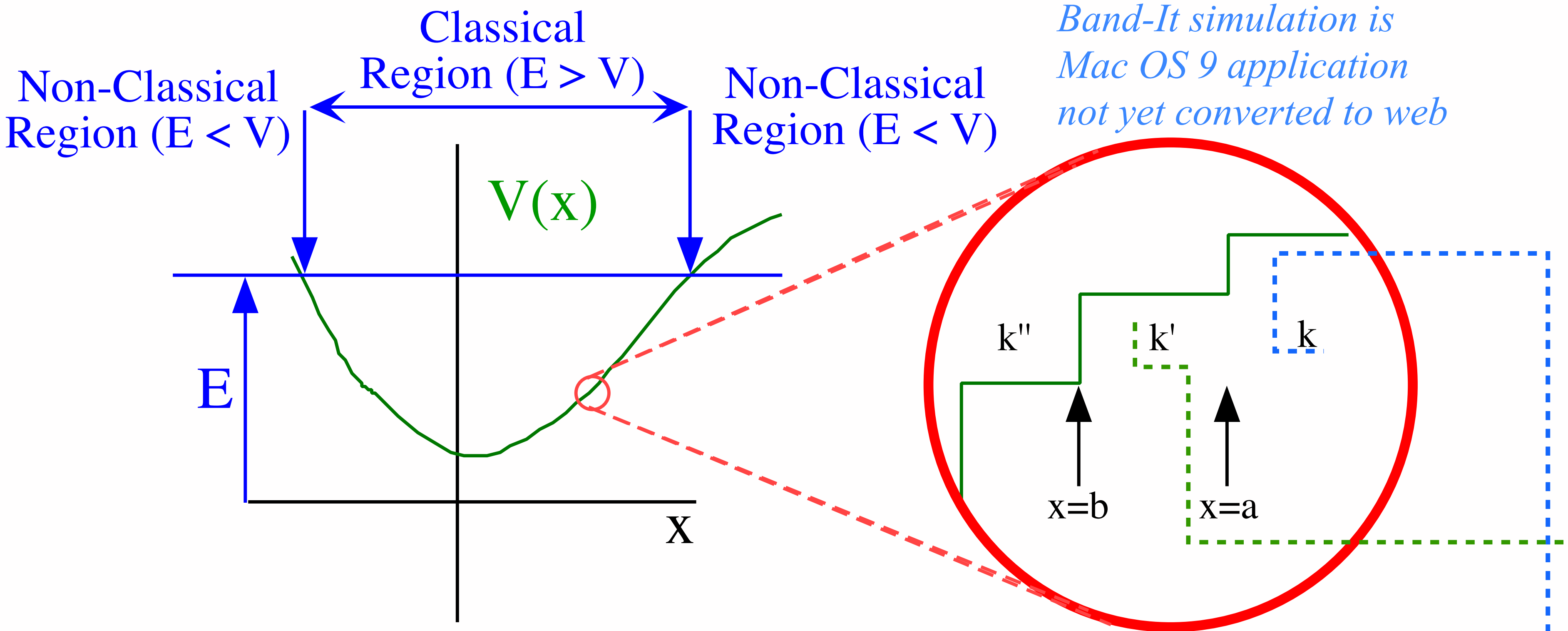

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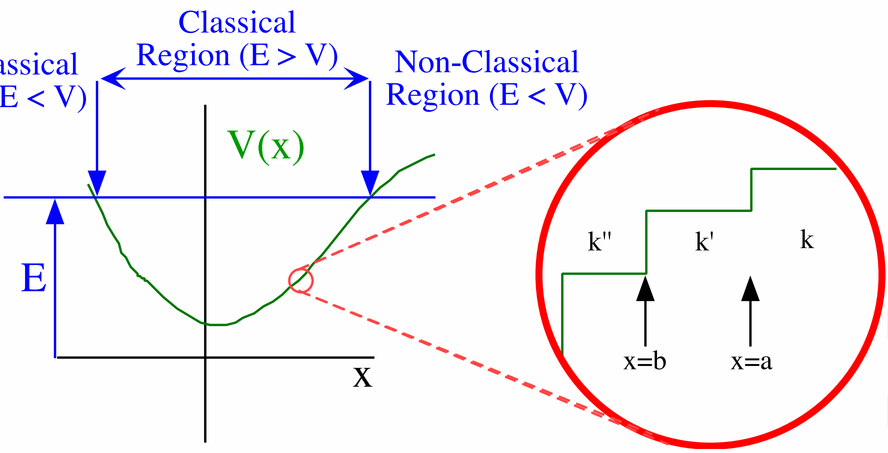
Relations on the other side of the step boundary just below $x=a$. *(Inverted)*

$$\begin{pmatrix} \Psi' \\ D\Psi' \end{pmatrix} = \begin{pmatrix} e^{ik'x} & e^{-ik'x} \\ ik'e^{ik'x} & -ik'e^{-ik'x} \end{pmatrix} \begin{pmatrix} R' \\ L' \end{pmatrix}, \qquad \begin{pmatrix} R' \\ L' \end{pmatrix} = \frac{i}{2k'} \begin{pmatrix} -ik'e^{-ik'x} & -e^{-ik'x} \\ -ik'e^{ik'x} & e^{ik'x} \end{pmatrix} \begin{pmatrix} \Psi' \\ D\Psi' \end{pmatrix}$$

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

Wave function and derivative at $x=a-\varepsilon$ equals that at $x=a+\varepsilon$.



$$\begin{pmatrix}\Psi'\\ D\Psi'\end{pmatrix}_{x=a-\varepsilon}=\begin{pmatrix}\Psi\\ D\Psi\end{pmatrix}_{x=a+\varepsilon}$$

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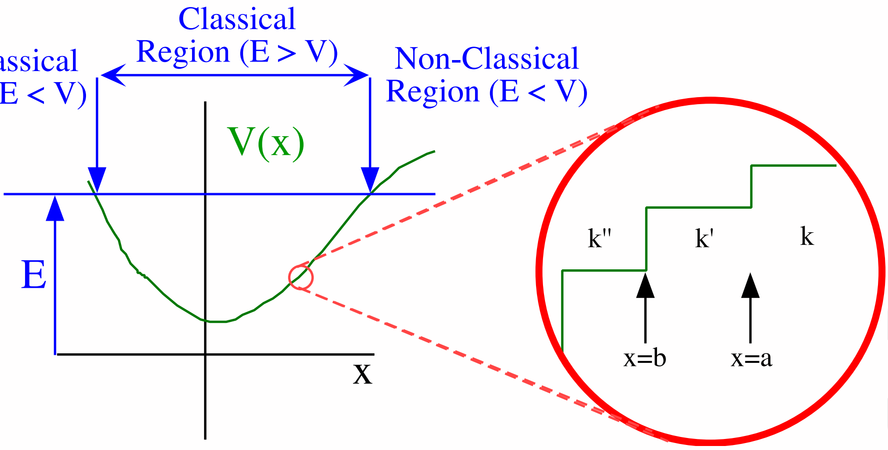
How Band-It simulation works (from QTfCA Unit 4 Chapter 13)



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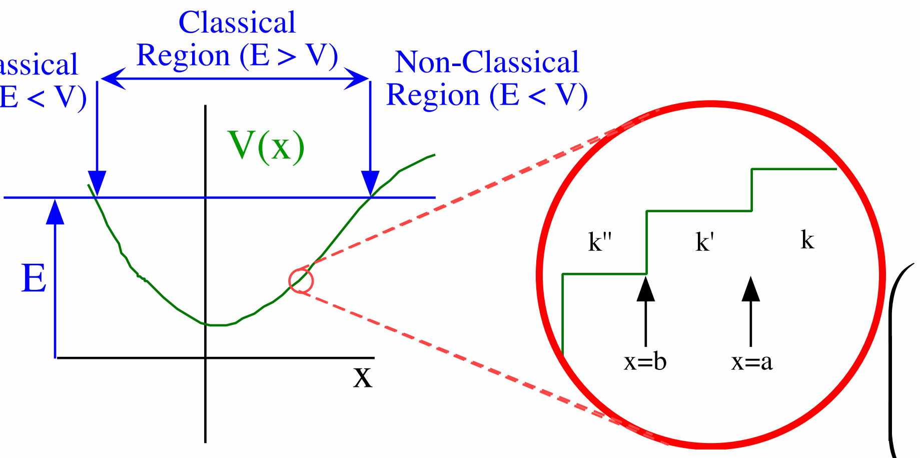
How Band-It simulation works (from QTfCA Unit 4 Chapter 13)



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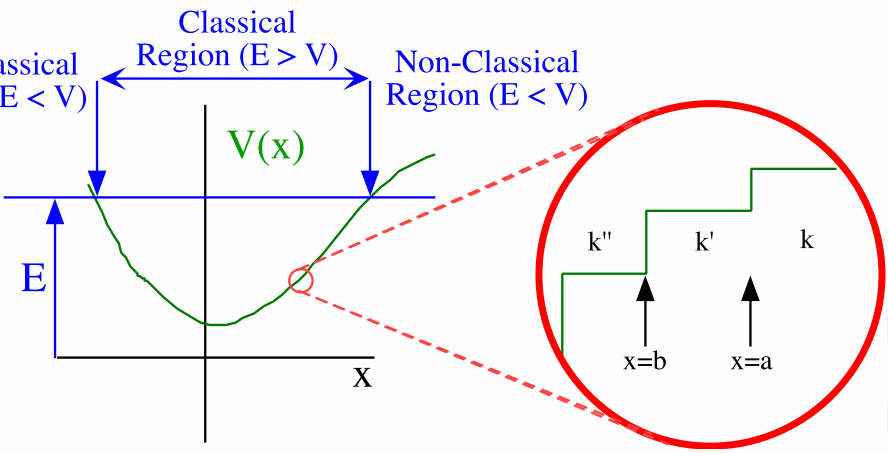

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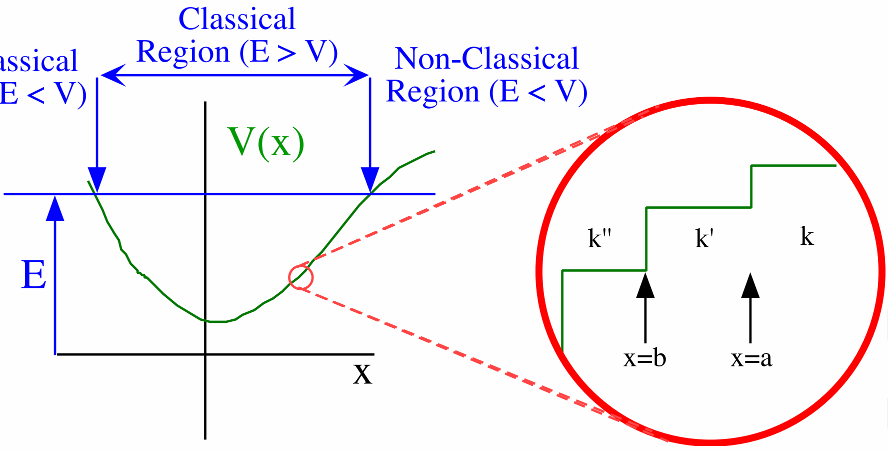
A special case: *single input conditions* with no sources or reflectors on one side (say, right hand side) so no incoming waves exist there (say, $L=0$ but $R=Outgoing\neq 0$.)

How Band-It simulation works (from QTfCA Unit 4 Chapter 13)



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How Band-It simulation works (from QTfCA Unit 4 Chapter 13)

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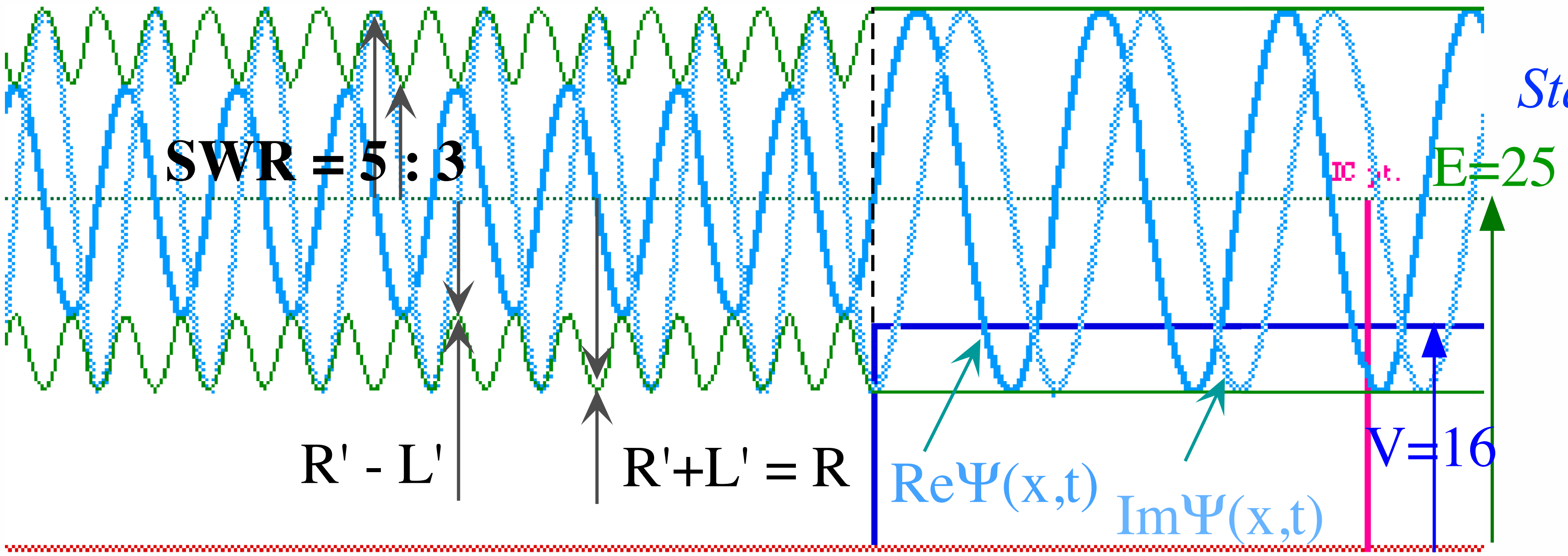
This gives *transmitted or output amplitude R* and *reflected amplitude L'* given an *input amplitude R'*.

$$R = \frac{2k'}{(k+k')} R' e^{i(k'-k)a} \quad , \qquad L' = \frac{(k'-k)}{(k+k')} R' e^{2ik'a}$$

The *transmission coefficient $T_{transmit}$* and *reflection coefficient $T_{reflect}$* (for $a=0$)

$$T_{transmit} = \frac{|R|^2}{|R'|^2} = \frac{4|k'|^2}{|k+k'|^2} \quad , \qquad T_{reflect} = \frac{|L'|^2}{|R'|^2} = \frac{|k'-k|^2}{|k'+k|^2} \qquad SWR = \frac{L'-R'}{L'+R'} = \frac{\frac{2kR'}{k+k'}}{\frac{2k'R'}{k+k'}} = \frac{k}{k'} = \frac{\sqrt{E-V}}{\sqrt{E}}$$



Standing Wave Ratio (SWR)

Breaking C_N cyclic coupling into linear chains

- *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
- *Breaking C_{2N+2} to approximate linear N-chain*
  - *Band-It simulation: Intro to scattering approach to quantum symmetry*

Breaking C_{2N} cyclic coupling down to C_N symmetry

- *Acoustical modes vs. Optical modes*
- *Intro to other examples of band theory*
- *Avoided crossing view of band-gaps*

Finally! Symmetry groups that are not just C_N

- *The "4-Group(s)" D_2 and C_{2v}*
- *Spectral decomposition of D_2*
  - *Some D_2 modes*
- *Outer product properties and the Group Zoo*

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.6 PSDS

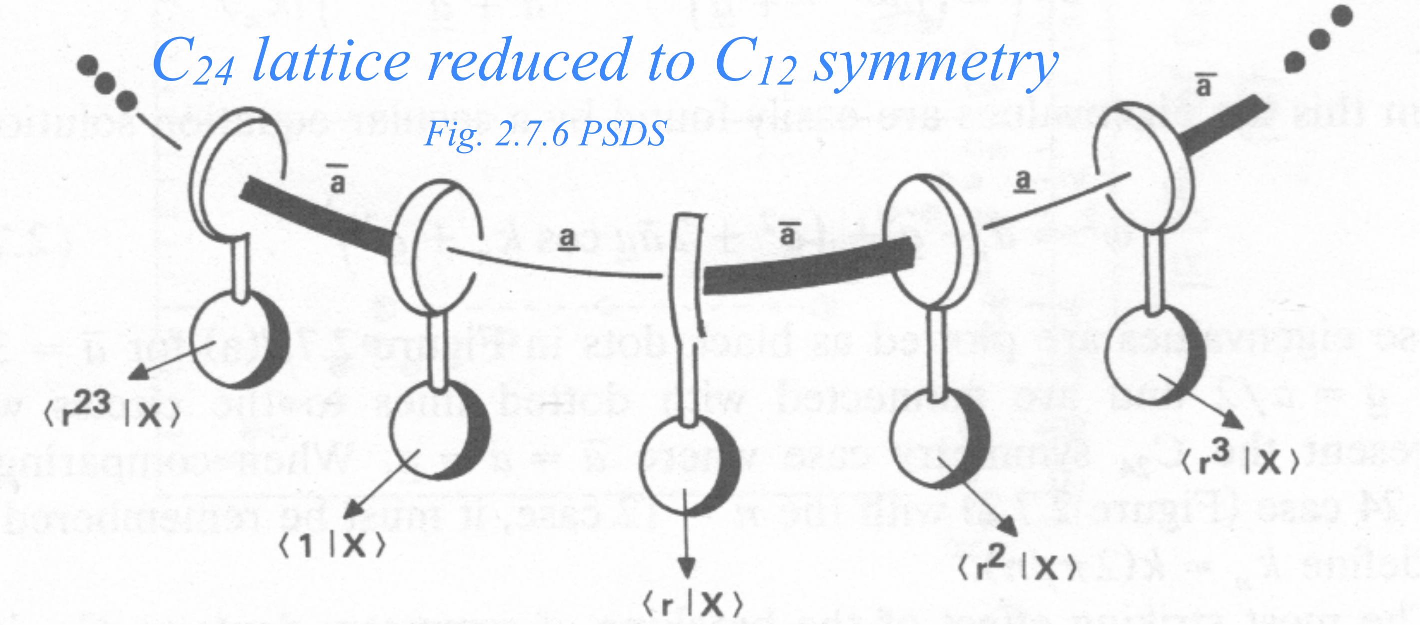


Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

C_{24} lattice reduced to C_{12} symmetry

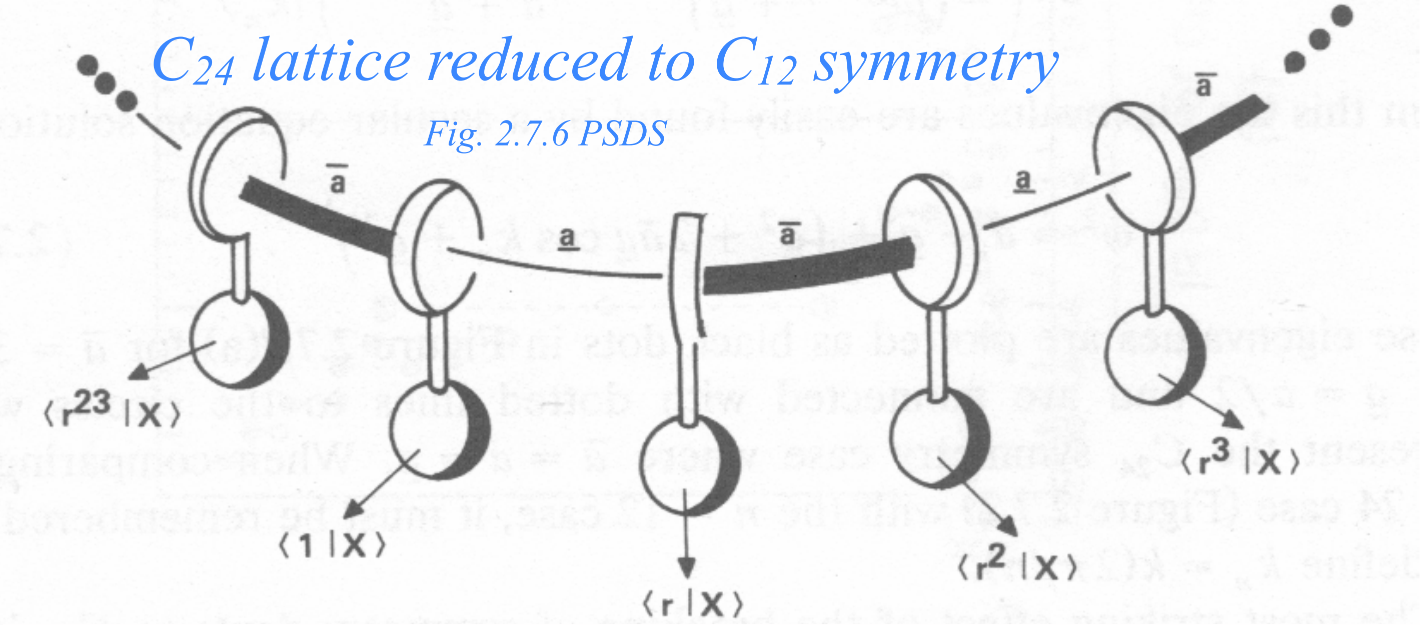


Fig. 2.7.6 PSDS

Fig. 2.7.6 PrinciplesSymmetryDynamics&Spectroscopy

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \dots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a}+\bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a}+\bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

C_{24} lattice reduced to C_{12} symmetry

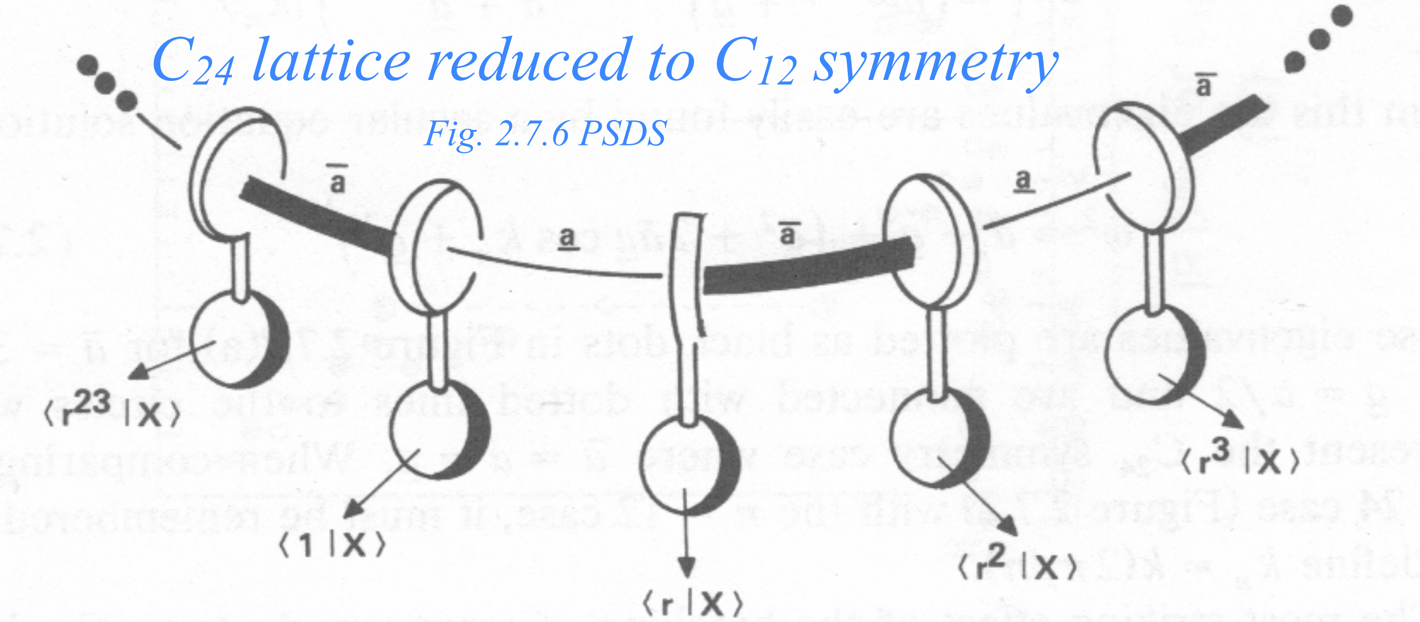


Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \dots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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Only C_{12} symmetry projectors commute with **K***-matrix if* $\underline{a}\neq\bar{a}$. *Then C_{24}-symmetry is broken !*

C_{24} lattice reduced to C_{12} symmetry

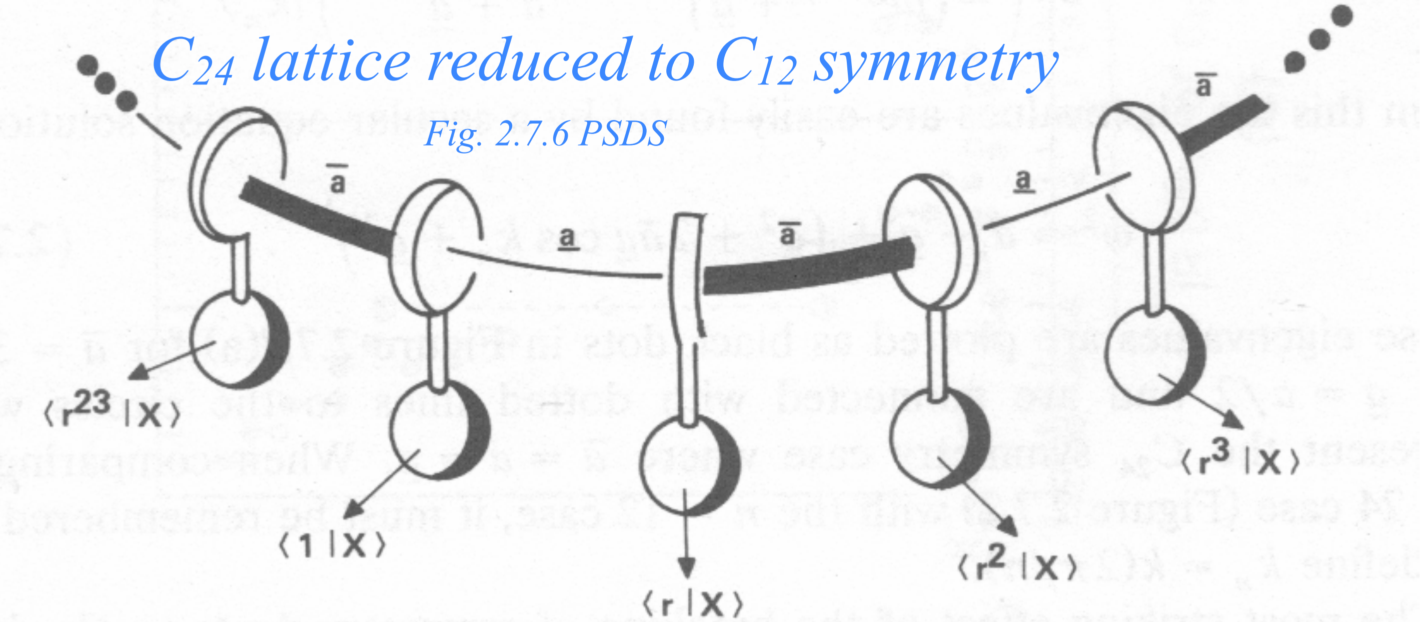

Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \ldots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \ldots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a}+\bar{a} & -\underline{a} & 0 & \ldots & -\bar{a} \\ -\underline{a} & \underline{a}+\bar{a} & -\bar{a} & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with $\mathbf{K}$*-matrix if* $\underline{a} \neq \bar{a}$. *Then C_{24}-symmetry is broken !*

$$\mathbf{P}^{(m)} = \frac{1}{12}\left(\mathbf{1} + e^{-ik_m}\mathbf{r}^{2} + e^{-2ik_m}\mathbf{r}^{4} + e^{-3ik_m}\mathbf{r}^{6} + \ldots + e^{+2ik_m}\mathbf{r}^{-4} + e^{+ik_m}\mathbf{r}^{-2}\right) \text{ where: } \quad k_m = \frac{2\pi m}{12}$$

C_{24} lattice reduced to C_{12} symmetry

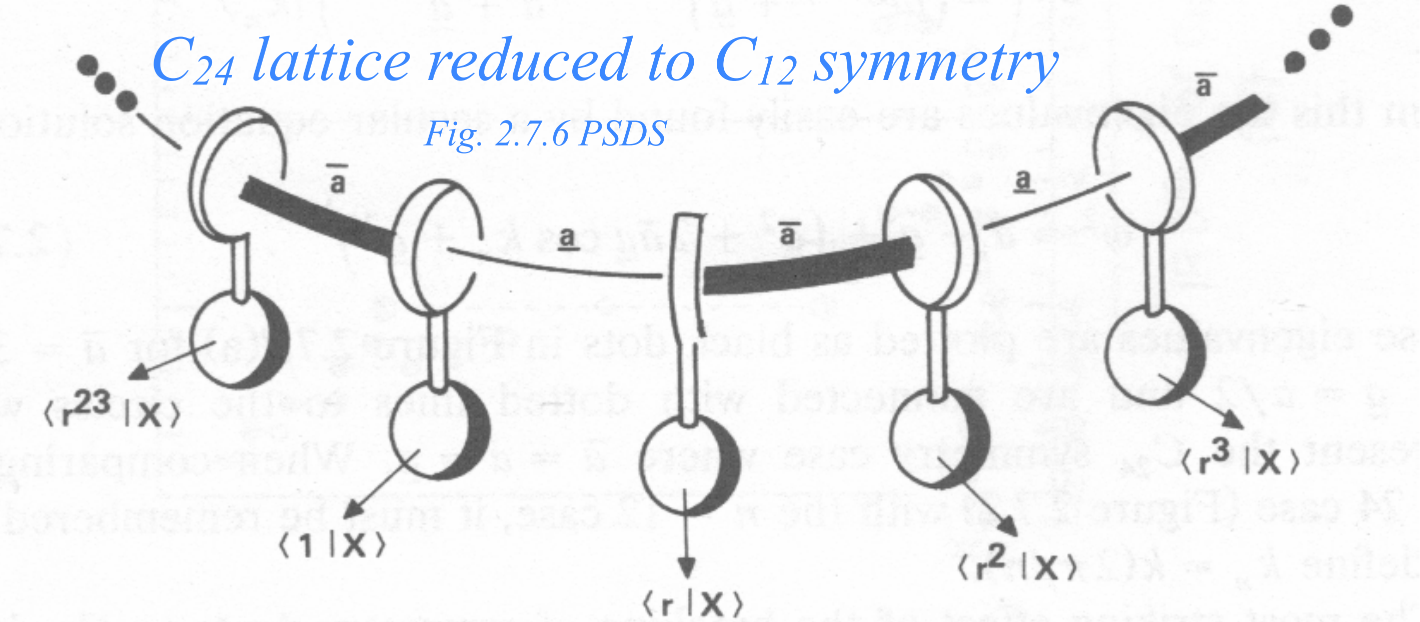

Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \dots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a}+\bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a}+\bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with **K**-matrix if $\underline{a} \neq \bar{a}$. Then C_{24}-symmetry is broken !

$$\mathbf{P}^{(m)} = \frac{1}{12}\left(\mathbf{1} + e^{-ik_m}\mathbf{r}^{2} + e^{-2ik_m}\mathbf{r}^{4} + e^{-3ik_m}\mathbf{r}^{6} + \dots + e^{+2ik_m}\mathbf{r}^{-4} + e^{+ik_m}\mathbf{r}^{-2}\right) \quad \text{where:} \quad k_m = \frac{2\pi m}{12}$$

Two kinds of C_{12} symmetry m-states are coupled by **K**-matrix.

C_{24} lattice reduced to C_{12} symmetry

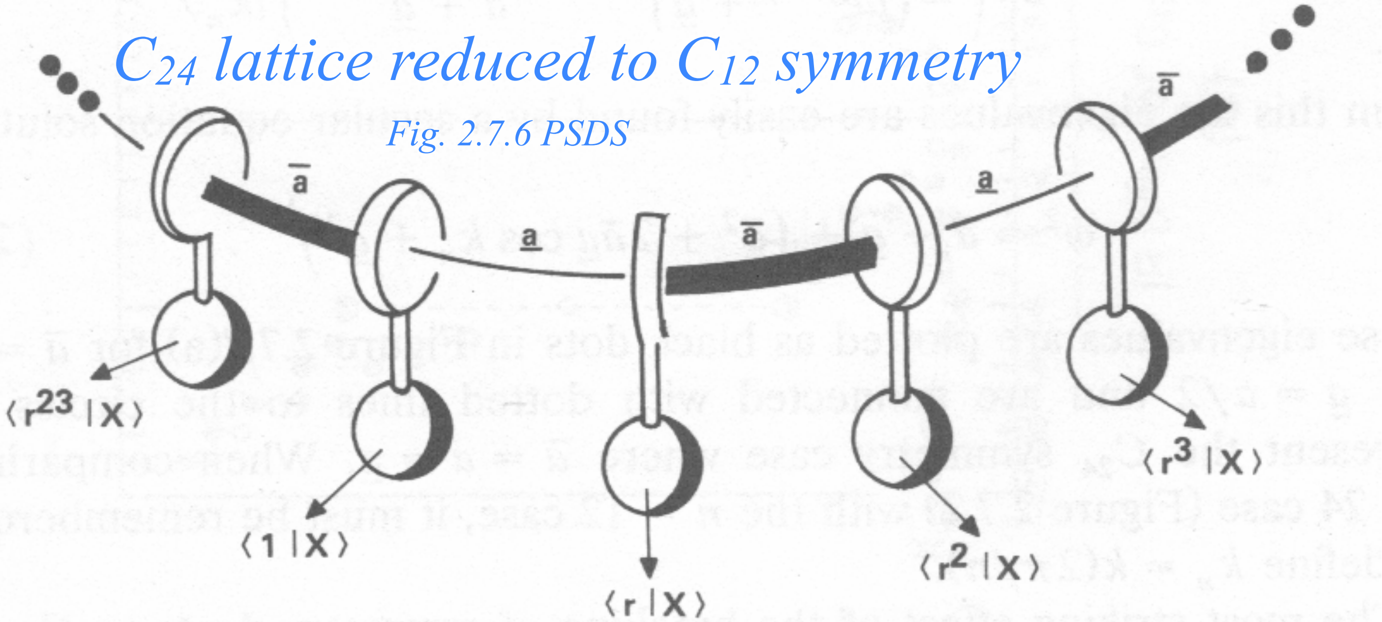

Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \dots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a}+\bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a}+\bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Only C_{12} symmetry projectors commute with **K**-*matrix if* $\underline{a} \neq \bar{a}$. *Then C_{24}-symmetry is broken !*

$$\mathbf{P}^{(m)} = \frac{1}{12}\left(\mathbf{1} + e^{-ik_m}\mathbf{r}^{2} + e^{-2ik_m}\mathbf{r}^{4} + e^{-3ik_m}\mathbf{r}^{6} + \dots + e^{+2ik_m}\mathbf{r}^{-4} + e^{+ik_m}\mathbf{r}^{-2}\right) \quad \text{where:} \quad k_m = \frac{2\pi m}{12}$$

Two kinds of C_{12} symmetry ***m****-states are coupled by* **K**-*matrix: Even $|r^{even}\rangle$ and odd $|r^{odd}\rangle$ p-points.*

$$|k_m\rangle = \mathbf{P}^{(m)}|r^0\rangle \cdot \sqrt{12} = \left(|r^0\rangle + e^{-ik_m}|r^2\rangle + e^{-2ik_m}|r^4\rangle + \dots\right)/\sqrt{12} \qquad |k'_m\rangle = \mathbf{P}^{(m)}|r^1\rangle \cdot \sqrt{12} = \left(|r^1\rangle + e^{-ik_m}|r^3\rangle + e^{-2ik_m}|r^5\rangle + \dots\right)/\sqrt{12}$$

C₂₄ lattice reduced to C₁₂ symmetry

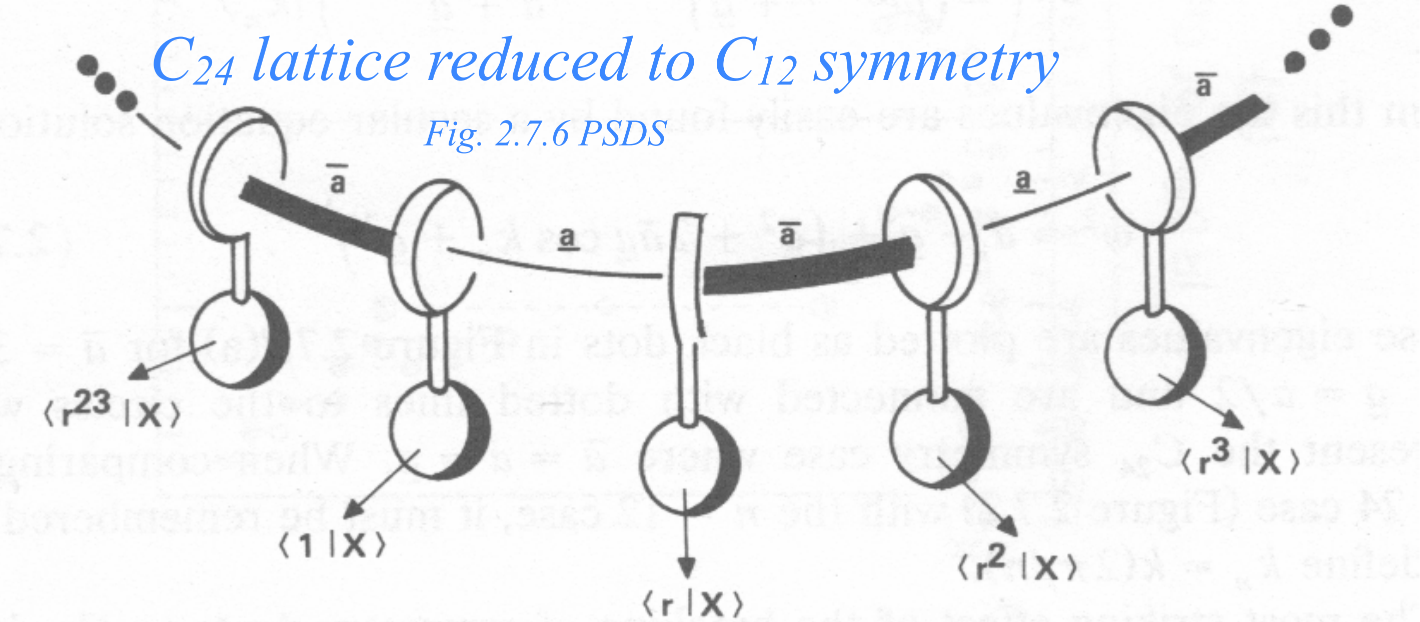

Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \dots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \dots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a}+\bar{a} & -\underline{a} & 0 & \dots & -\bar{a} \\ -\underline{a} & \underline{a}+\bar{a} & -\bar{a} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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$$\mathbf{P}^{(m)} = \frac{1}{12}\left(\mathbf{1} + e^{-ik_m}\mathbf{r}^{2} + e^{-2ik_m}\mathbf{r}^{4} + e^{-3ik_m}\mathbf{r}^{6} + \dots + e^{+2ik_m}\mathbf{r}^{-4} + e^{+ik_m}\mathbf{r}^{-2}\right) \quad \text{where:} \quad k_m = \frac{2\pi m}{12}$$

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$$\begin{aligned} \langle k_m|\mathbf{K}|k_m\rangle &= \langle r^0|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 = \langle r^0|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 \\ &= \langle r^0|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^0|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^0|\mathbf{K}|r^4\rangle|r^5\rangle + \dots \\ &= \quad \underline{a}+\bar{a} \quad + \quad 0 \quad + \quad 0 \quad + \dots \end{aligned}$$

C_{24} lattice reduced to C_{12} symmetry

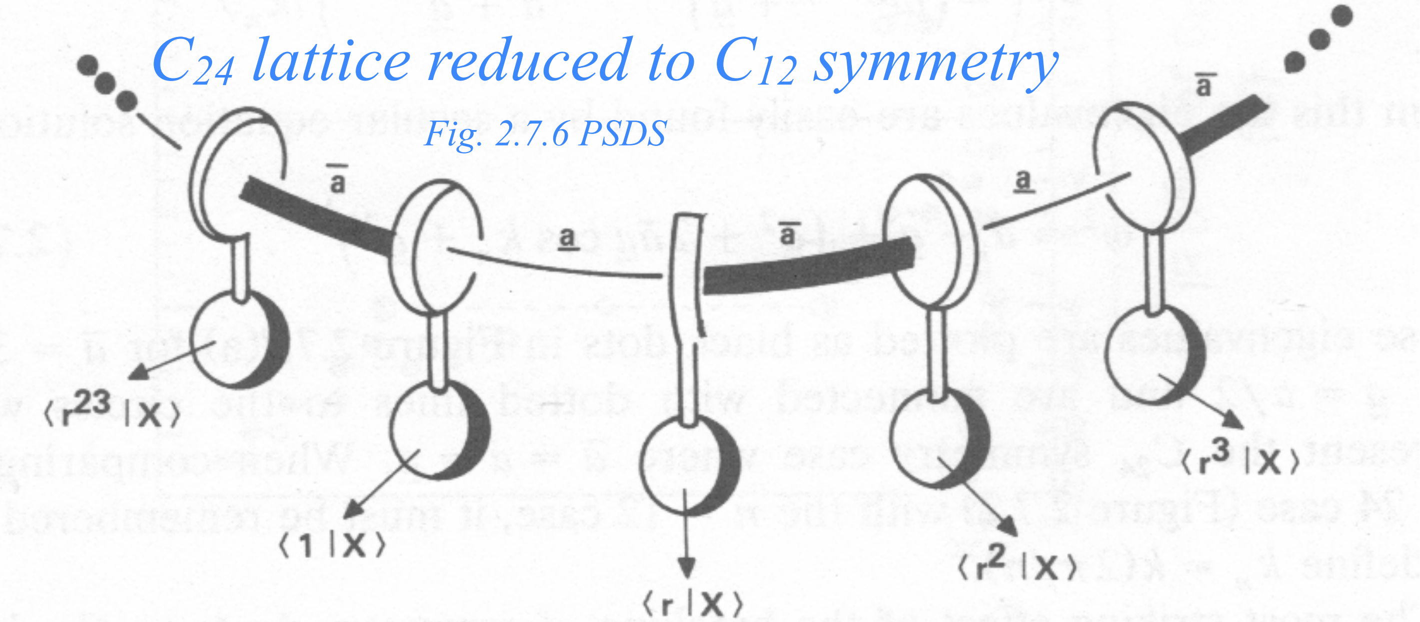

Fig. 2.7.6 PSDS

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$$\langle k_m|\mathbf{K}|k_m\rangle = \langle r^0|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 = \langle r^0|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12$$

$$= \langle r^0|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^0|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^0|\mathbf{K}|r^4\rangle|r^5\rangle + \ldots$$

$$= \underline{a}+\bar{a} \quad + \quad 0 \quad + \quad 0 \quad + \ldots$$

$$\langle k'_m|\mathbf{K}|k_m\rangle = \langle r^1|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 = \langle r^1|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12$$

$$= \langle r^1|\mathbf{K}|r^0\rangle + e^{-ik_m}\langle r^1|\mathbf{K}|r^2\rangle + e^{-2ik_m}\langle r^1|\mathbf{K}|r^4\rangle|r^5\rangle + \ldots$$

$$= \quad -\underline{a} \quad + \; e^{-ik_m} \quad (-\bar{a}) \quad + \quad 0 \quad + \ldots$$

$$= \quad -(\underline{a} \quad + \; e^{-ik_m}\bar{a}) \quad = \quad \langle k_m|\mathbf{K}|k'_m\rangle^*$$

C_{24} lattice reduced to C_{12} symmetry

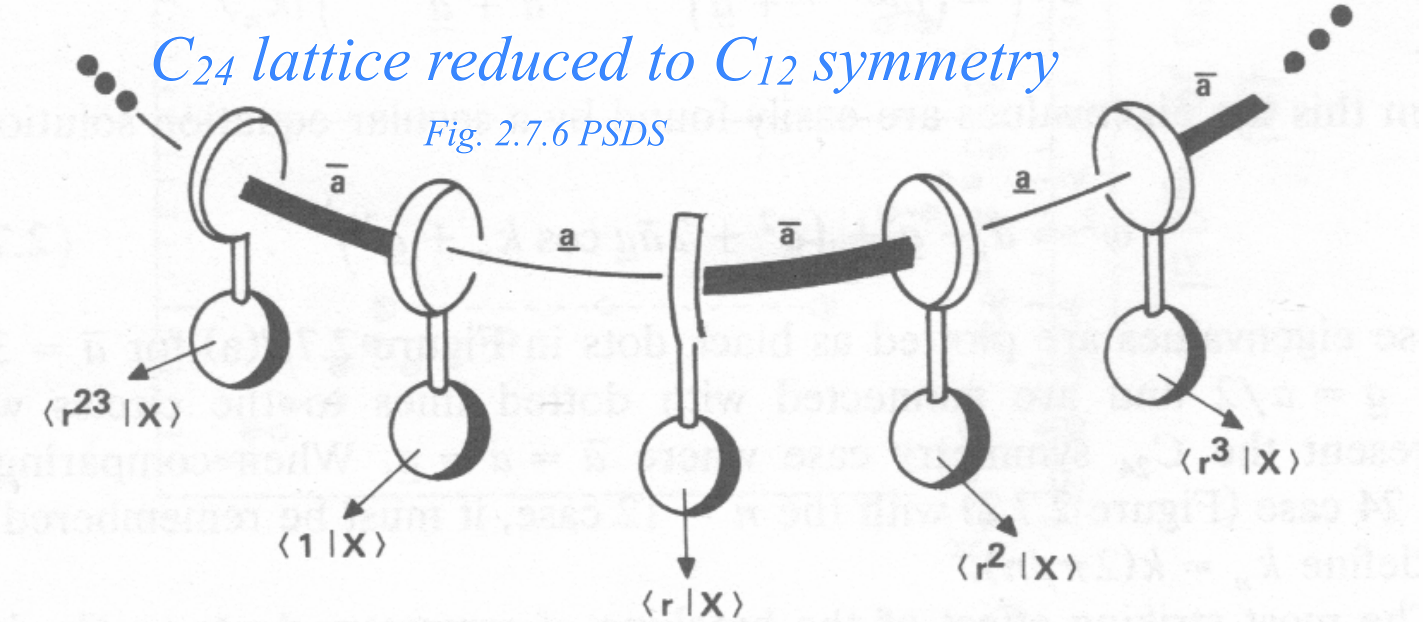

Fig. 2.7.6 PSDS

$$\begin{pmatrix} \langle r^0|\mathbf{K}|r^0\rangle & \langle r^0|\mathbf{K}|r^1\rangle & \langle r^0|\mathbf{K}|r^2\rangle & \ldots & \langle r^0|\mathbf{K}|r^{-1}\rangle \\ \langle r^1|\mathbf{K}|r^0\rangle & \langle r^1|\mathbf{K}|r^1\rangle & \langle r^1|\mathbf{K}|r^2\rangle & \ldots & \langle r^1|\mathbf{K}|r^{-1}\rangle \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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$$\langle\mathbf{K}\rangle^{k_m}=\begin{pmatrix} \langle k_m|\mathbf{K}|k_m\rangle & \langle k_m|\mathbf{K}|k'_m\rangle \\ \langle k'_m|\mathbf{K}|k_m\rangle & \langle k'_m|\mathbf{K}|k'_m\rangle \end{pmatrix}$$

$$=\begin{pmatrix} \underline{a}+\bar{a} & -(\underline{a}+e^{+ik_m}\bar{a}) \\ -(\underline{a}+e^{-ik_m}\bar{a}) & \underline{a}+\bar{a} \end{pmatrix}$$

$$\begin{aligned}\langle k'_m|\mathbf{K}|k_m\rangle &= \langle r^1|\mathbf{P}^{(m)}\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12=\langle r^1|\mathbf{K}\mathbf{P}^{(m)}|r^0\rangle\cdot 12 \\ &= \langle r^1|\mathbf{K}|r^0\rangle+e^{-ik_m}\langle r^1|\mathbf{K}|r^2\rangle+e^{-2ik_m}\langle r^1|\mathbf{K}|r^4\rangle|r^5\rangle+\ldots \\ &= -\underline{a} \quad + e^{-ik_m}(-\bar{a}) \quad + \quad 0 \quad +\ldots \\ &= -(\underline{a} \quad + e^{-ik_m}\bar{a}) \quad = \langle k_m|\mathbf{K}|k'_m\rangle^*\end{aligned}$$

Breaking C_N cyclic coupling into linear chains

Review of 1D-Bohr-ring related to infinite square well (and review of revival)

Breaking C_{2N+2} to approximate linear N-chain

Band-It simulation: Intro to scattering approach to quantum symmetry

Breaking C_{2N} cyclic coupling down to C_N symmetry

Acoustical modes vs. Optical modes

Intro to other examples of band theory

Type-AB avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N

The "4-Group(s)" D_2 and C_{2v}

Spectral decomposition of D_2

Some D_2 modes

Outer product properties and the Group Zoo

C_{24} lattice reduced to C_{12} symmetry

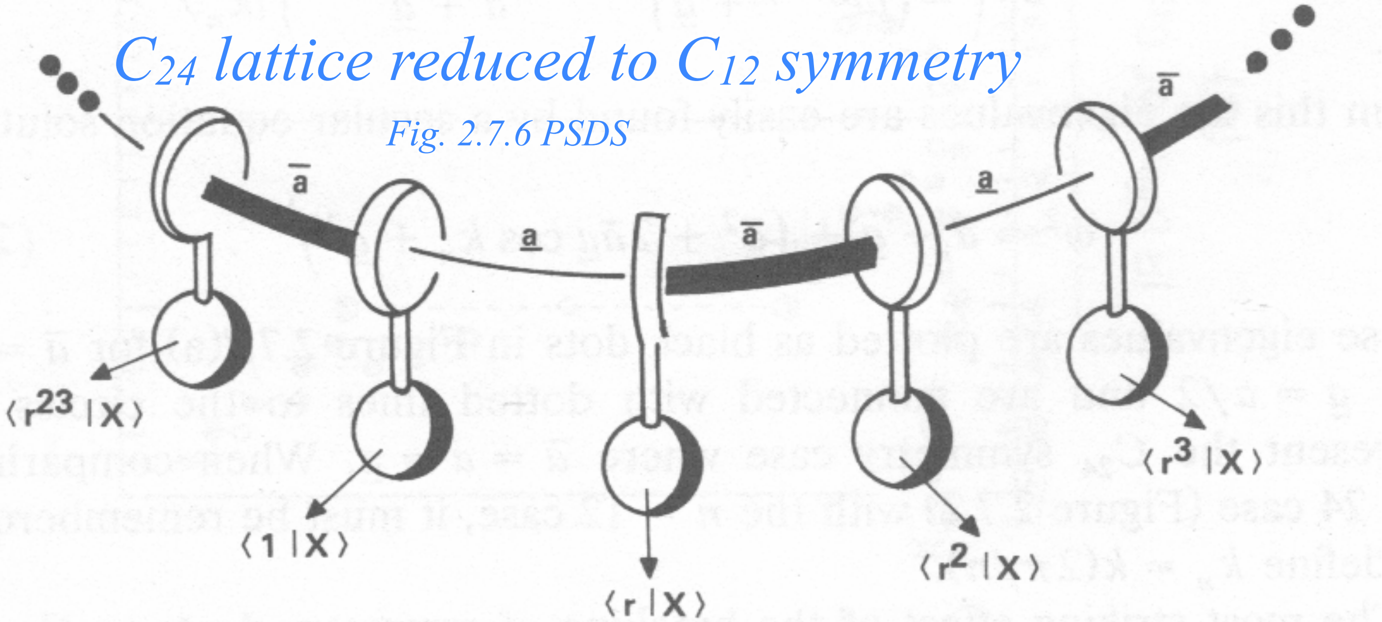

Fig. 2.7.6 PSDS

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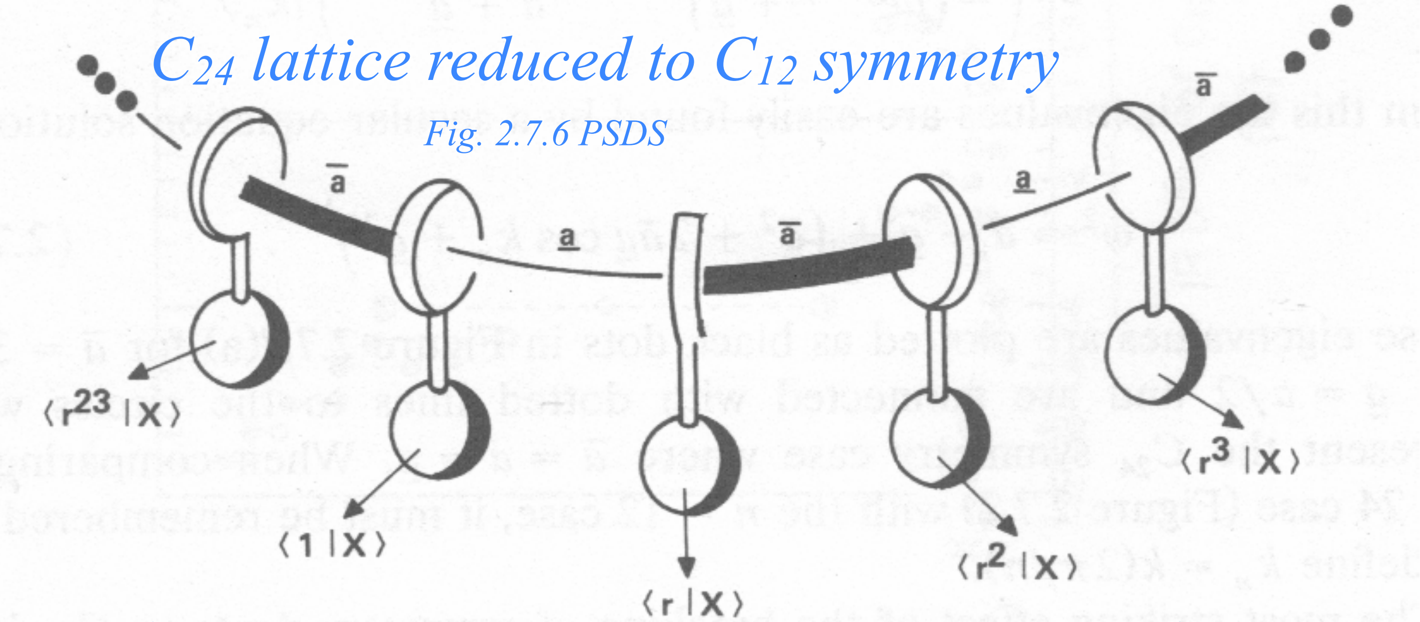
C_{24} lattice reduced to C_{12} symmetry



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Secular Eq.:

$$0 = \kappa^2 - \ Tr\langle\mathbf{K}\rangle^{k_m} + \ Det\langle\mathbf{K}\rangle^{k_m}$$

$$0 = \kappa^2 - 2(\underline{a}+\bar{a})\kappa + (\underline{a}+\bar{a})^2 - (\underline{a}+e^{+ik_m}\bar{a})(\underline{a}+e^{-ik_m}\bar{a})$$

$$0 = \kappa^2 - 2(\underline{a}+\bar{a})\kappa + (\underline{a}+\bar{a})^2 - \underline{a}^2 - \bar{a}^2 - 2\bar{a}\underline{a}\cos k_m$$

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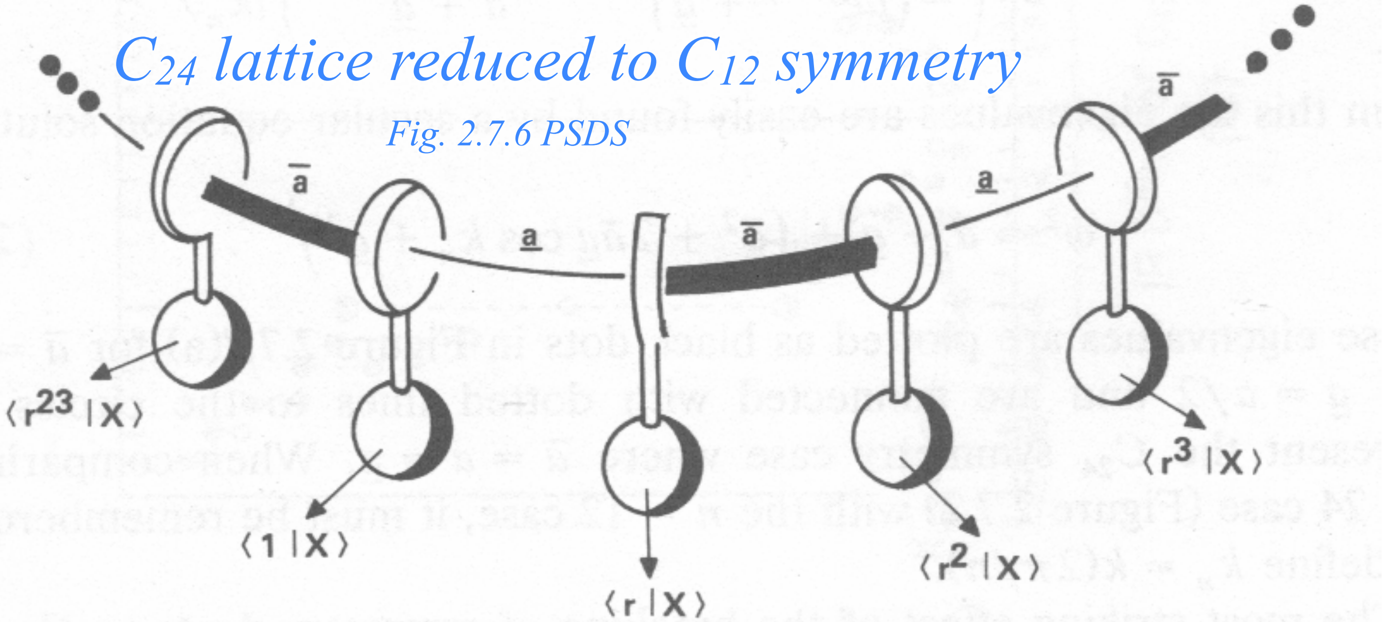
C₂₄ lattice reduced to C₁₂ symmetry



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Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a}+\bar{a} \pm \sqrt{\underline{a}^2 + 2\bar{a}\underline{a}\cos k_m + \bar{a}^2}$$

C_{24} lattice reduced to C_{12} symmetry

Fig. 2.7.7 PSDS

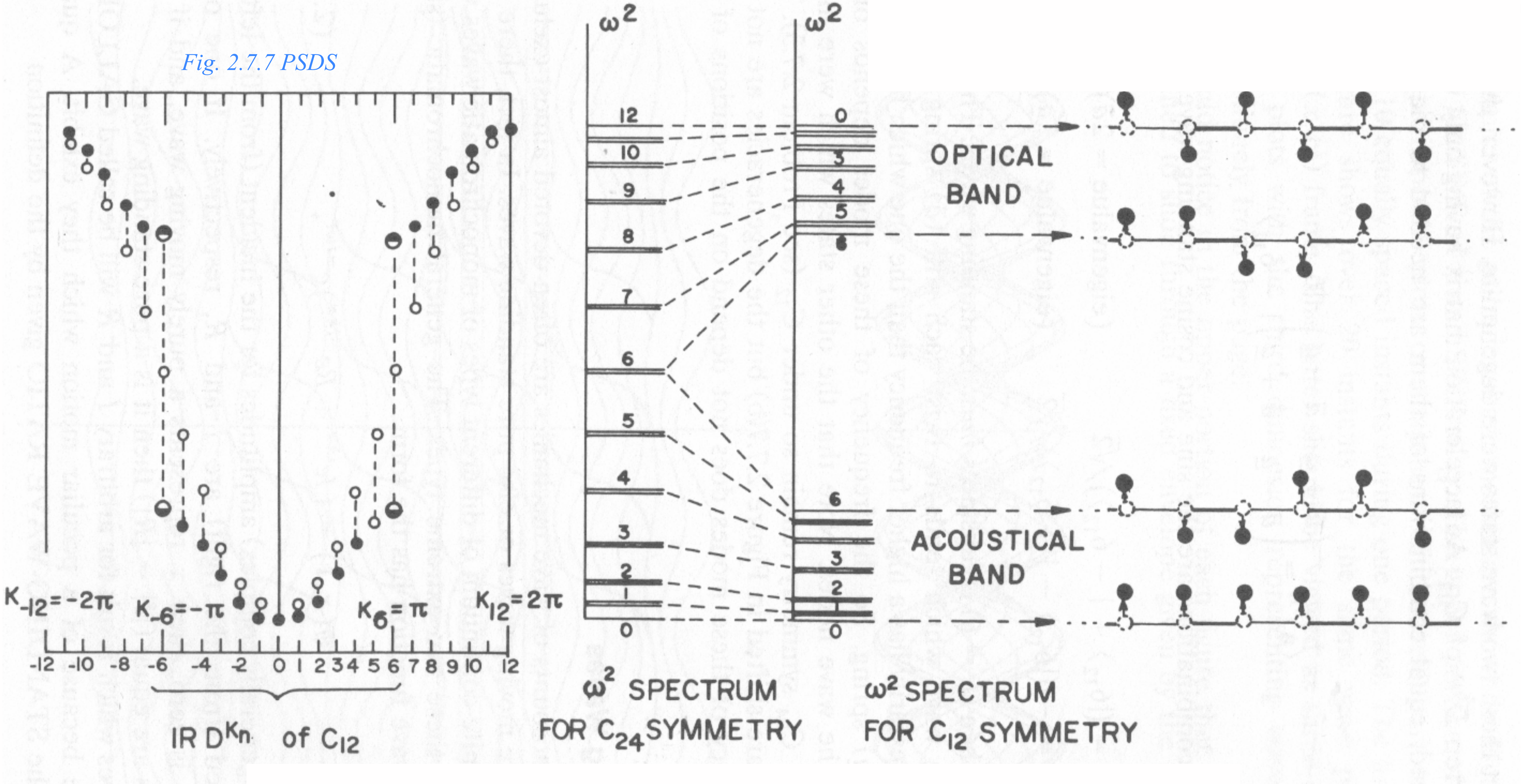

Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\bar{a}\underline{a}\cos k_m + \bar{a}^2}$$

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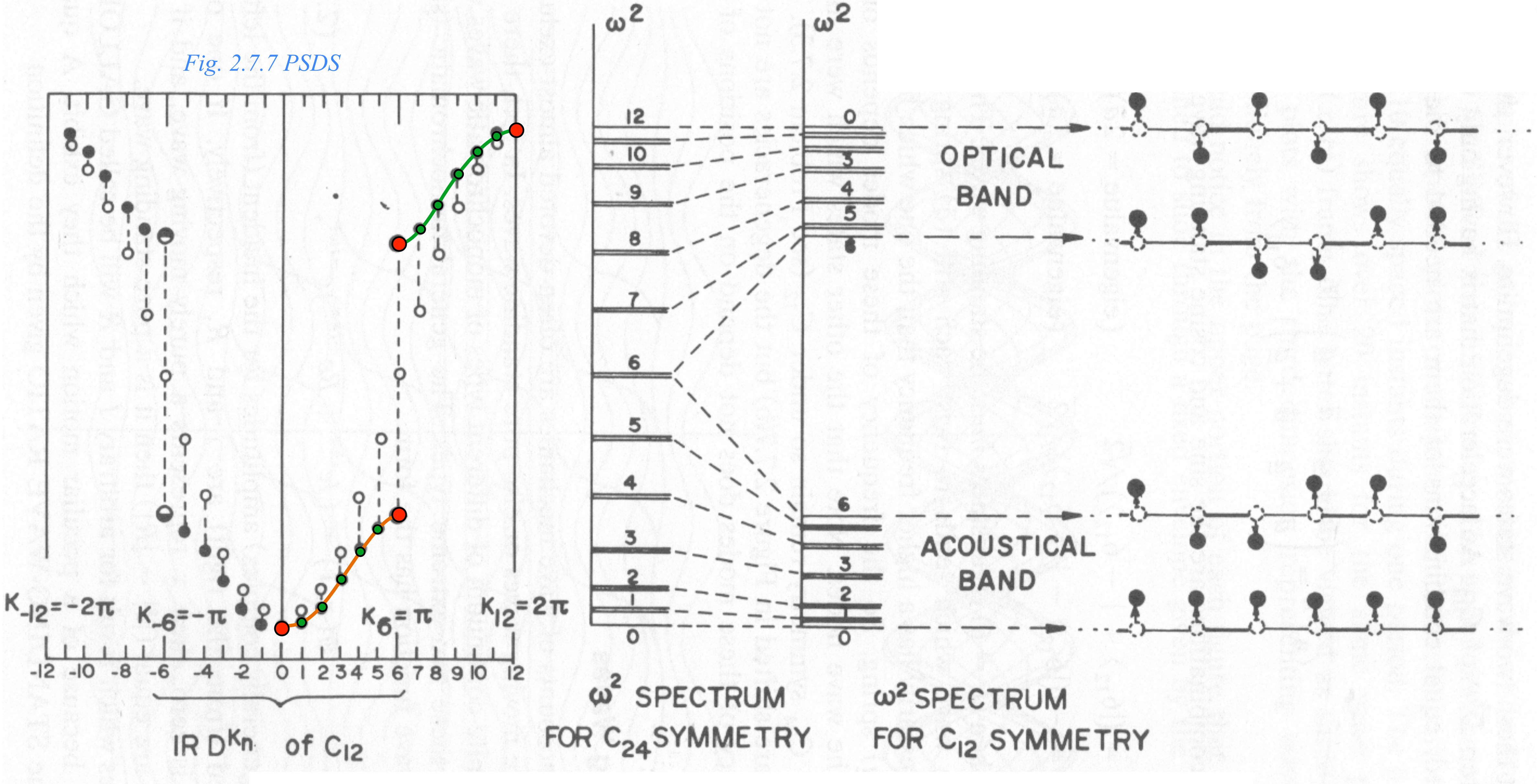
C_{24} lattice reduced to C_{12} symmetry



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$$= \begin{pmatrix} \underline{a} + \bar{a} & -(\underline{a} + e^{+ik_m}\bar{a}) \\ -(\underline{a} + e^{-ik_m}\bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$

C_{24} lattice reduced to C_{12} symmetry

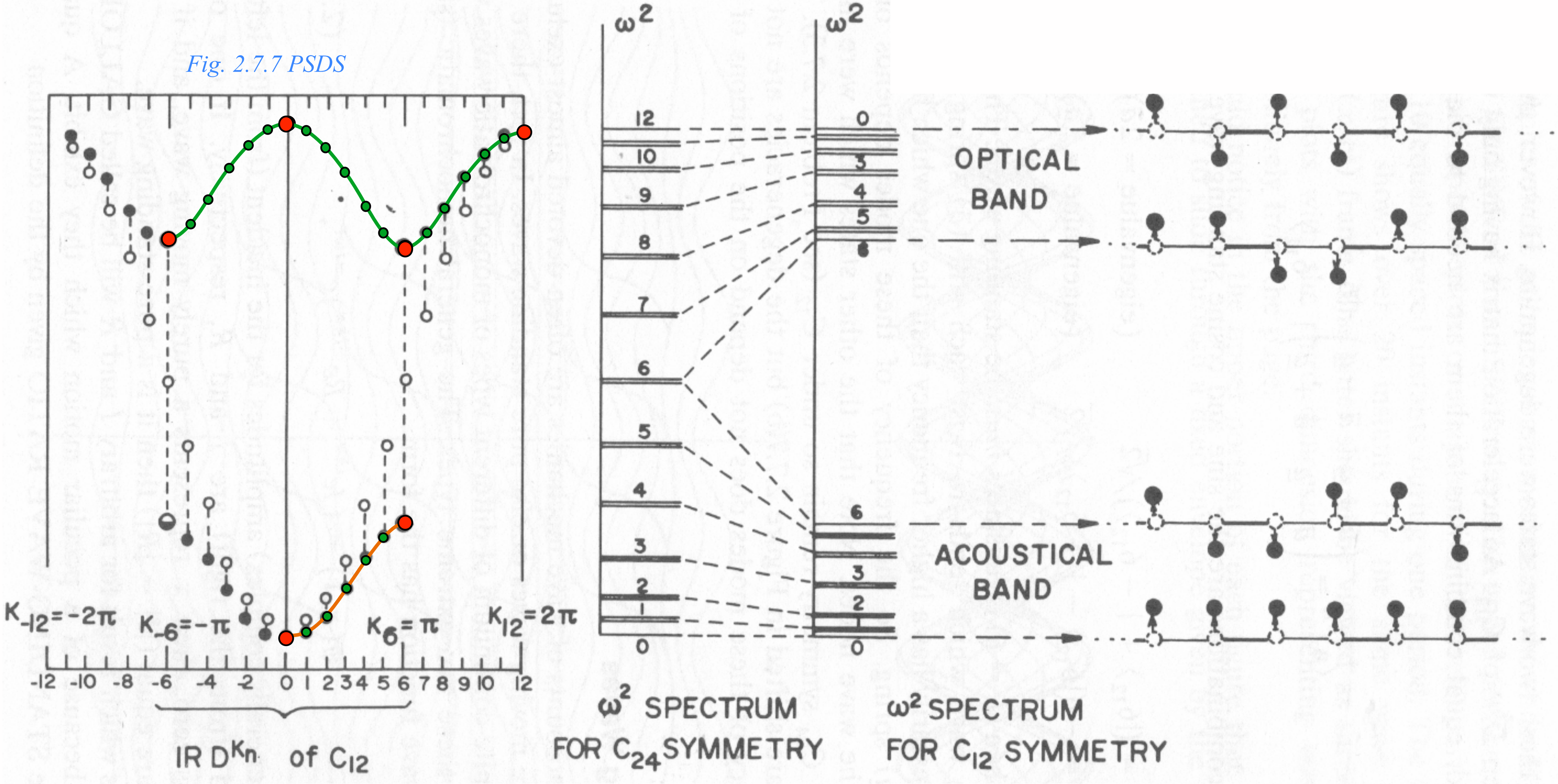


Figure 2.7.7 Band splitting due to C_{24}–C_{12} symmetry breaking.

Eigenvalues:

$$\kappa = \omega_{k_m}^2 = \underline{a} + \bar{a} \pm \sqrt{\underline{a}^2 + 2\bar{a}\underline{a}\cos k_m + \bar{a}^2}$$

$$\langle \mathbf{K} \rangle^{k_m} = \begin{pmatrix} \langle k_m | \mathbf{K} | k_m \rangle & \langle k_m | \mathbf{K} | k'_m \rangle \\ \langle k'_m | \mathbf{K} | k_m \rangle & \langle k'_m | \mathbf{K} | k'_m \rangle \end{pmatrix}$$

$$= \begin{pmatrix} \underline{a} + \bar{a} & \text{-}(\underline{a} + e^{+ik_m}\bar{a}) \\ \text{-}(\underline{a} + e^{-ik_m}\bar{a}) & \underline{a} + \bar{a} \end{pmatrix}$$

Breaking C_N cyclic coupling into linear chains
Review of 1D-Bohr-ring related to infinite square well (and review of revival)
Breaking C_{2N+2} to approximate linear N-chain
Band-It simulation: Intro to scattering approach to quantum symmetry

Breaking C_{2N} cyclic coupling down to C_N symmetry
Acoustical modes vs. Optical modes
➡ *Intro to other examples of band theory* ⬅
Type-AB avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N
The "4-Group(s)" D_2 and C_{2v}
Spectral decomposition of D_2
Some D_2 modes
Outer product properties and the Group Zoo

Intro to other examples of band theory

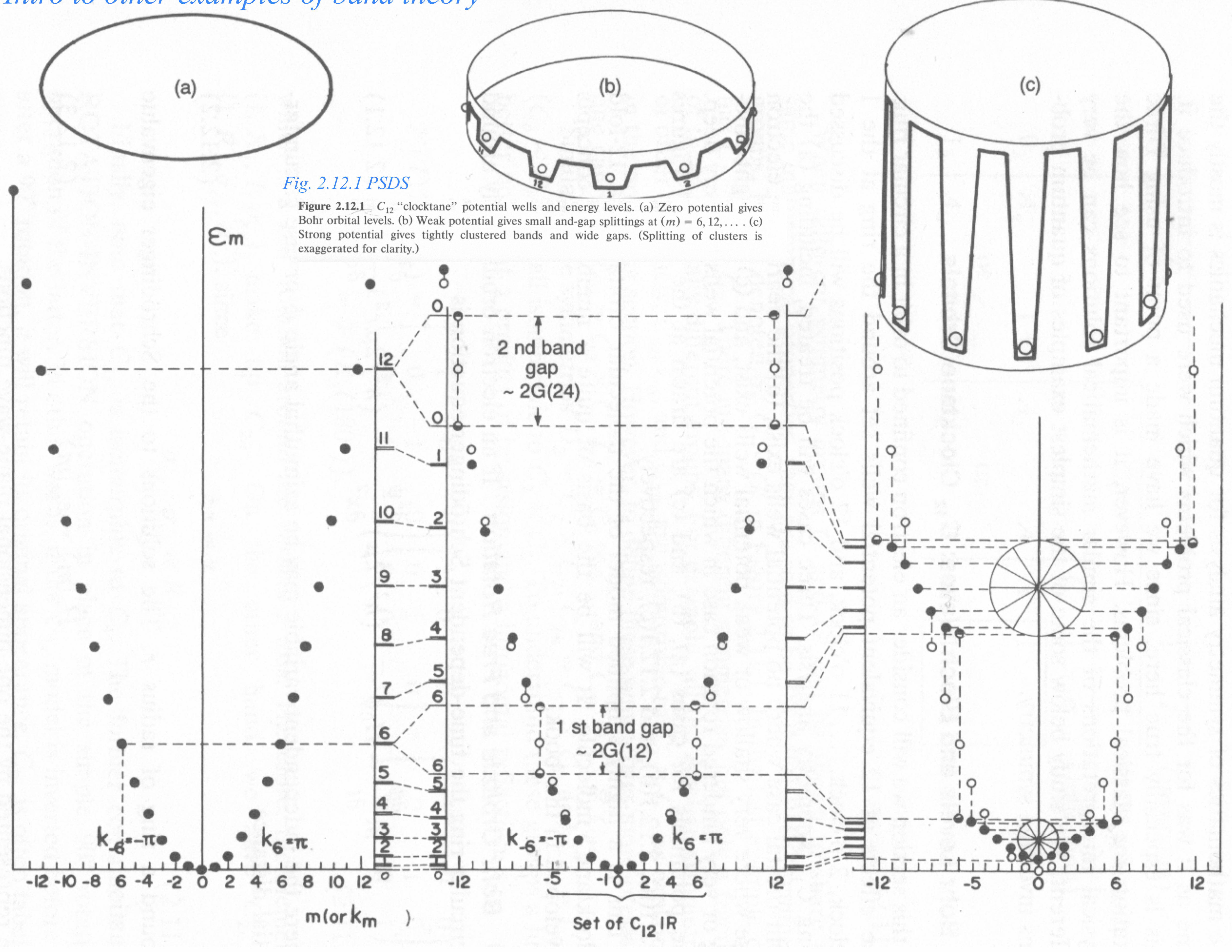


Fig. 2.12.1 PSDS

Figure 2.12.1 C_{12} "clocktane" potential wells and energy levels. (a) Zero potential gives Bohr orbital levels. (b) Weak potential gives small and-gap splittings at $(m) = 6, 12, \ldots$ (c) Strong potential gives tightly clustered bands and wide gaps. (Splitting of clusters is exaggerated for clarity.)

Crossing equations for a pair of humps

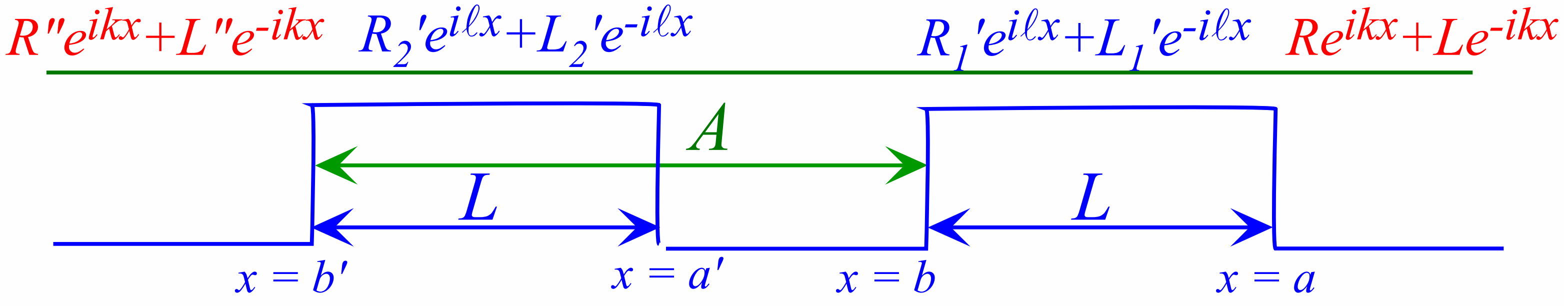


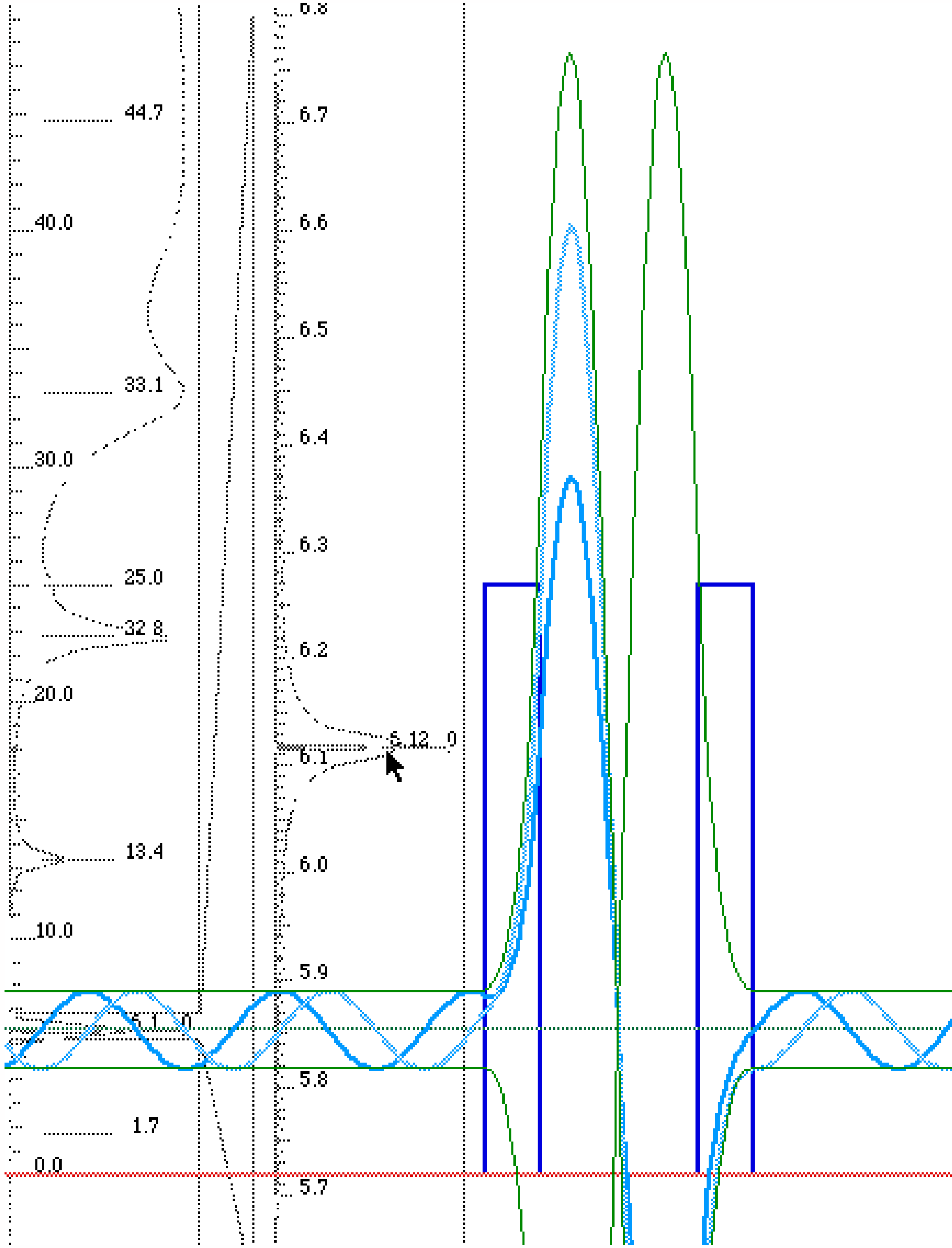
Fig. 14.1.5 C₂-symmetric double barrier .

$$\begin{pmatrix} R'' \\ L'' \end{pmatrix} = \begin{pmatrix} e^{i2kL}\chi^{*2}+e^{-i2kA}\xi^{2} & -i\xi\left(e^{-i2kb}\chi^{*}+e^{-i2ka'}\chi\right) \\ i\xi\left(e^{i2kb}\chi+e^{i2ka'}\chi^{*}\right) & e^{-i2kL}\chi^{2}+e^{i2kA}\xi^{2} \end{pmatrix} \begin{pmatrix} R \\ L \end{pmatrix}$$

$\chi = \cosh \kappa L - i \sinh 2\beta \;\, \sinh \kappa L$, and: $\xi = \cosh 2\beta \;\, \sinh \kappa L$

$$\cosh 2\beta = \frac{1}{2}\left(\frac{\kappa}{k}+\frac{k}{\kappa}\right) = \frac{\kappa^2+k^2}{2k\kappa}, \qquad \sinh 2\beta = \frac{1}{2}\left(\frac{\kappa}{k}-\frac{k}{\kappa}\right) = \frac{\kappa^2-k^2}{2k\kappa}$$

Fig. 14.1.7 Second (E= 6.117) resonance in L=0.5 well between two width=0.5 barriers(V=25) .



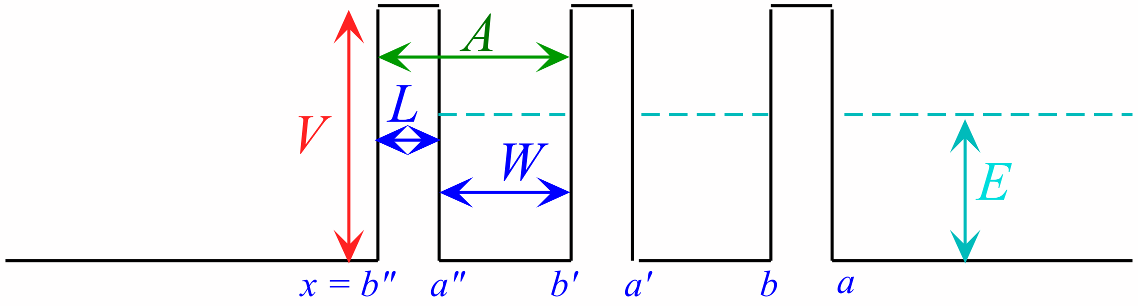
Intro to other examples of band theory

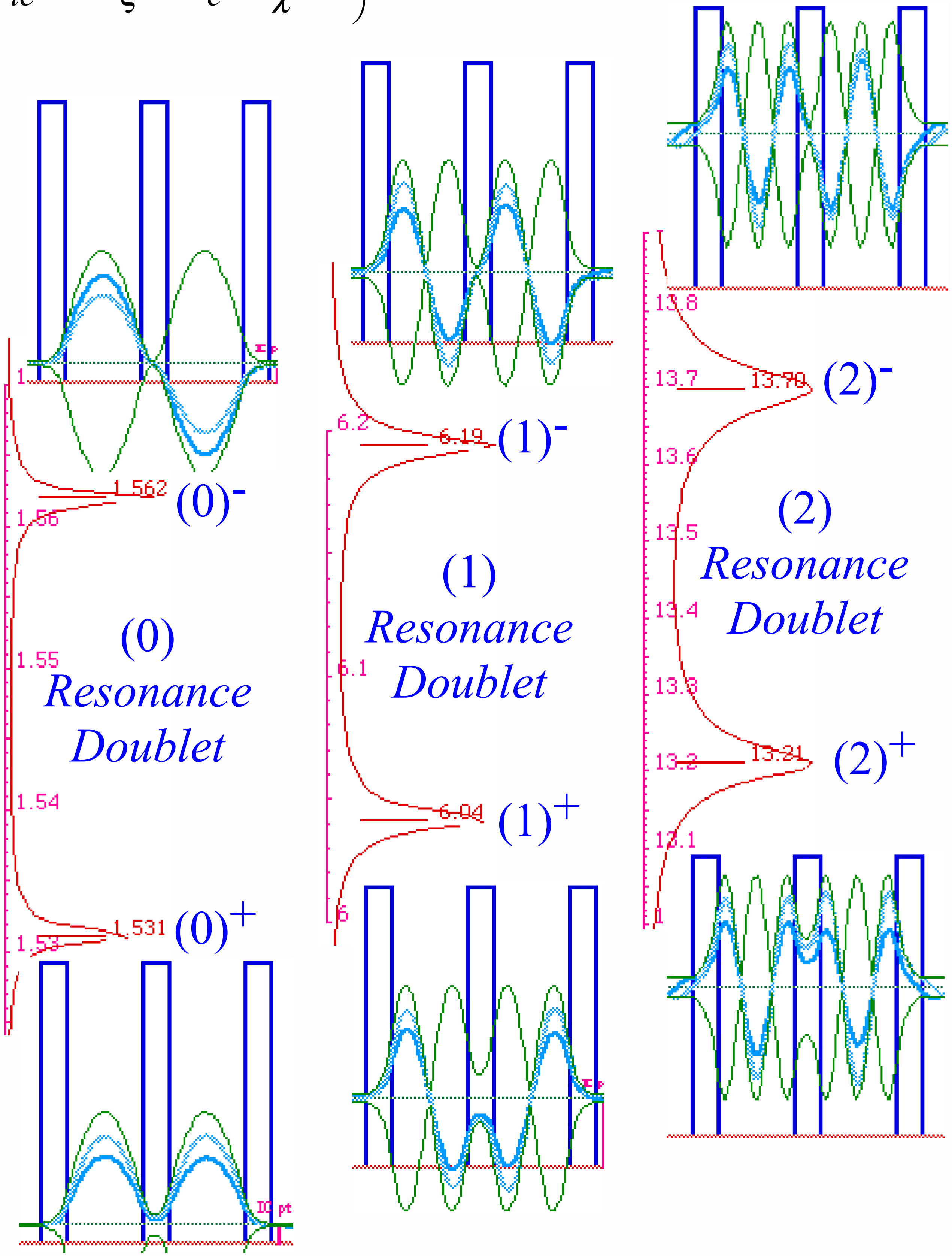
$$C^{3-barrier} = C''\cdot C'\cdot C$$

$$= \begin{pmatrix} e^{ikL}\chi^* & -ie^{-ik(a''+b'')}\xi \\ ie^{ik(a''+b'')}\xi & e^{-ikL}\chi \end{pmatrix}\cdot\begin{pmatrix} e^{ikL}\chi^* & -ie^{-ik(a'+b')}\xi \\ ie^{ik(a'+b')}\xi & e^{-ikL}\chi \end{pmatrix}\cdot\begin{pmatrix} e^{ikL}\chi^* & -ie^{-ik(a+b)}\xi \\ ie^{ik(a+b)}\xi & e^{-ikL}\chi \end{pmatrix}$$

Crossing equations for three humps

Fig. 14.1.10 Triple-barrier double-well potential





Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

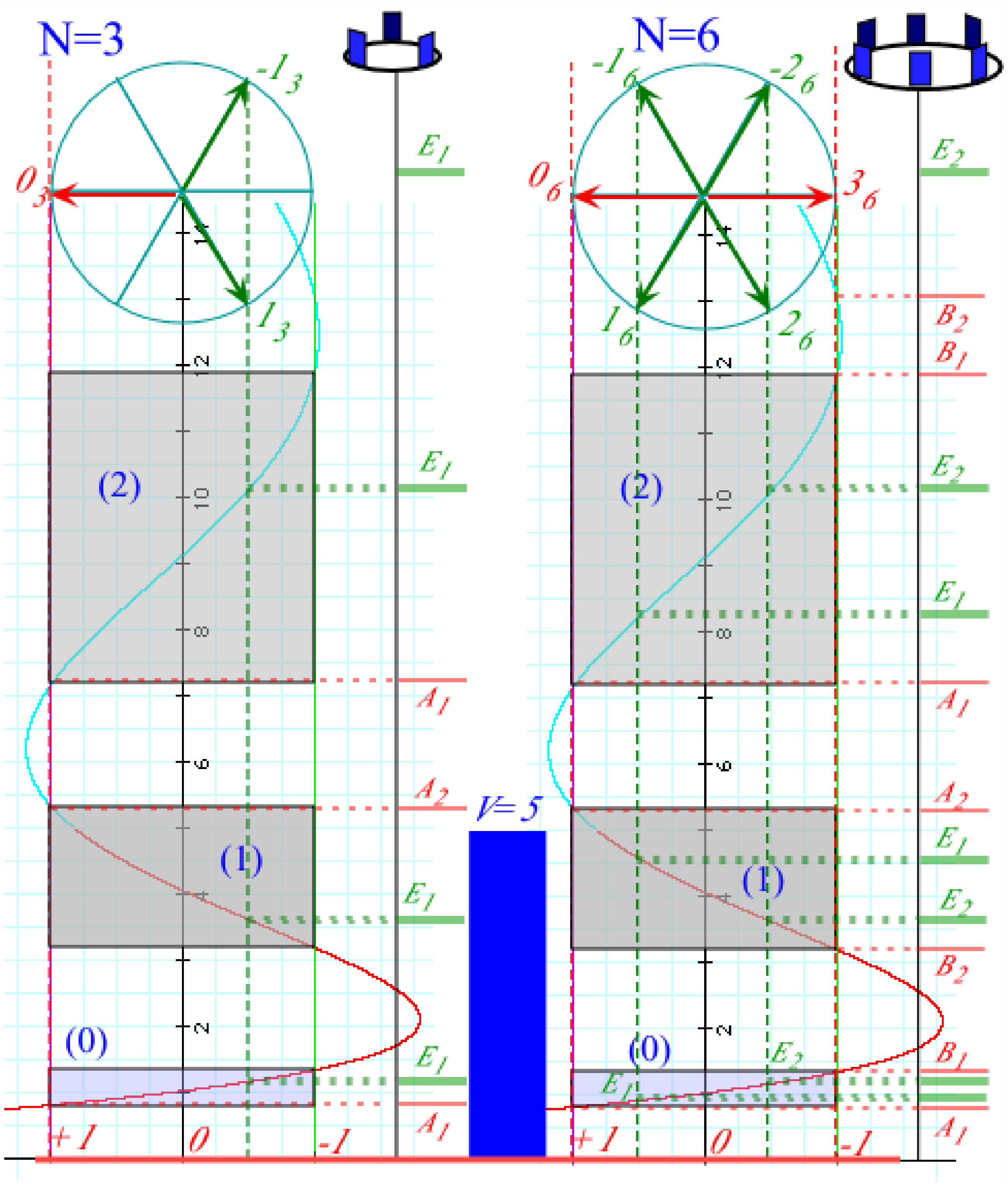


Fig. 14.2.8 Multiplets for V=5.
(W=15nm well ,L=5nm barrier) for (N=3)-ring and (N=6)-ring.

Intro to other examples of band theory

Bohr-It simulations assume ring-periodic-boundary conditions

Band-It simulations line-non-periodic scattering conditions

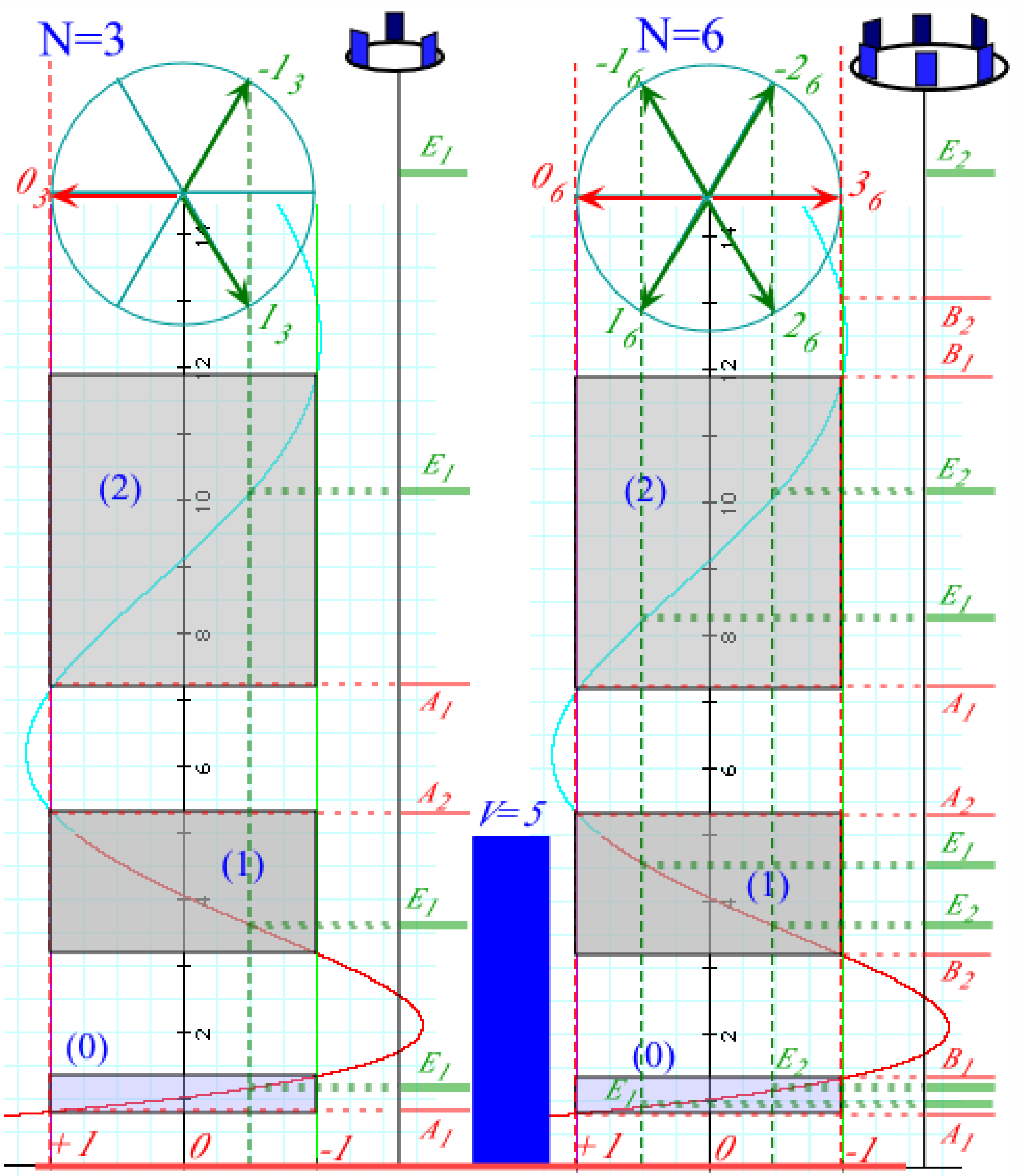


Fig. 14.2.8 Multiplets for V=5.
(W=15nm well ,L=5nm barrier) for (N=3)-ring and (N=6)-ring.

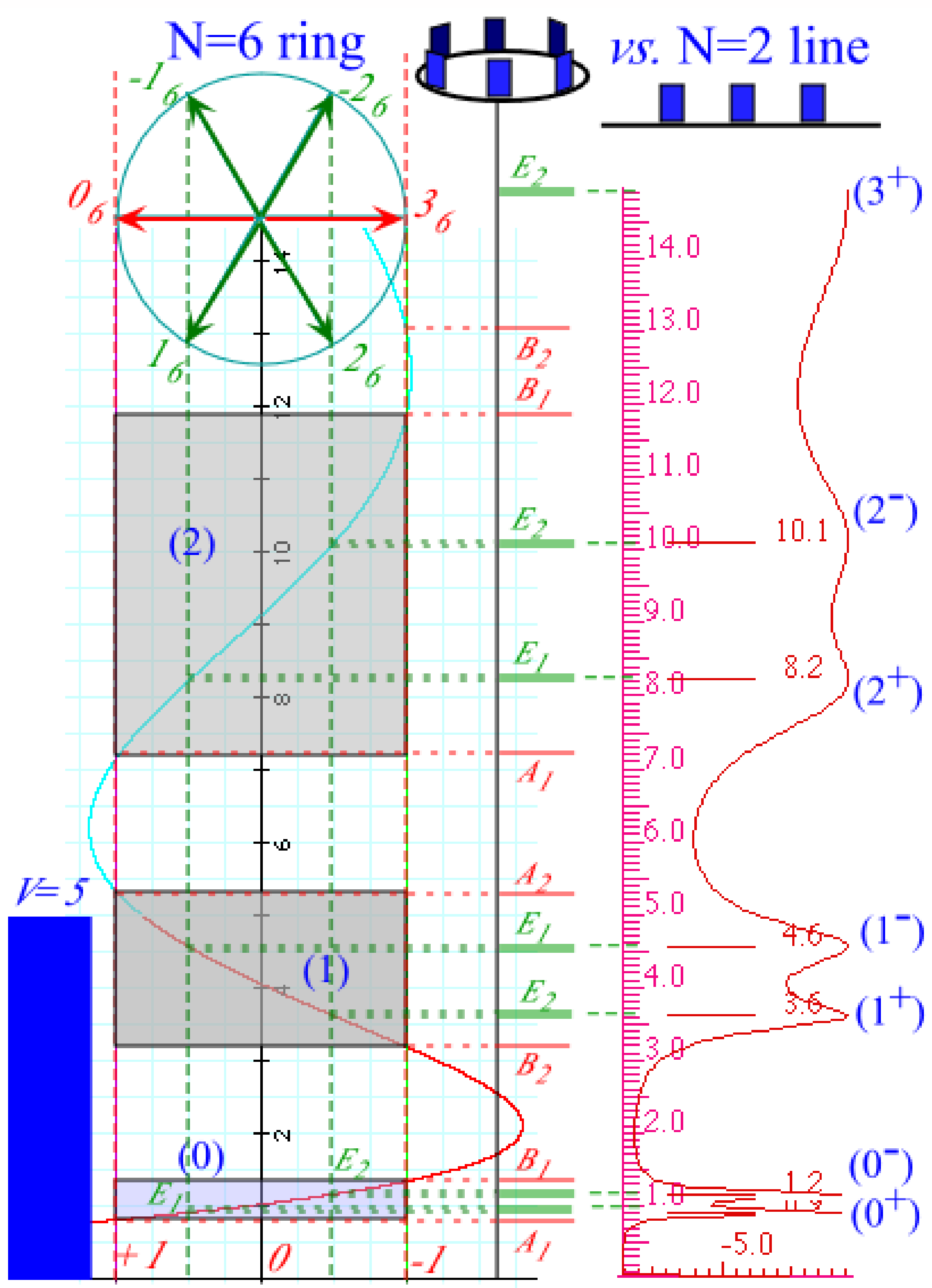


Fig. 14.2.9 (N=6)-ring and (N=2)-line potential.
(V=5, W=15nm well ,L=5nm barrier)

Breaking C_N cyclic coupling into linear chains

- *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
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  - *Band-It simulation: Intro to scattering approach to quantum symmetry*

Breaking C_{2N} cyclic coupling down to C_N symmetry

- *Acoustical modes vs. Optical modes*
- *Intro to other examples of band theory*
- ➡ *Type-*AB *avoided crossing view of band-gaps* ⬅

Finally! Symmetry groups that are not just C_N

- *The "4-Group(s)" D_2 and C_{2v}*
- *Spectral decomposition of D_2*
  - *Some D_2 modes*
- *Outer product properties and the Group Zoo*

Pure Type-B Hamiltonian

NH_3 (Ammonia)

Fig. 2.12.7 PSDS

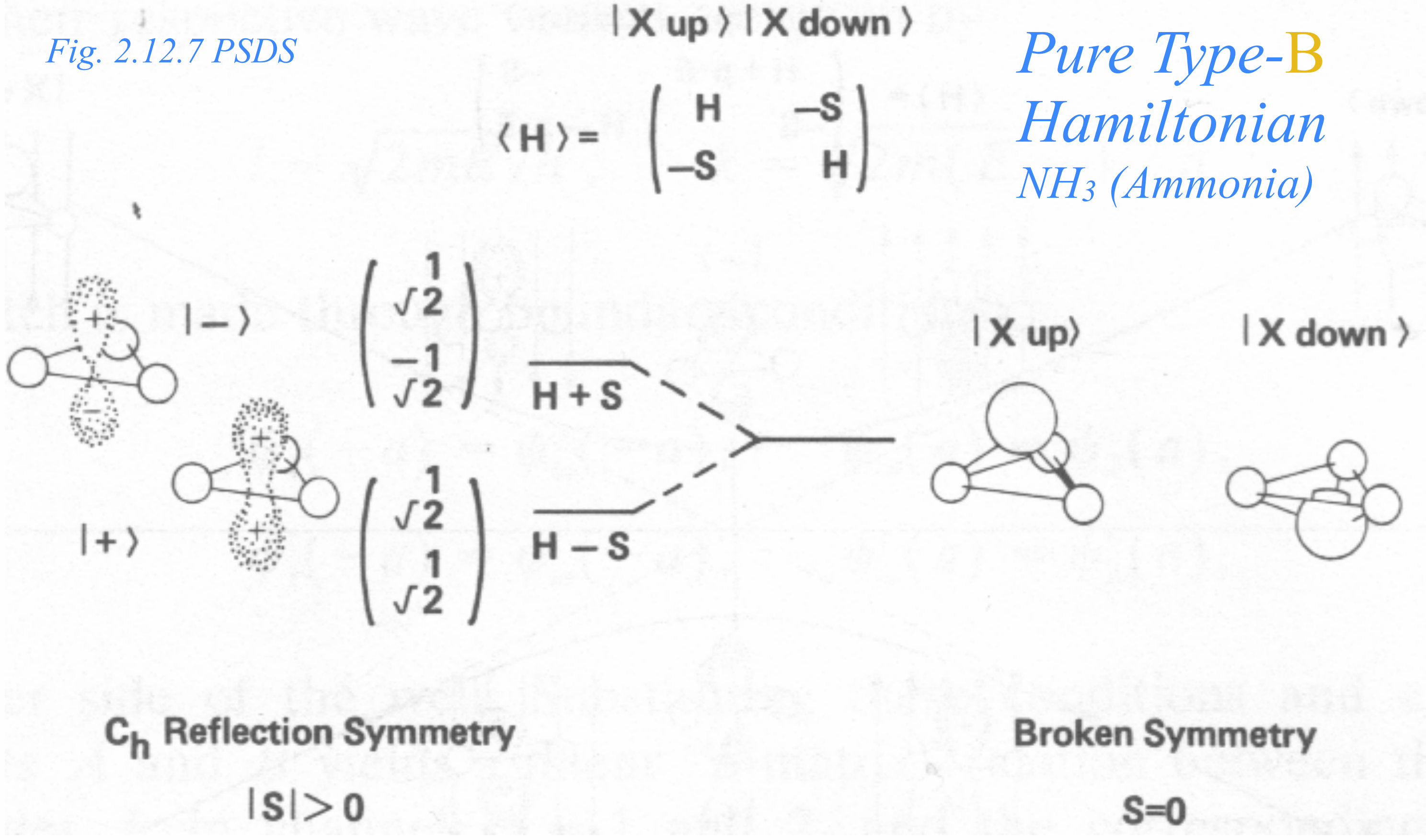
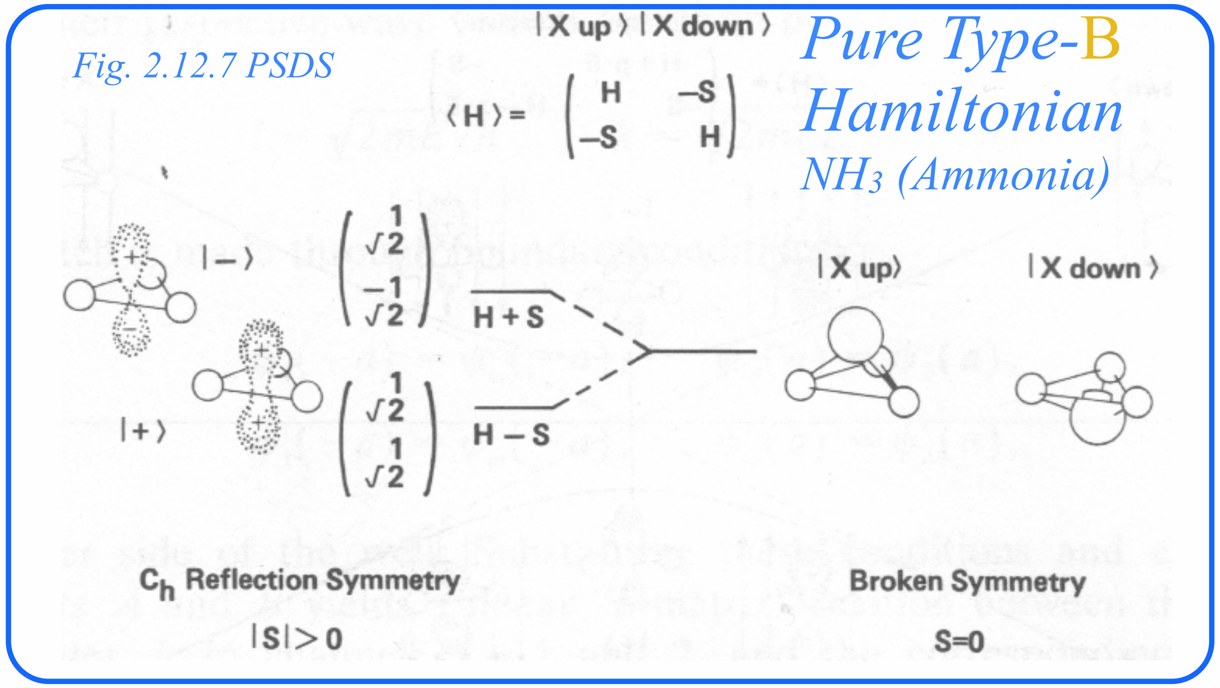


Fig. 2.12.7 PSDS



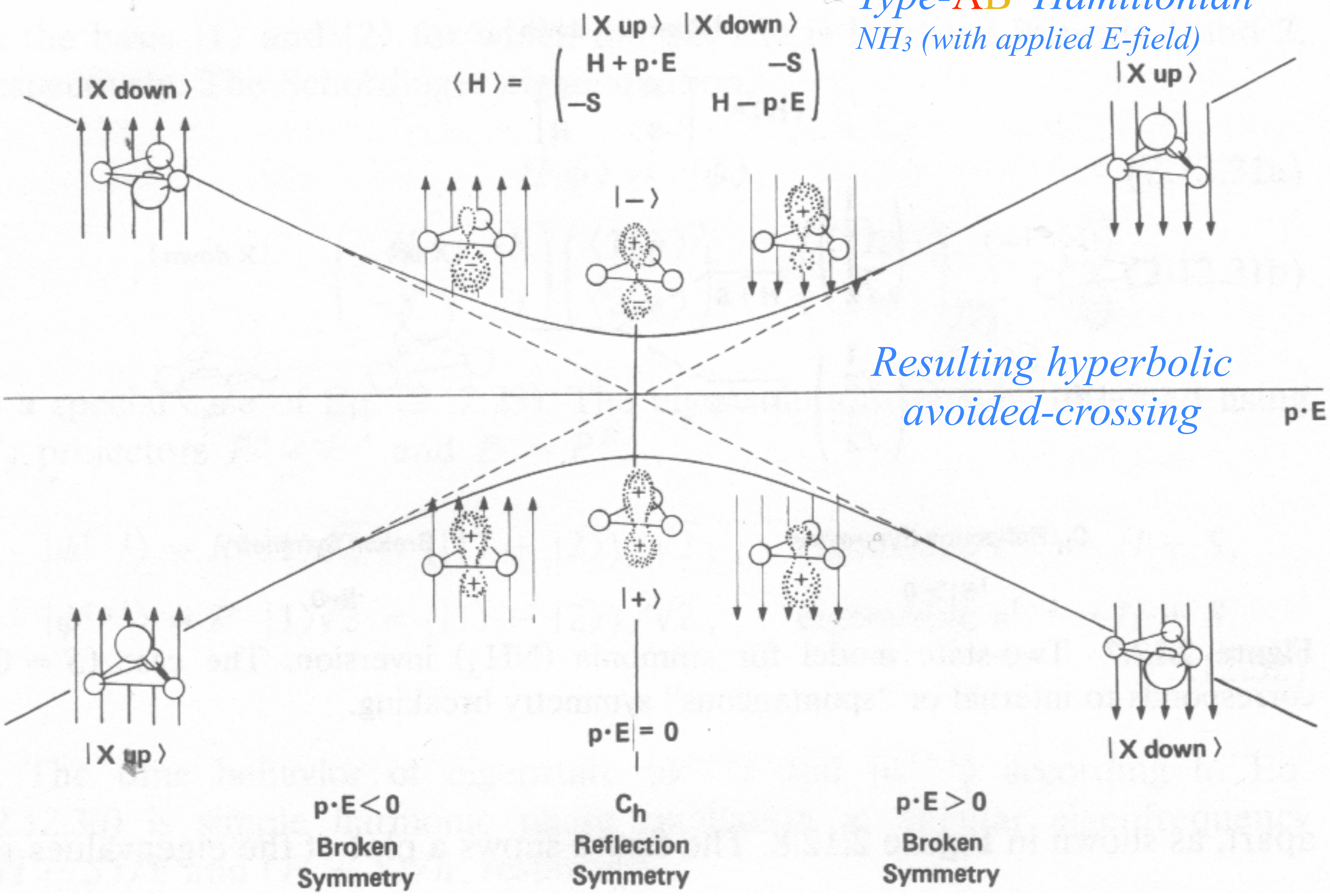
Pure Type-B Hamiltonian

NH₃ (Ammonia)

Type-AB Hamiltonian

NH₃ (with applied E-field)

Fig. 2.12.8 PSDS



Resulting hyperbolic avoided-crossing

Transform $\mathbf{H}(A-basis)$ *into* $\mathbf{H}(B-basis)$

$$\frac{\begin{pmatrix}1&1\\1&-1\end{pmatrix}}{\sqrt{2}}\begin{pmatrix}+A&B\\B&-A\end{pmatrix}\frac{\begin{pmatrix}1&1\\1&-1\end{pmatrix}}{\sqrt{2}}$$

$$=\frac{1}{2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\begin{pmatrix}+A&B\\B&-A\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

$$=\frac{1}{2}\begin{pmatrix}+A+B&B-A\\+A-B&B+A\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

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

$$=\begin{pmatrix}+B&A\\A&-B\end{pmatrix}$$

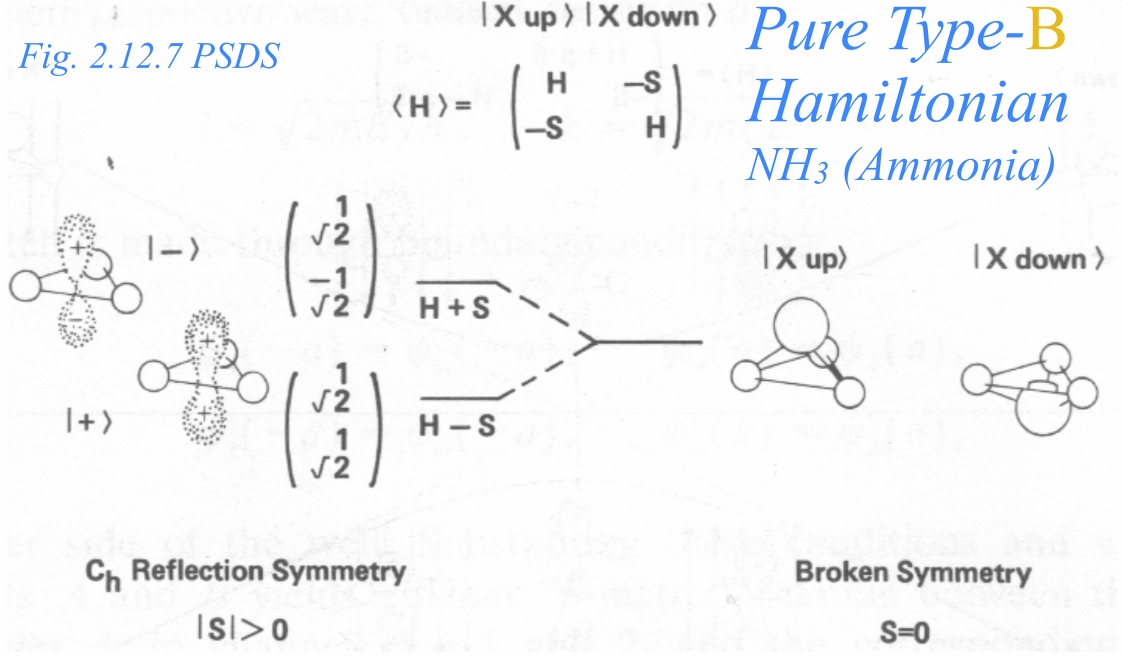


Fig. 2.12.7 PSDS

Pure Type-B Hamiltonian

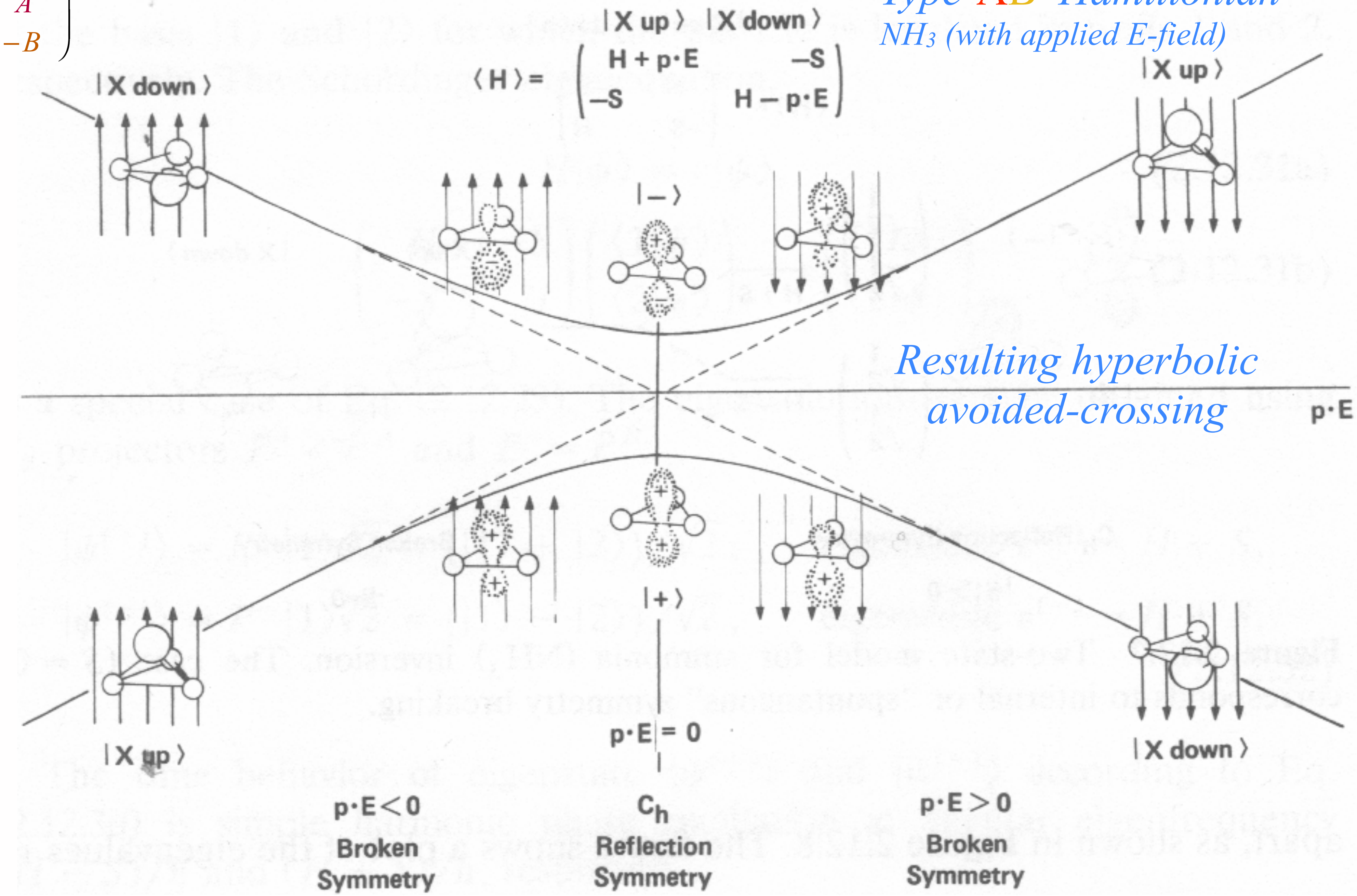
NH$_3$ (Ammonia)

Type-AB Hamiltonian

NH$_3$ (with applied E-field)

Review of
Lecture 10
p. 65 to 73

Fig. 2.12.8 PSDS



Resulting hyperbolic avoided-crossing

A to B to A Symmetry breaking described by hyperbolic eigenvalues of $A\boldsymbol{\sigma}_A+B\boldsymbol{\sigma}_B=\mathbf{H}=\begin{pmatrix}+A & B\\ B & -A\end{pmatrix}$

$\mathbf{H}=\begin{pmatrix}+A & B\\ B & -A\end{pmatrix}$ Secular equation: $\varepsilon^2-0\cdot\varepsilon-(A^2+B^2)$ gives *hyperbolic* energy levels: $\varepsilon=\pm\sqrt{A^2+B^2}$

$\mathbf{H}(B-basis)$ $\qquad$ $\mathbf{H}(A-basis)$

$$\begin{pmatrix}? & ?\\ ? & ?\end{pmatrix}=\frac{\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}}{\sqrt{2}}\begin{pmatrix}+A & B\\ B & -A\end{pmatrix}\frac{\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}}{\sqrt{2}}$$

$$=\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}+A & B\\ B & -A\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$=\frac{1}{2}\begin{pmatrix}+A+B & B-A\\ +A-B & B+A\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

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

$$=\begin{pmatrix}+B & A\\ A & -B\end{pmatrix}$$

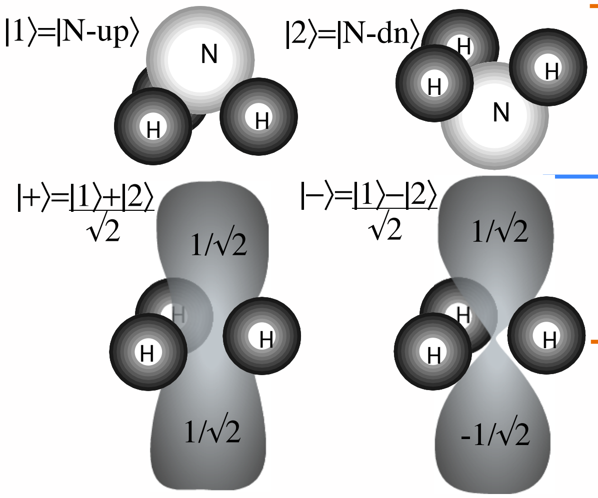
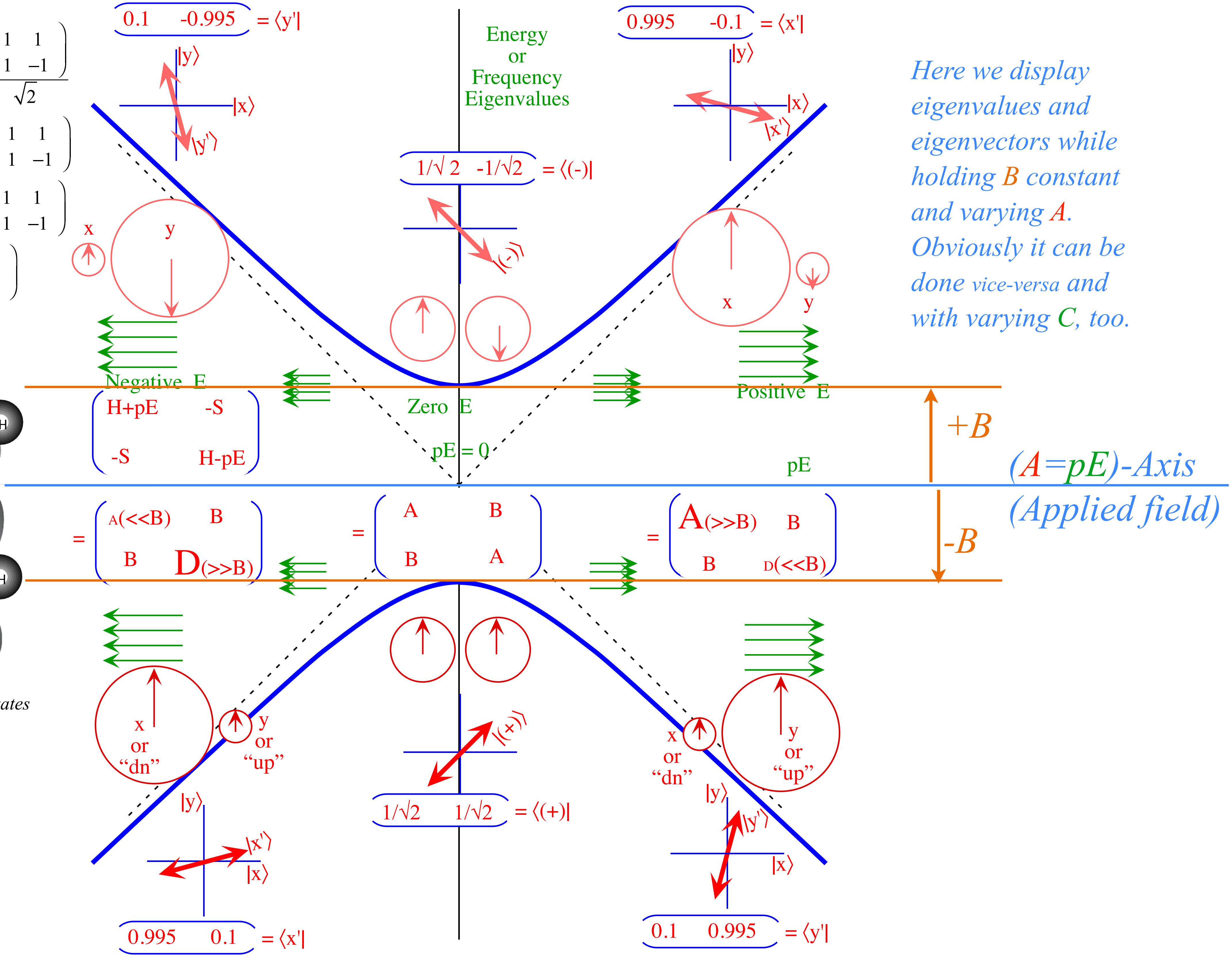


Fig. 10.3.2 Ammonia (NH_3) inversion states
(a) Base states (b) C_2-Eigenstates



Here we display eigenvalues and eigenvectors while holding B constant and varying A. Obviously it can be done vice-versa and with varying C, too.

Fig. 10.3.1 (b) Wigner avoided level crossing. (Fixed tunneling B=-S and variable A-D=pE field.)

Review of
Lecture 10
p. 73

- *Breaking C_N cyclic coupling into linear chains*
  - *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
  - *Breaking C_{2N+2} to approximate linear N-chain*
    - *Band-It simulation: Intro to scattering approach to quantum symmetry*

- *Breaking C_{2N} cyclic coupling down to C_N symmetry*
  - *Acoustical modes vs. Optical modes*
  - *Intro to other examples of band theory*
  - *Type-AB avoided crossing view of band-gaps*

- *Finally! Symmetry groups that are not just C_N*
  - *The "4-Group(s)" D_2 and C_{2v}*
  - *Spectral decomposition of D_2*
    - *Some D_2 modes*
  - *Outer product properties and the Crystal-Point Group Zoo*

Finally! Symmetry groups that are not just C_N (And some that are)

Fig. 2.11.1 PSDS

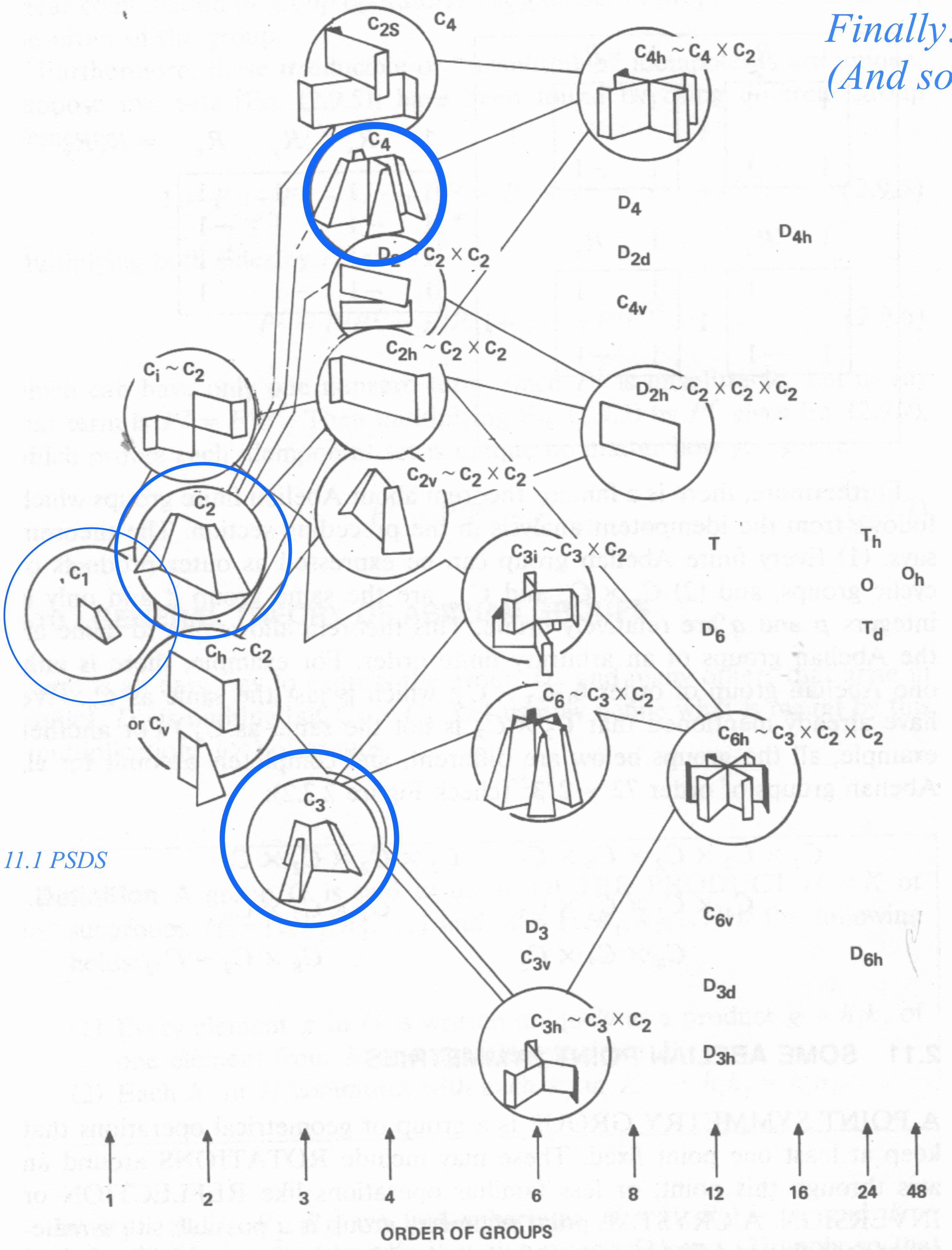


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Finally! Symmetry groups that are not just C_N

(And some that are)

Starting with D_2

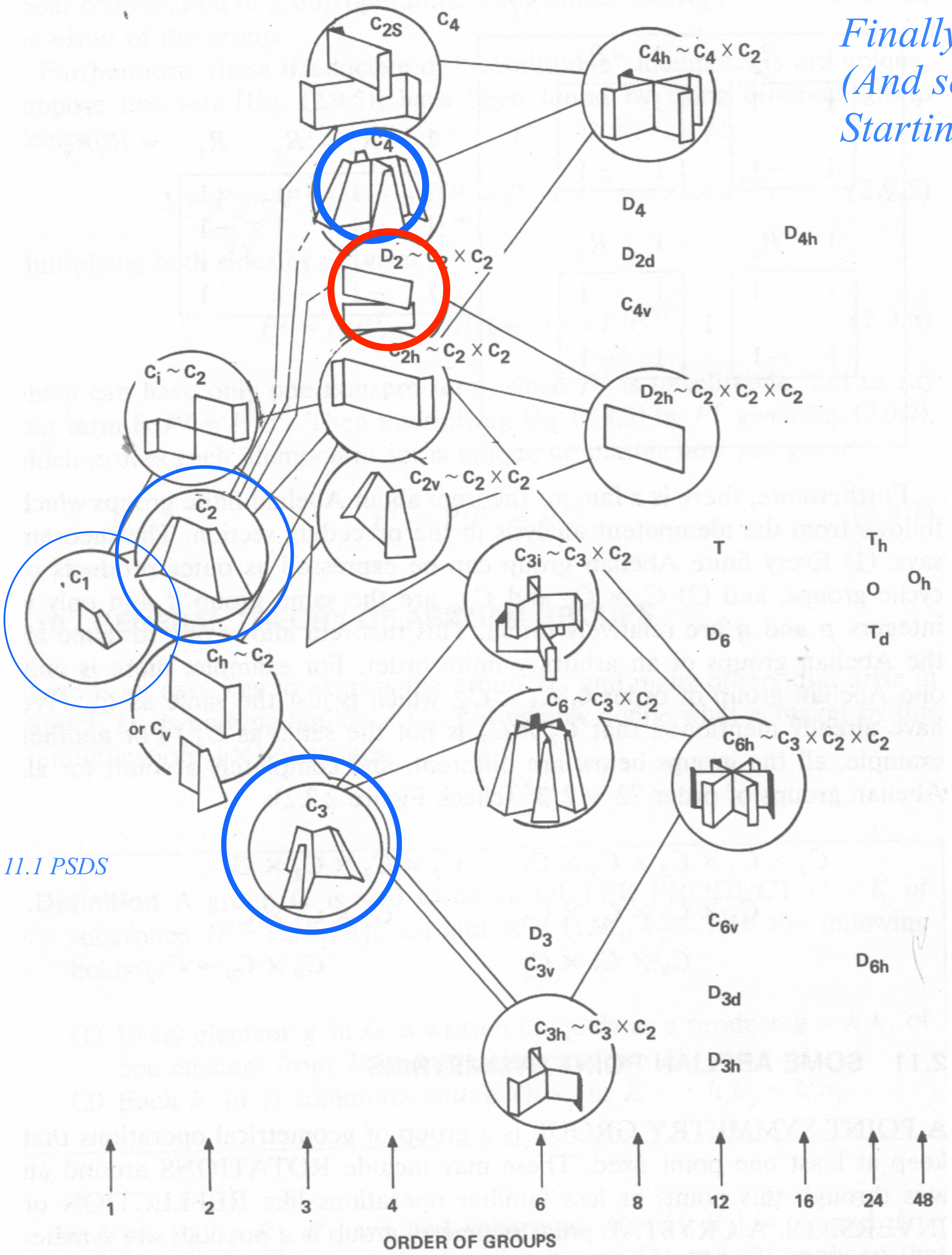


Fig. 2.11.1 PSDS

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Finally! Symmetry groups that are not just C_N
(And some that are)
Starting with D_2 and C_{2h} and C_{2v}

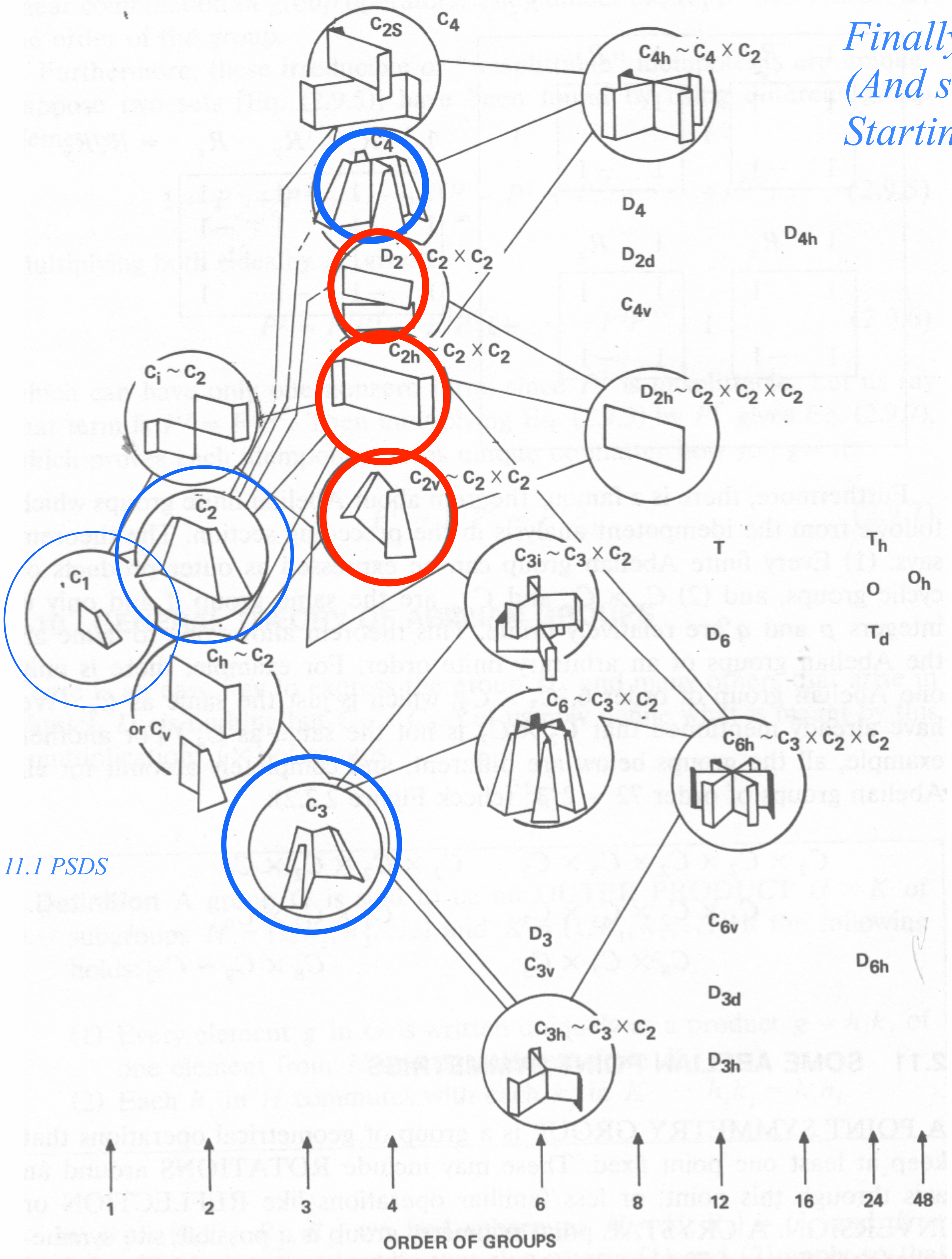
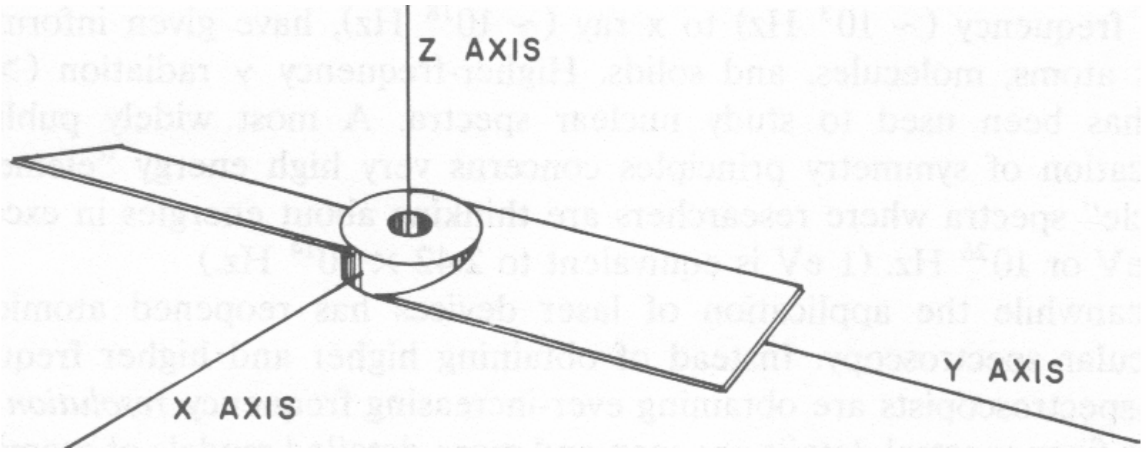


Fig. 2.11.1 PSDS

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

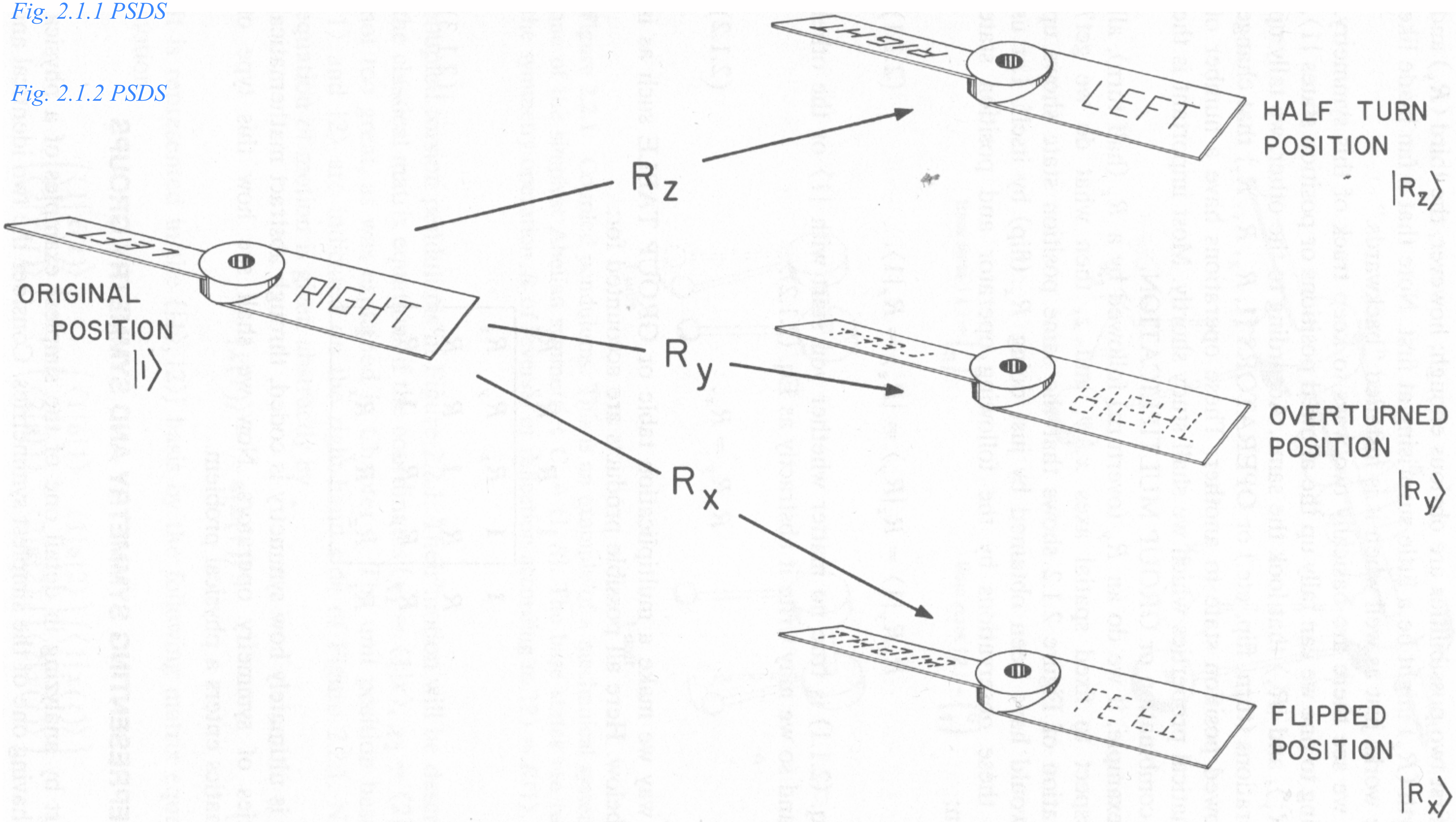
D_2 Symmetry (The 4-Group)



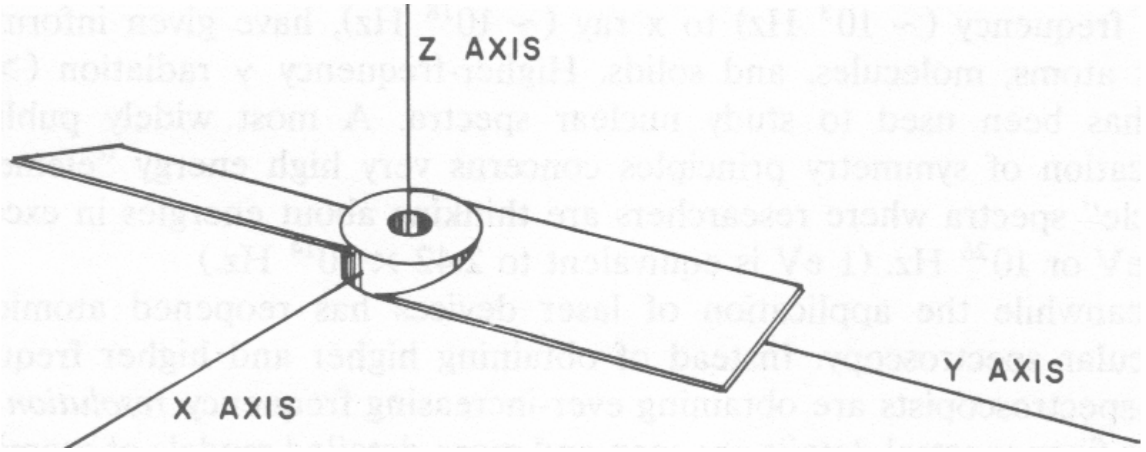
1 :	THE ORIGINAL POSITION	Don't touch the fan blade.
R_z:	THE HALF-TURN POSITION	Rotate it by 180° around its axle or the z axis.
R_y:	THE OVERTURNED POSITION	Overturn it 180° around the y axis.
R_x:	THE FLIPPED POSITION	Flip it 180° around the x axis.

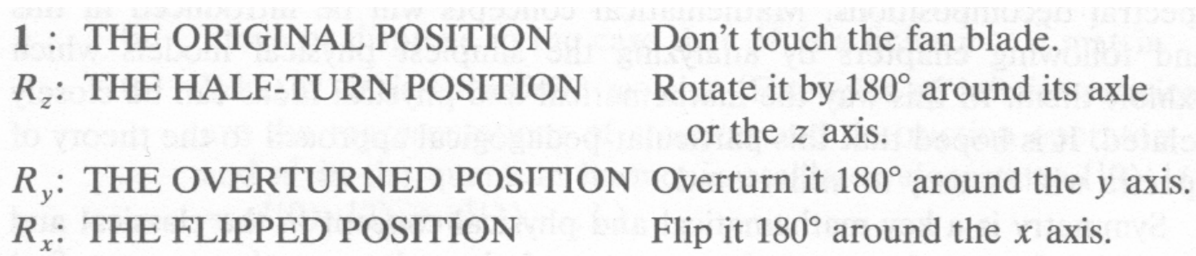
Fig. 2.1.1 PSDS

Fig. 2.1.2 PSDS



D_2 Symmetry (The 4-Group)




1 : THE ORIGINAL POSITION Don't touch the fan blade.

R_z: THE HALF-TURN POSITION Rotate it by 180° around its axle or the z axis.

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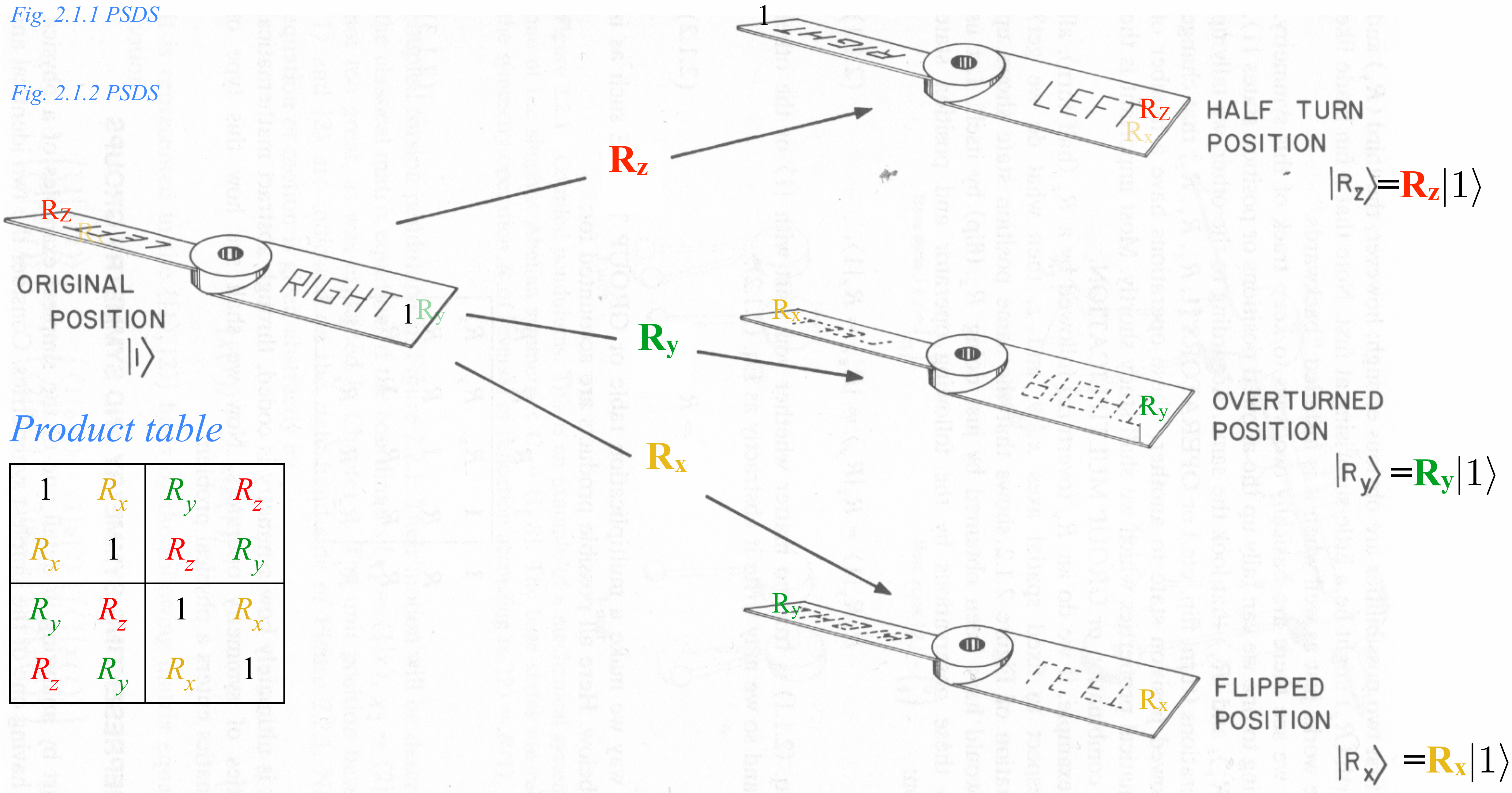
Fig. 2.1.1 PSDS

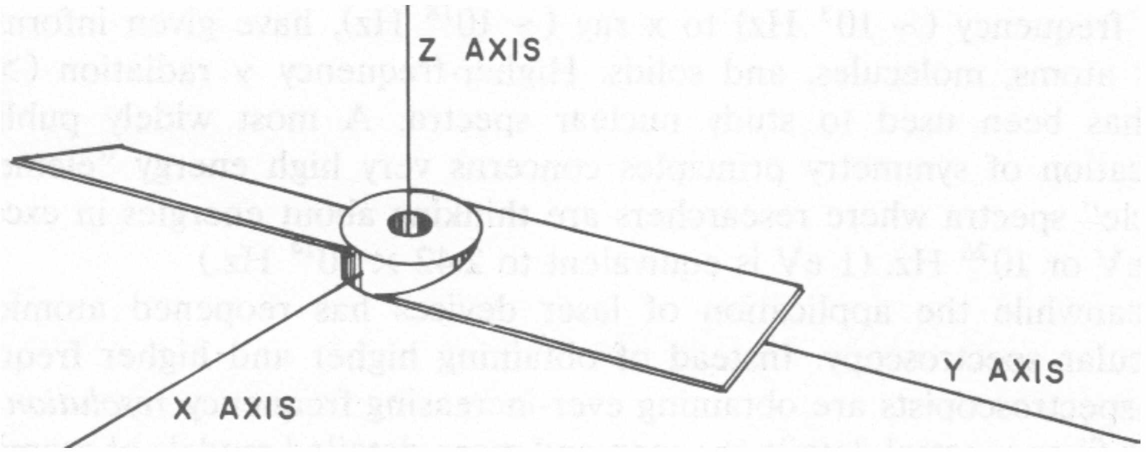
Fig. 2.1.2 PSDS



D_2 Product table

1	R_x	R_y	R_z
R_x	1	R_z	R_y
R_y	R_z	1	R_x
R_z	R_y	R_x	1

D_2 Symmetry (The 4-Group)



1 :	THE ORIGINAL POSITION	Don't touch the fan blade.
R_z:	THE HALF-TURN POSITION	Rotate it by 180° around its axle or the z axis.
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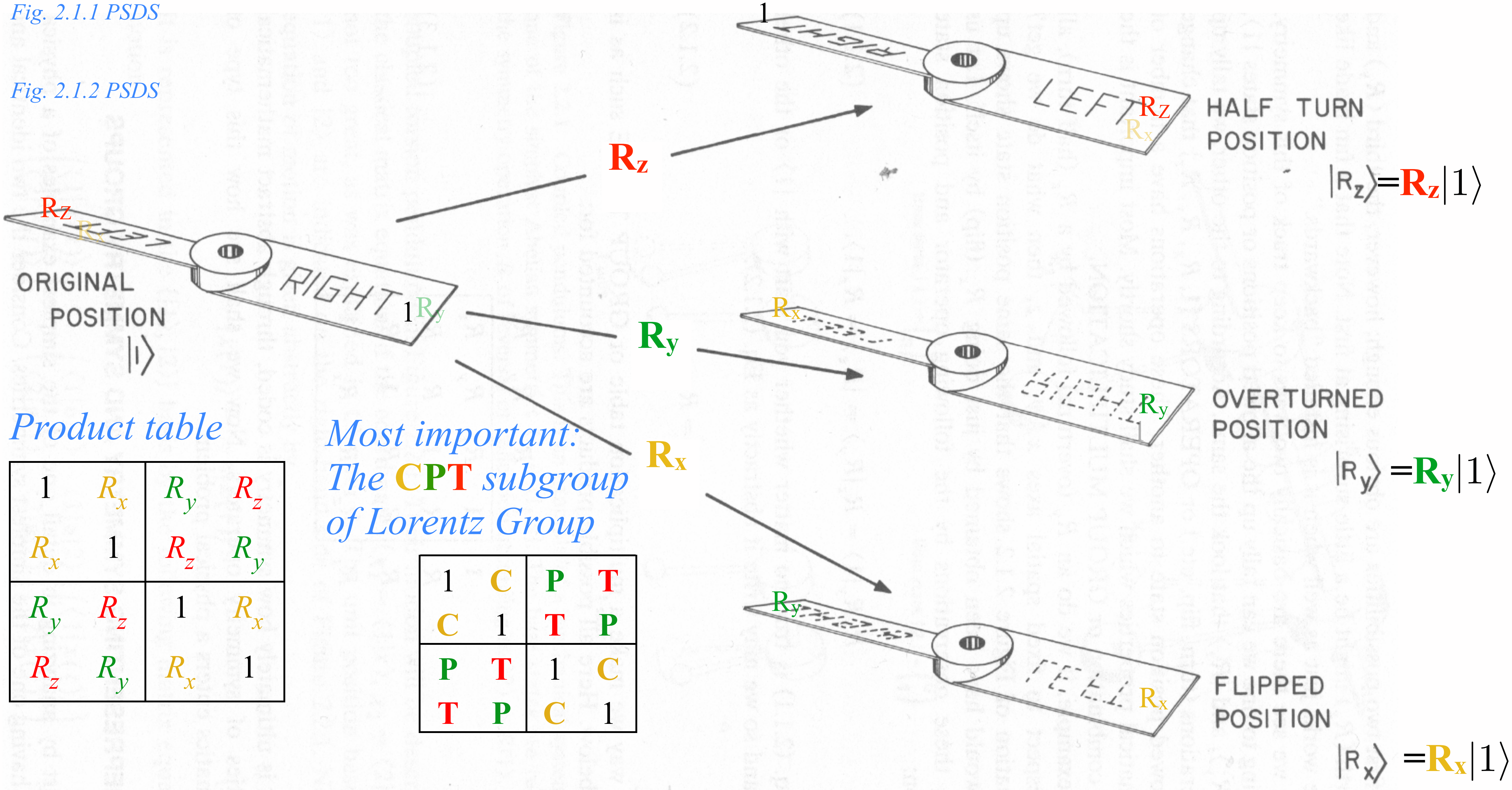
R_x:	THE FLIPPED POSITION	Flip it 180° around the x axis.

Fig. 2.1.1 PSDS

Fig. 2.1.2 PSDS



D_2 Product table

1	R_x	R_y	R_z
R_x	1	R_z	R_y
R_y	R_z	1	R_x
R_z	R_y	R_x	1

Most important:
*The **CPT** subgroup*
of Lorentz Group

1	**C**	**P**	**T**
C	1	**T**	**P**
P	**T**	1	**C**
T	**P**	**C**	1

Breaking C_N cyclic coupling into linear chains
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- *The "4-Group(s)" D_2 and C_{2v}*
- → *Spectral decomposition of D_2* ←
  - *Some D_2 modes*
- *Outer product properties and the Crystal-Point Group Zoo*

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations:

$\mathbf{R_x}^2 \mathbf{- 1 = 0}$, $\mathbf{R_y}^2 \mathbf{- 1 = 0}$.

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R}_y^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1} + \mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1} + \mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{P}_x^- = \frac{\mathbf{1} - \mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1} - \mathbf{R}_y}{2}$$

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R}_y^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R}_y^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

Spec.decomps

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$\mathbf{R_x}^2 - \mathbf{1} = \mathbf{0}$,

$\mathbf{R_y}^2 - \mathbf{1} = \mathbf{0}$.

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

Spec.decomps

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^+ + \mathbf{P}_x^-\right)\cdot\left(\mathbf{P}_y^+ + \mathbf{P}_y^-\right) = \mathbf{P}_x^+\cdot\mathbf{P}_y^+ + \mathbf{P}_x^-\cdot\mathbf{P}_y^+ + \mathbf{P}_x^+\cdot\mathbf{P}_y^- + \mathbf{P}_x^-\cdot\mathbf{P}_y^-$ *gives irrep projectors*

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$\mathbf{R}_x^2 - \mathbf{1} = \mathbf{0},$ $\mathbf{R}_y^2 - \mathbf{1} = \mathbf{0}.$

$$\mathbf{P}_x^{+} = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{+} = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^{-} = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{-} = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{1} = \mathbf{P}_x^{+} + \mathbf{P}_x^{-} \qquad \mathbf{1} = \mathbf{P}_y^{+} + \mathbf{P}_y^{-}$$

$$\mathbf{R}_x = \mathbf{P}_x^{+} - \mathbf{P}_x^{-} \qquad \mathbf{R}_y = \mathbf{P}_y^{+} - \mathbf{P}_y^{-}$$

Completeness Spec.decomps

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^{+} + \mathbf{P}_x^{-}\right)\cdot\left(\mathbf{P}_y^{+} + \mathbf{P}_y^{-}\right) = \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+} + \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+} + \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-} + \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-}$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+} = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+} = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-} = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-} = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R}_x{}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R}_y{}^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^+ + \mathbf{P}_x^-\right)\cdot\left(\mathbf{P}_y^+ + \mathbf{P}_y^-\right) = \mathbf{P}_x^+\cdot\mathbf{P}_y^+ + \mathbf{P}_x^-\cdot\mathbf{P}_y^+ + \mathbf{P}_x^+\cdot\mathbf{P}_y^- + \mathbf{P}_x^-\cdot\mathbf{P}_y^-$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

$(\textit{completeness is first})$

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

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R}_x{}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R}_y{}^2 - \mathbf{1} = \mathbf{0}.$$

reducible projectors

$$\mathbf{P}_x^{+} = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{+} = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^{-} = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{-} = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

Completeness

$$\mathbf{1} = \mathbf{P}_x^{+} + \mathbf{P}_x^{-} \qquad \mathbf{1} = \mathbf{P}_y^{+} + \mathbf{P}_y^{-}$$

Spec.decomps

$$\mathbf{R}_x = \mathbf{P}_x^{+} - \mathbf{P}_x^{-} \qquad \mathbf{R}_y = \mathbf{P}_y^{+} - \mathbf{P}_y^{-}$$

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^{+} + \mathbf{P}_x^{-}\right)\cdot\left(\mathbf{P}_y^{+} + \mathbf{P}_y^{-}\right) = \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+} + \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+} + \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-} + \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-}$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+} = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+} = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-} = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-} = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

(*then R_x eigenvalues*)

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

$$\mathbf{R}_x = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (+1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R_x}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R_y}^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^{+} = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{+} = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{P}_x^{-} = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^{-} = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

$$\mathbf{1} = \mathbf{P}_x^{+} + \mathbf{P}_x^{-} \qquad \mathbf{1} = \mathbf{P}_y^{+} + \mathbf{P}_y^{-}$$

Completeness

Spec.decomps

$$\mathbf{R}_x = \mathbf{P}_x^{+} - \mathbf{P}_x^{-} \qquad \mathbf{R}_y = \mathbf{P}_y^{+} - \mathbf{P}_y^{-}$$

The old "**1=1•1** trick" $\mathbf{1}=\mathbf{1}\cdot\mathbf{1}=\left(\mathbf{P}_x^{+}+\mathbf{P}_x^{-}\right)\cdot\left(\mathbf{P}_y^{+}+\mathbf{P}_y^{-}\right)=\mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+}+\mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+}+\mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-}+\mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-}$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{+} = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{+} = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^{+}\cdot\mathbf{P}_y^{-} = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^{-}\cdot\mathbf{P}_y^{-} = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

(*...and so forth*)

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

$$\mathbf{R}_x = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (+1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_y = (+1)\mathbf{P}^{++} + (+1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R_x}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R_y}^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Completeness

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

Spec.decomps

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^+ + \mathbf{P}_x^-\right)\cdot\left(\mathbf{P}_y^+ + \mathbf{P}_y^-\right) = \mathbf{P}_x^+\cdot\mathbf{P}_y^+ + \mathbf{P}_x^-\cdot\mathbf{P}_y^+ + \mathbf{P}_x^+\cdot\mathbf{P}_y^- + \mathbf{P}_x^-\cdot\mathbf{P}_y^-$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot 2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

(*completeness is first*)

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

$$\mathbf{R}_x = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (+1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_y = (+1)\mathbf{P}^{++} + (+1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$-\cdot+$	$1\cdot 1$	$-1\cdot 1$	$1\cdot 1$	$-1\cdot 1$
$+\cdot-$	$1\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot 1$	$-1\cdot 1$	$1\cdot(-1)$	$-1\cdot(-1)$

Shortcut notation for getting D_2 character table

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$+\cdot+$	1	1	1	1
$-\cdot+$	1	-1	1	-1
$+\cdot-$	1	1	-1	-1
$-\cdot-$	1	-1	-1	1

$$\mathbf{R_x}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R_y}^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

Completeness Spec.decomps

The old "**1=1•1** trick" $\mathbf{1} = \mathbf{1}\cdot\mathbf{1} = \left(\mathbf{P}_x^+ + \mathbf{P}_x^-\right)\cdot\left(\mathbf{P}_y^+ + \mathbf{P}_y^-\right) = \mathbf{P}_x^+\cdot\mathbf{P}_y^+ + \mathbf{P}_x^-\cdot\mathbf{P}_y^+ + \mathbf{P}_x^+\cdot\mathbf{P}_y^- + \mathbf{P}_x^-\cdot\mathbf{P}_y^-$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}+\mathbf{R}_y\right)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}+\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{\left(\mathbf{1}-\mathbf{R}_x\right)\cdot\left(\mathbf{1}-\mathbf{R}_y\right)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

$(\textit{completeness is first})$

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

$$\mathbf{R}_x = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (+1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_y = (+1)\mathbf{P}^{++} + (+1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

Shortcut notation for getting D_2 character table

D_2 spectral decomposition: The old "1=1•1 trick" again

Two C_2 subgroup minimal equations and their projectors:

$$\mathbf{R_x}^2 - \mathbf{1} = \mathbf{0}, \qquad \mathbf{R_y}^2 - \mathbf{1} = \mathbf{0}.$$

$$\mathbf{P}_x^+ = \frac{\mathbf{1}+\mathbf{R}_x}{2} \qquad \mathbf{P}_y^+ = \frac{\mathbf{1}+\mathbf{R}_y}{2}$$

reducible projectors

$$\mathbf{P}_x^- = \frac{\mathbf{1}-\mathbf{R}_x}{2} \qquad \mathbf{P}_y^- = \frac{\mathbf{1}-\mathbf{R}_y}{2}$$

Completeness

$$\mathbf{1} = \mathbf{P}_x^+ + \mathbf{P}_x^- \qquad \mathbf{1} = \mathbf{P}_y^+ + \mathbf{P}_y^-$$

Spec.decomps

$$\mathbf{R}_x = \mathbf{P}_x^+ - \mathbf{P}_x^- \qquad \mathbf{R}_y = \mathbf{P}_y^+ - \mathbf{P}_y^-$$

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++=A_1$	1	1	1	1
$-+=A_2$	1	-1	1	-1
$+-=B_1$	1	1	-1	-1
$--=B_2$	1	-1	-1	1

Note common notation

The old "**1=1•1** trick" $\mathbf{1}=\mathbf{1}\cdot\mathbf{1}=\left(\mathbf{P}_x^+ + \mathbf{P}_x^-\right)\cdot\left(\mathbf{P}_y^+ + \mathbf{P}_y^-\right)=\mathbf{P}_x^+\cdot\mathbf{P}_y^+ + \mathbf{P}_x^-\cdot\mathbf{P}_y^+ + \mathbf{P}_x^+\cdot\mathbf{P}_y^- + \mathbf{P}_x^-\cdot\mathbf{P}_y^-$ *gives irrep projectors*

$$\mathbf{P}^{++} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x+\mathbf{R}_y+\mathbf{R}_z\right)$$

$$\mathbf{P}^{-+} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^+ = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}+\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x+\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{+-} \equiv \mathbf{P}_x^+\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}+\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}+\mathbf{R}_x-\mathbf{R}_y-\mathbf{R}_z\right)$$

$$\mathbf{P}^{--} \equiv \mathbf{P}_x^-\cdot\mathbf{P}_y^- = \frac{(\mathbf{1}-\mathbf{R}_x)\cdot(\mathbf{1}-\mathbf{R}_y)}{2\cdot2} = \frac{1}{4}\left(\mathbf{1}-\mathbf{R}_x-\mathbf{R}_y+\mathbf{R}_z\right)$$

$(completeness\ is\ first)$

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

$$\mathbf{R}_x = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (+1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_y = (+1)\mathbf{P}^{++} + (+1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (-1)\mathbf{P}^{--}$$

$$\mathbf{R}_z = (+1)\mathbf{P}^{++} + (-1)\mathbf{P}^{-+} + (-1)\mathbf{P}^{+-} + (+1)\mathbf{P}^{--}$$

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

Shortcut notation for getting D_2 character table

- *Breaking C_N cyclic coupling into linear chains*
    - *Review of 1D-Bohr-ring related to infinite square well (and review of revival)*
    - *Breaking C_{2N+2} to approximate linear N-chain*
        - *Band-It simulation: Intro to scattering approach to quantum symmetry*

- *Breaking C_{2N} cyclic coupling down to C_N symmetry*
    - *Acoustical modes vs. Optical modes*
    - *Intro to other examples of band theory*
    - *Avoided crossing view of band-gaps*

- *Finally! Symmetry groups that are not just C_N*
    - *The "4-Group(s)" D_2 and C_{2v}*
    - *Spectral decomposition of D_2*
        - → *Some D_2 modes* ←
    - *Outer product properties and the Crystal-Point Group Zoo*

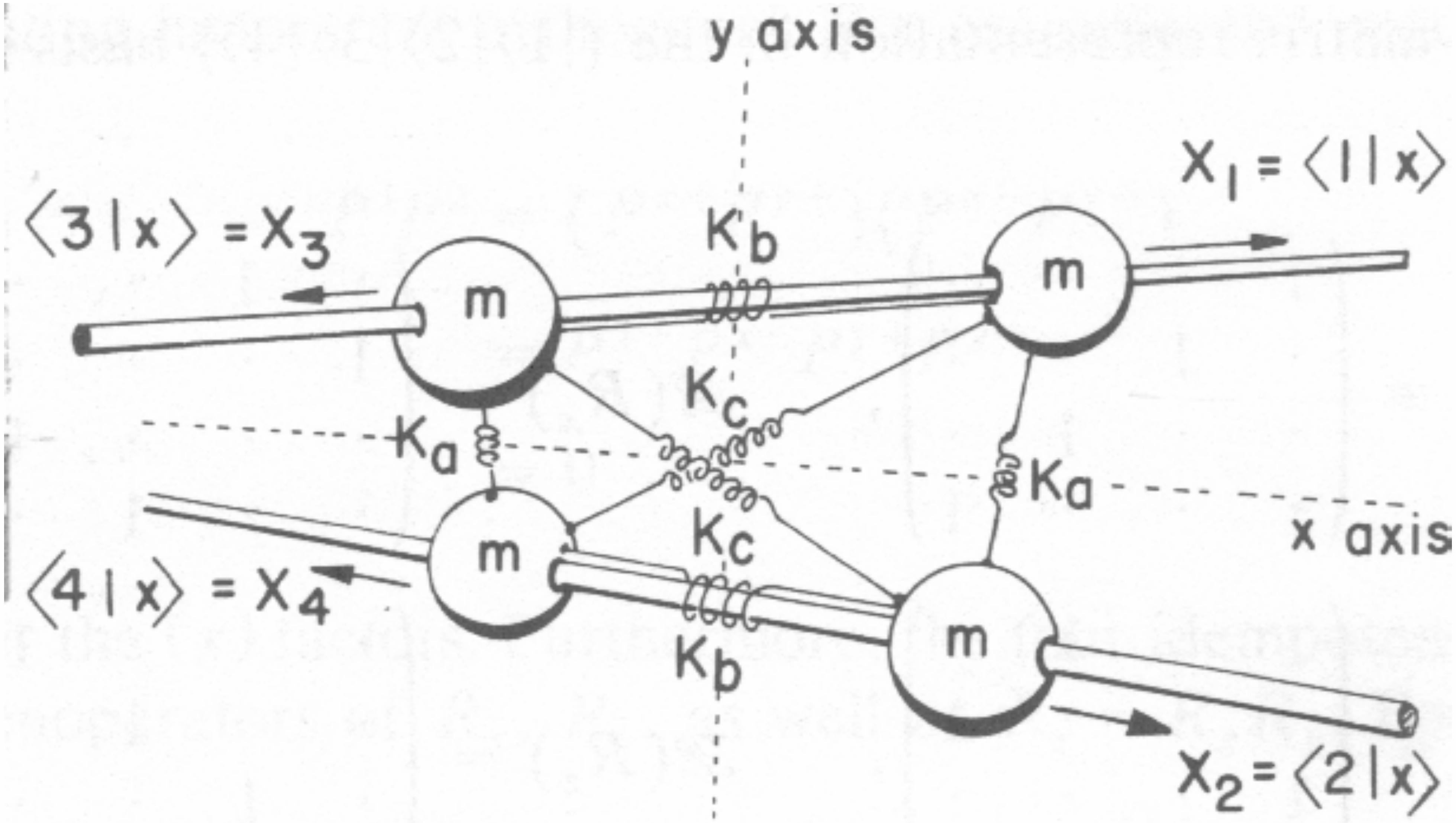


Fig. 2.8.1 PSDS

$$\begin{pmatrix} \langle 1|\ddot{x}\rangle \\ \langle 2|\ddot{x}\rangle \\ \langle 3|\ddot{x}\rangle \\ \langle 4|\ddot{x}\rangle \end{pmatrix} = \begin{pmatrix} A & a & b & c \\ a & A & c & b \\ b & c & A & a \\ c & b & a & A \end{pmatrix} \begin{pmatrix} \langle 1|x\rangle \\ \langle 2|x\rangle \\ \langle 3|x\rangle \\ \langle 4|x\rangle \end{pmatrix}$$

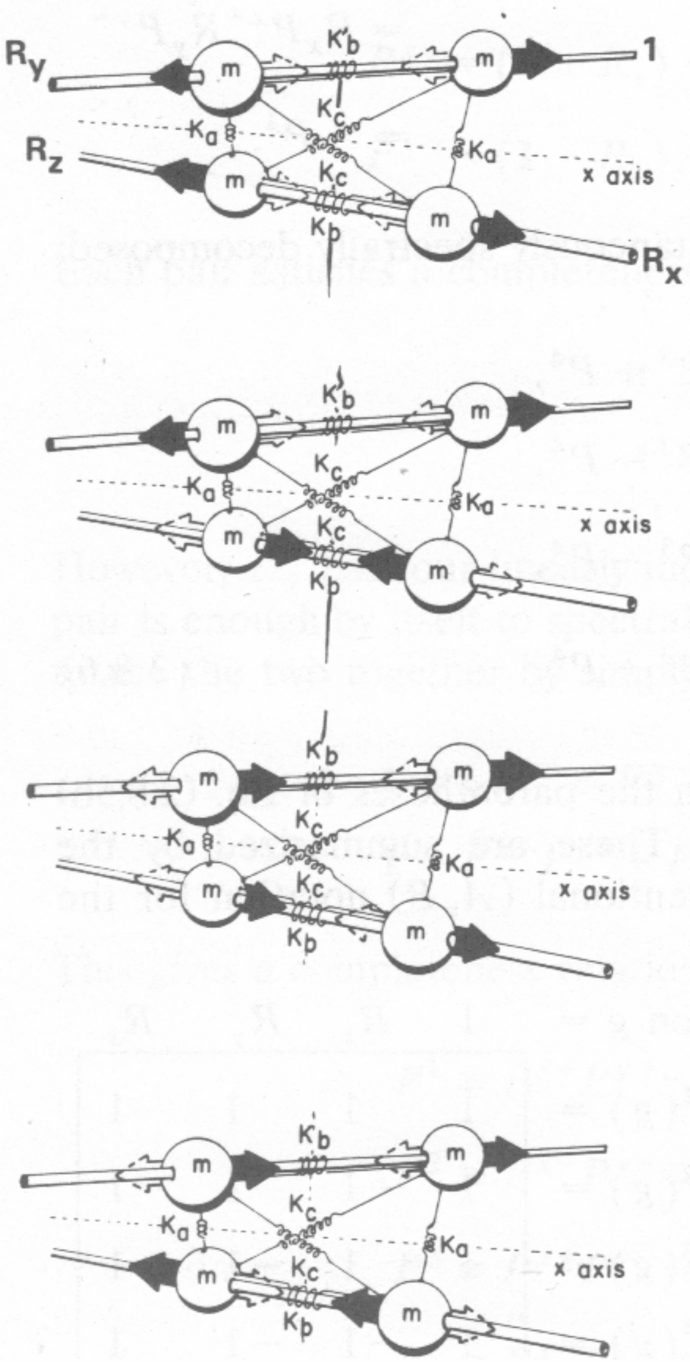
$$A = -\left(k_a \cos^2(a,b) + k_b + k_c \cos^2(b,c)\right)/m,$$
$$a = -k_a \cos^2(a,b)/m,$$
$$b = -k_b/m,$$
$$c = -k_c \cos^2(b,c)/m.$$

$$|e^{A_1}\rangle \equiv |e^1\rangle = P^1|1\rangle\sqrt{4} = (|1\rangle + |2\rangle + |3\rangle + |4\rangle)/2,$$

$$|e^{B_2}\rangle \equiv |e^2\rangle = P^2|1\rangle\sqrt{4} = (|1\rangle - |2\rangle + |3\rangle - |4\rangle)/2,$$

$$|e^{B_1}\rangle \equiv |e^3\rangle = P^3|1\rangle\sqrt{4} = (|1\rangle + |2\rangle - |3\rangle - |4\rangle)/2,$$

$$|e^{A_2}\rangle \equiv |e^4\rangle = P^4|1\rangle\sqrt{4} = (|1\rangle - |2\rangle - |3\rangle + |4\rangle)/2,$$



$$\begin{pmatrix}1\\1\\1\\1\end{pmatrix}/2 \qquad (A+a+b+c)^{1/2}$$

$$\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix}/2 \qquad (A-a+b-c)^{1/2}$$

$$\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix}/2 \qquad (A+a-b-c)^{1/2}$$

$$\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}/2 \qquad (A-a-b+c)^{1/2}$$

Fig. 2.8.2 PSDS

Breaking C_N cyclic coupling into linear chains
Review of 1D-Bohr-ring related to infinite square well (and review of revival)
Breaking C_{2N+2} to approximate linear N-chain
Band-It simulation: Intro to scattering approach to quantum symmetry

Breaking C_{2N} cyclic coupling down to C_N symmetry
Acoustical modes vs. Optical modes
Intro to other examples of band theory
Avoided crossing view of band-gaps

Finally! Symmetry groups that are not just C_N
The "4-Group(s)" D_2 and C_{2v}
Spectral decomposition of D_2
Some D_2 modes
Outer product properties and the Crystal-Point Group Zoo

Crystal-Point Group Zoo
having 32 groups
(Showing
16 Abelian
Crystal Groups)

Fig. 2.11.1 PSDS

The other 16
crystal-point groups
are
Non-Abelian

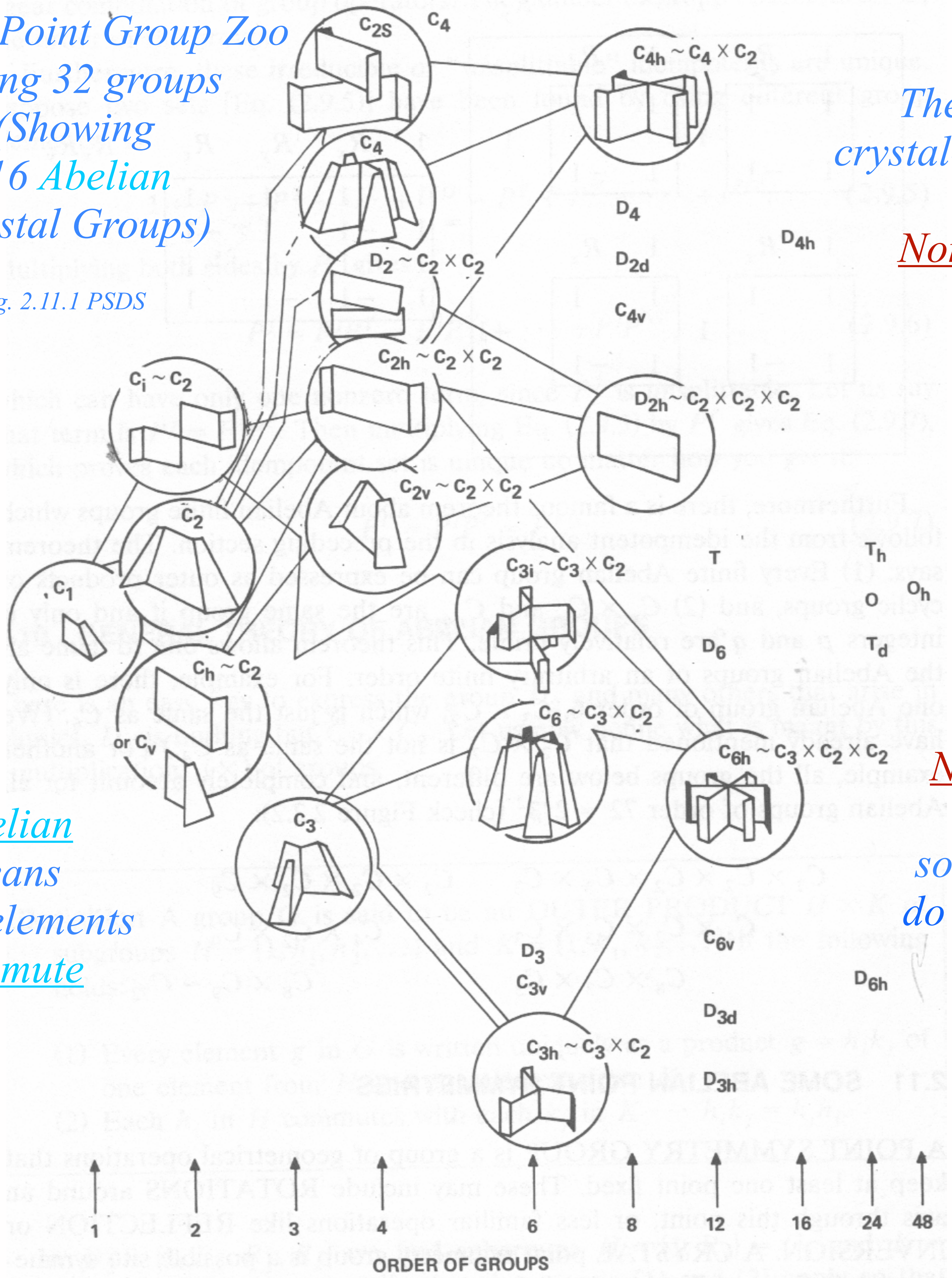


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

Abelian
means
all its elements
commute

Non-Abelian
means
some elements
do not commute

Crystal-Point Group Zoo
having 32 groups
(Showing
16 Abelian
Crystal Groups)

Fig. 2.11.1 PSDS

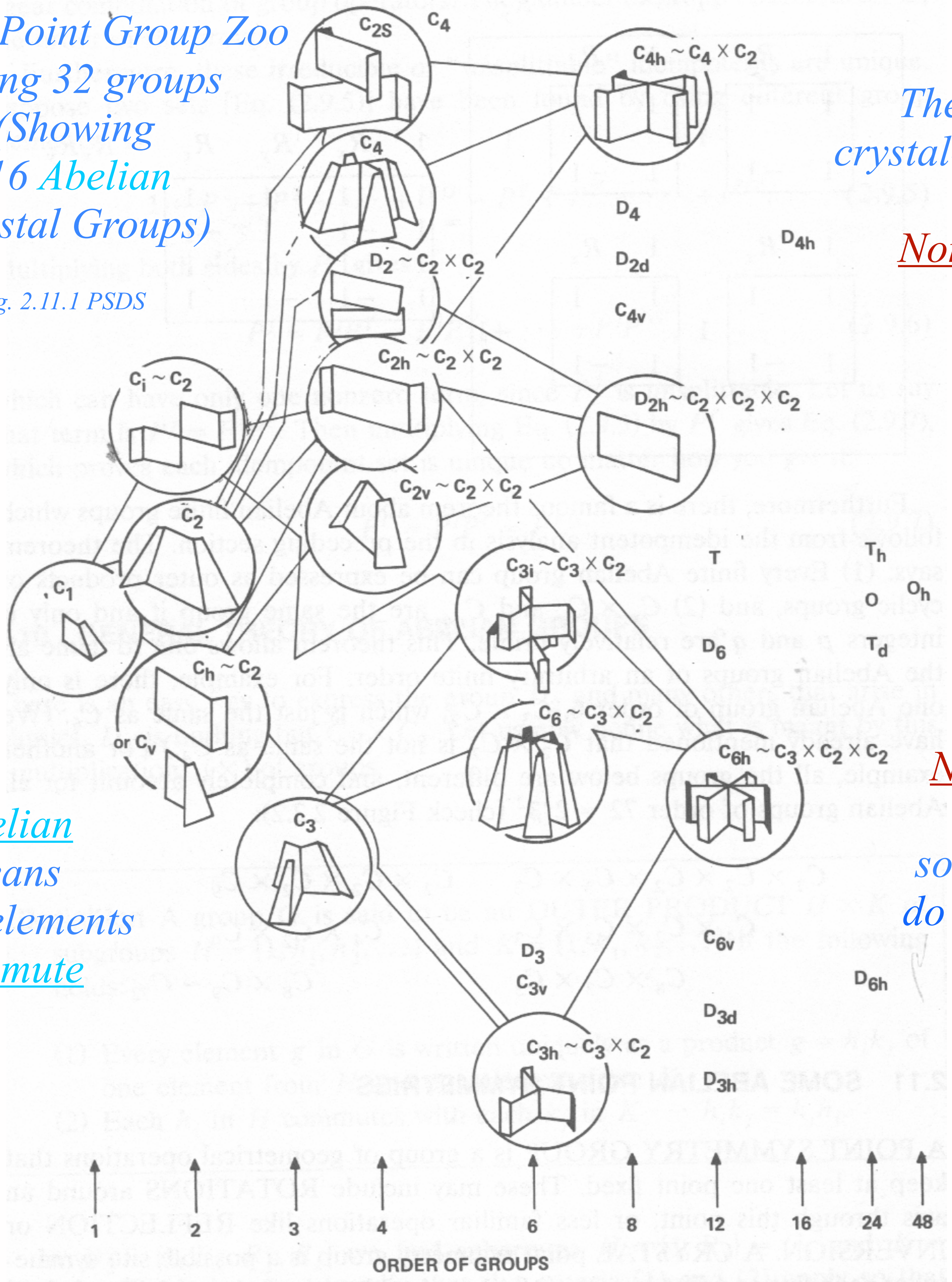


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

The other 16
crystal-point groups
are
Non-Abelian

From Lecture 12.6 p. 134
Character Trace of
n-fold rotation
where: $\ell^j = 2j+1$
is U(2) irrep dimension

$$\boxed{\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}}$$

Abelian
means
all its elements
commute

Non-Abelian
means
some elements
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Crystal-Point Group Zoo having 32 groups (Showing 16 Abelian Crystal Groups)

Fig. 2.11.1 PSDS

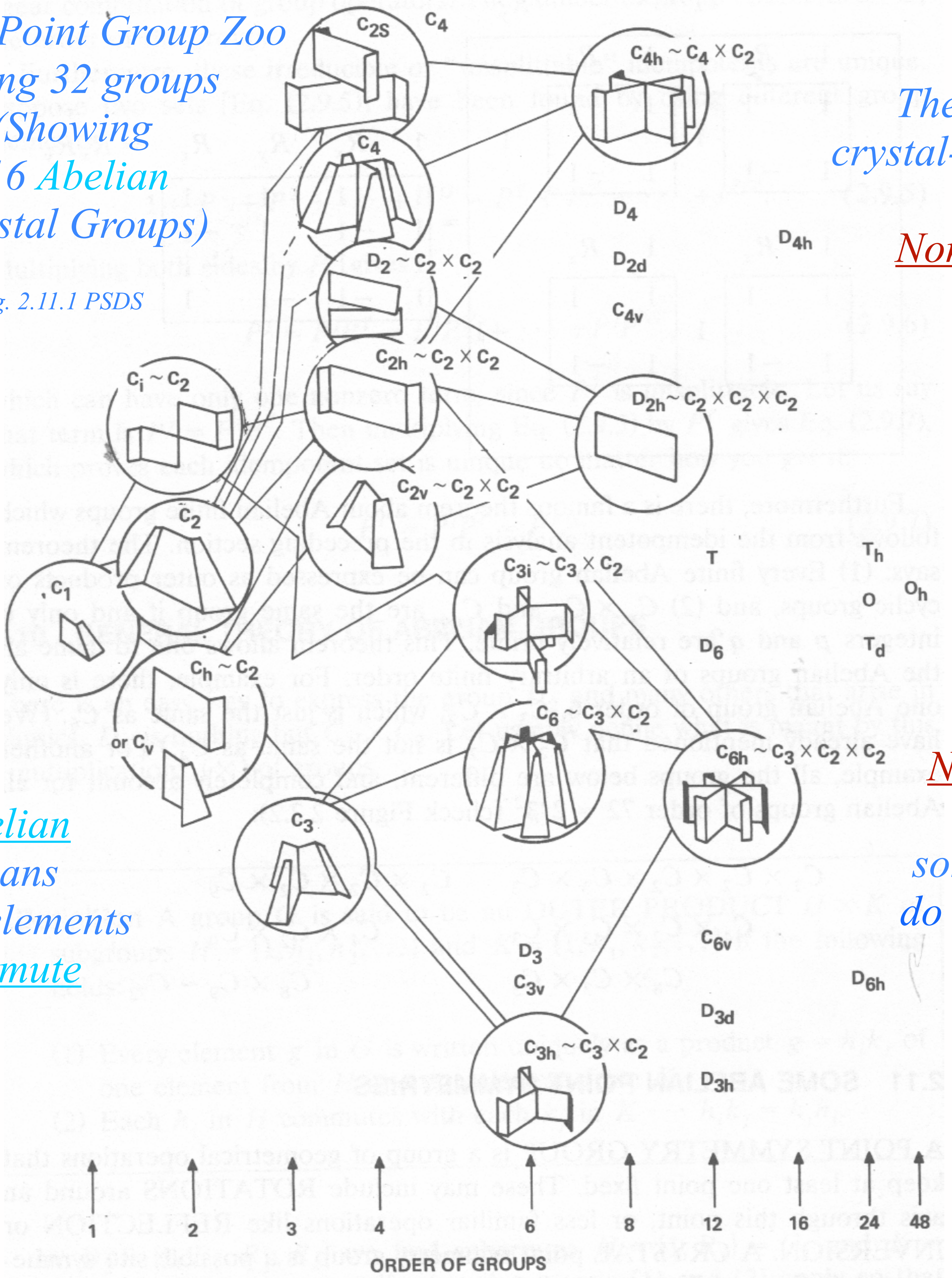

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

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From Lecture 12.6 p. 134
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$$\boxed{\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}}$$

To be a crystal-point group
the Character Trace of
n-fold vector rotation
for: $\ell^1 = 2+1 = 3$
must be an integer

$$\chi^1\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{1}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{3\pi}{n}}{\sin\frac{\pi}{n}} = \text{integer}$$

$$\frac{\sin\frac{3\pi}{2}}{\sin\frac{\pi}{2}} = -1 \ (n{=}2 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{3}}{\sin\frac{\pi}{3}} = +1 \ (n{=}3 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{4}}{\sin\frac{\pi}{4}} = +1 \ (n{=}4 \text{ ok})$$

$$\frac{\sin\frac{3\pi}{5}}{\sin\frac{\pi}{5}} = G^+ \ (n{=}5 \text{ NO!})$$

$$\frac{\sin\frac{3\pi}{6}}{\sin\frac{\pi}{6}} = +2 \ (n{=}6 \text{ ok})$$

Abelian means all its elements commute

Non-Abelian means some elements do not commute

Crystal-Point Group Zoo having 32 groups (Showing 16 Abelian Crystal Groups)

Fig. 2.11.1 PSDS

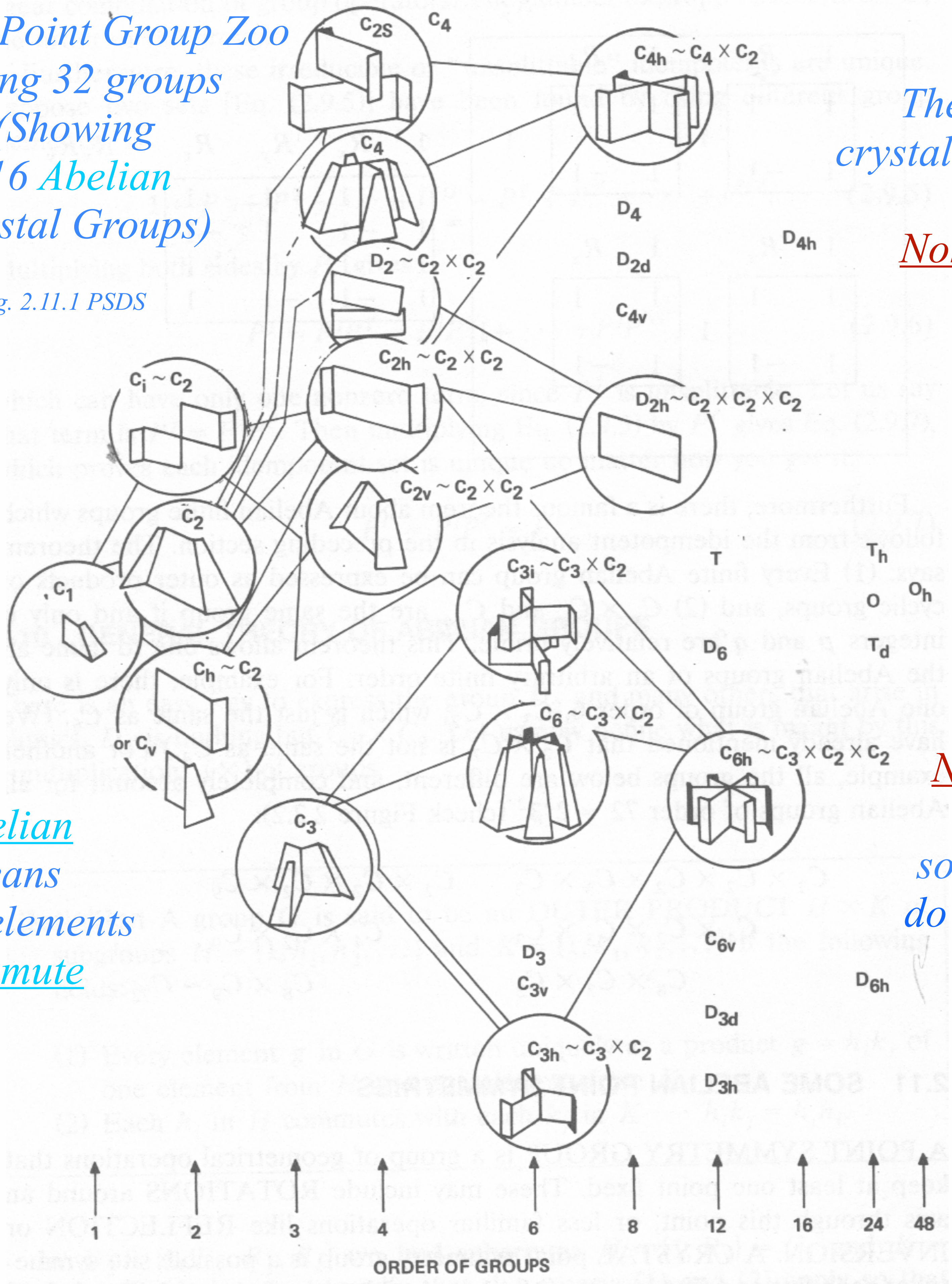


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

The other 16 crystal-point groups are Non-Abelian

Abelian means all its elements commute

Non-Abelian means some elements do not commute

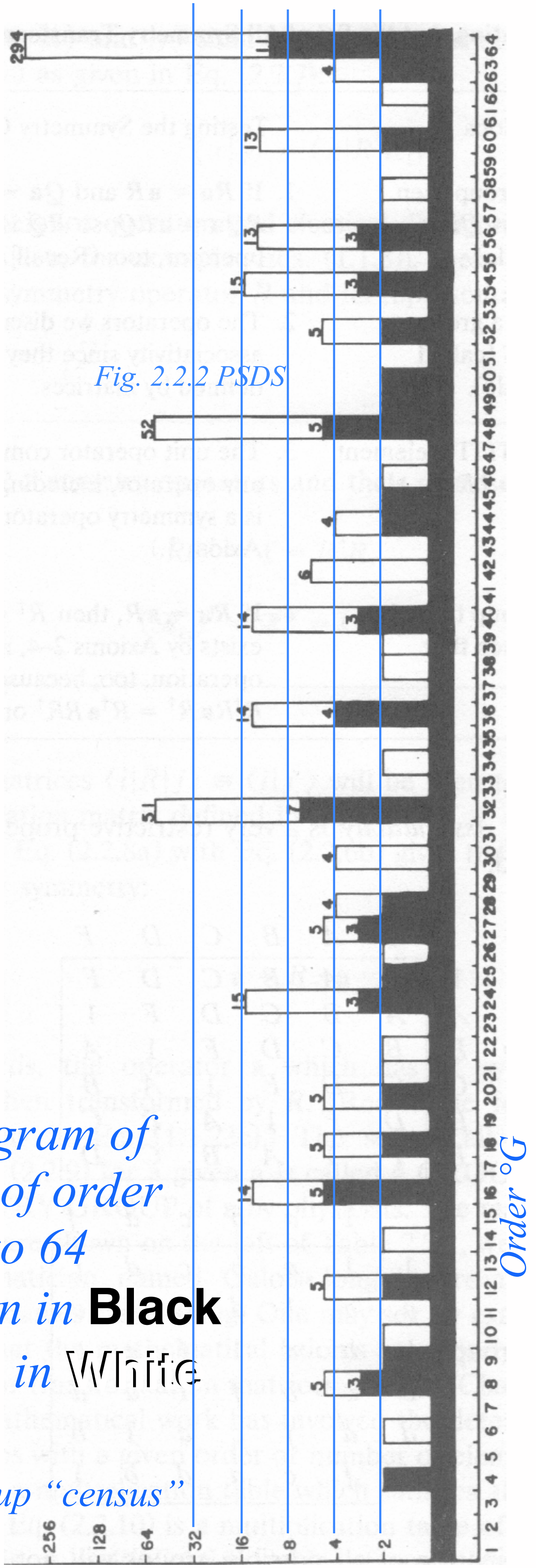


Fig. 2.2.2 PSDS

Log-histogram of all groups of order °G=1 to 64

Abelian shown in **Black**

Non-Abelian in White

Group "census"

Crystal-Point Group Zoo having 32 groups (Showing 16 Non-Abelian Crystal Groups)

Fig. 2.11.1 PSDS

The other 16 crystal-point groups are Abelian

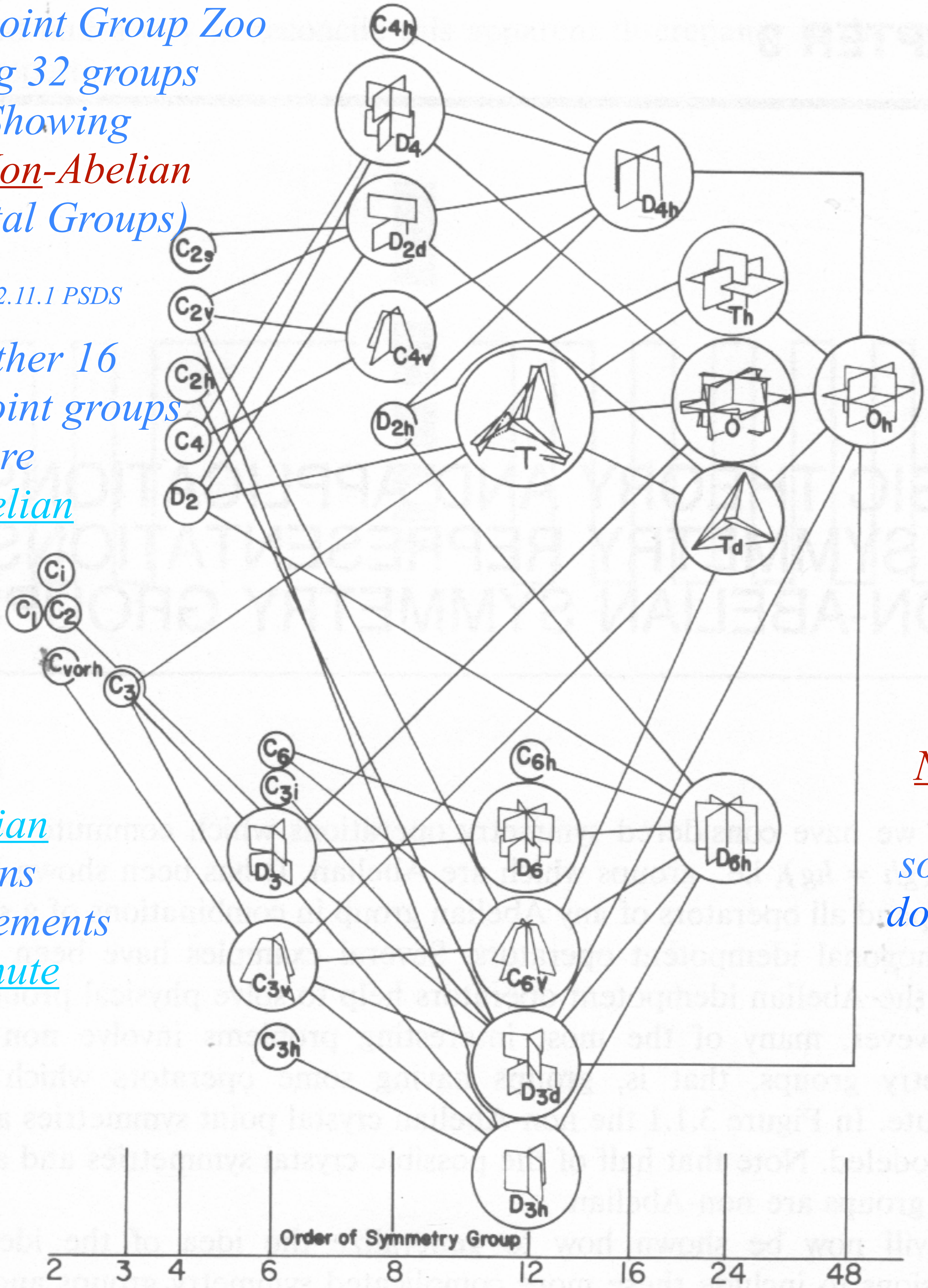


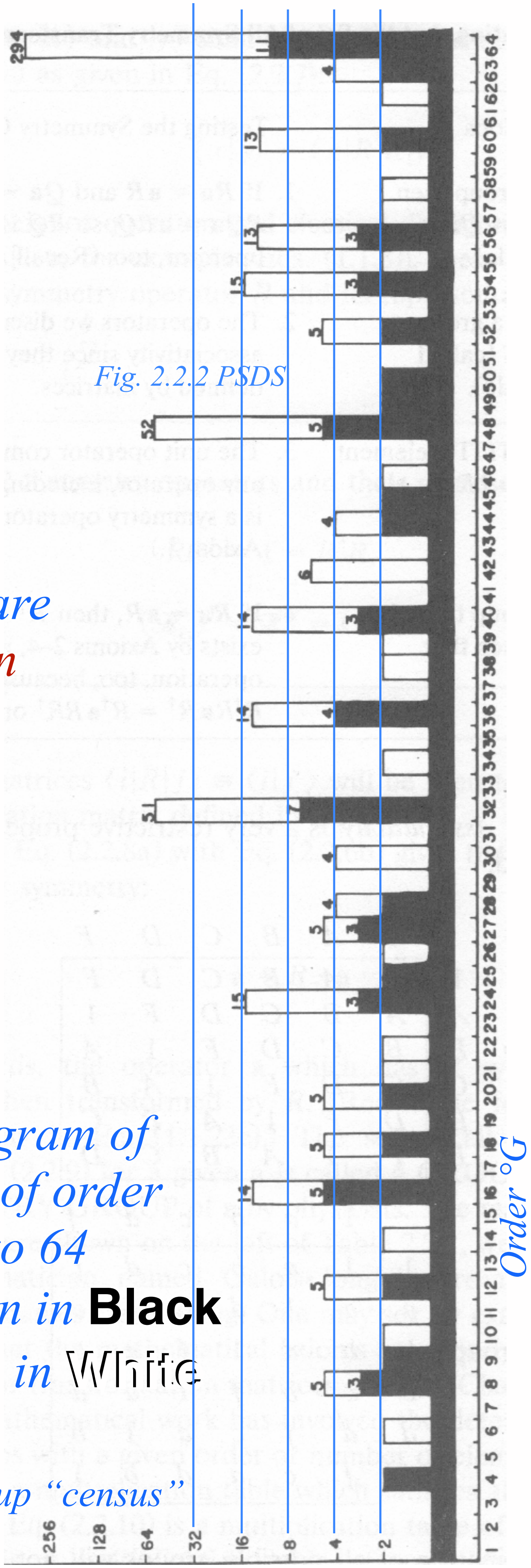
Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

Abelian means all its elements commute

Clearly most groups are Non-Abelian

Non-Abelian means some elements do not commute

Fig. 2.2.2 PSDS



Log-histogram of all groups of order °G=1 to 64

Abelian shown in **Black**

Non-Abelian in White

Group "census"

C_6 is product $C_3\times C_2$ *(but C_4 is NOT* $C_2\times C_2$*)*

C_3	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$(0)_3$	1	1	1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$

×

C_2	$\mathbf{1}$	$\mathbf{R}$
$(0)_2$	1	1
$(1)_2$	1	-1

=

$C_3\times C_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$	$\mathbf{1}\cdot\mathbf{R}$	$\mathbf{r}\cdot\mathbf{R}$	$\mathbf{r}^2\cdot\mathbf{R}$
$(0)_3\cdot(0)_2$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$(1)_3\cdot(0)_2$	$1\cdot 1$	$e^{2\pi i/3}\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot 1$	$e^{2\pi i/3}\cdot 1$	$e^{-2\pi i/3}\cdot 1$
$(2)_3\cdot(0)_2$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$e^{2\pi i/3}\cdot 1$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$e^{2\pi i/3}\cdot 1$
$(0)_3\cdot(1)_2$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$(1)_3\cdot(1)_2$	$1\cdot 1$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot(-1)$	$e^{2\pi i/3}\cdot(-1)$	$e^{-2\pi i/3}\cdot(-1)$
$(2)_3\cdot(1)_2$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$e^{-2\pi i/3}\cdot(-1)$	$e^{2\pi i/3}\cdot(-1)$

C_6 *is product* $\mathrm{C}_3\times \mathrm{C}_2$ *(but* C_4 *is NOT* $\mathrm{C}_2\times \mathrm{C}_2$*)*

C_3	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$(0)_3$	1	1	1
$(1)_3$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$

×

C_2	$\mathbf{1}$	$\mathbf{R}$
$(0)_2$	1	1
$(1)_2$	1	-1

=

$C_3 \times C_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$	$\mathbf{1}\cdot\mathbf{R}$	$\mathbf{r}\cdot\mathbf{R}$	$\mathbf{r}^2\cdot\mathbf{R}$
$(0)_3\cdot(0)_2$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$(1)_3\cdot(0)_2$	$1\cdot 1$	$e^{2\pi i/3}\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot 1$	$e^{2\pi i/3}\cdot 1$	$e^{-2\pi i/3}\cdot 1$
$(2)_3\cdot(0)_2$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$e^{2\pi i/3}\cdot 1$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$e^{2\pi i/3}\cdot 1$
$(0)_3\cdot(1)_2$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$(1)_3\cdot(1)_2$	$1\cdot 1$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot(-1)$	$e^{2\pi i/3}\cdot(-1)$	$e^{-2\pi i/3}\cdot(-1)$
$(2)_3\cdot(1)_2$	$1\cdot 1$	$e^{-2\pi i/3}\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$e^{-2\pi i/3}\cdot(-1)$	$e^{2\pi i/3}\cdot(-1)$

=

$C_3 \times C_2 = C_6$	$\mathbf{1}$	$\mathbf{r} = h^2$	$\mathbf{r}^2 = h^4$	$\mathbf{R} = \mathbf{h}^3$	$\mathbf{r}\cdot\mathbf{R} = h$	$\mathbf{r}^2\cdot\mathbf{R} = h^5$
$(0)_3\cdot(0)_2 = (0)_6$	1	1	1	1	1	1
$(1)_3\cdot(0)_2 = (2)_6$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
$(2)_3\cdot(0)_2 = (4)_6$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$
$(0)_3\cdot(1)_2 = (3)_6$	1	1	1	-1	-1	-1
$(1)_3\cdot(1)_2 = (5)_6$	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$	-1	$-e^{2\pi i/3}$	$-e^{-2\pi i/3}$
$(2)_3\cdot(1)_2 = (1)_6$	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$	-1	$-e^{-2\pi i/3}$	$-e^{2\pi i/3}$