1.16.15-19 class 1.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

AMOP reference links

Sketch of modern molecular spectroscopy

Spectral hierarchy of Born-Openheimer approximations to ***AMOP***

Example of16μm spectra of CF_4 1996 AMOP Handbook

2005 AMOP Handbook

Example of16μm spectra of SF_6 2018?AMOP Handbook

Example of ??μm spectra of C_{60} ?

Units of frequency (Hz), wavelength (m), and energy (eV)

Spectral windows in atmosphere due to molecules

Simple molecular-spectra models

2-well tunneling, Bohr mass-on-ring, 1D harmonic oscillator, Coulomb PE models

More advanced molecular-spectra models (Using symmetry-group theory)

2-state U(2)-spin tunneling models

3D R(3)-rotor and D-function lab-body wave models

2D harmonic oscillator and U(2) 2nd quantization

Bohr Mass-On-a-Ring *(model of rotation) and related* ***∞-Square Well*** *(model of quantum dots)*

Quantum levels of ∞-Square well and Bohr rotor

Example of CO_2 rotational (υ=0)⇔(υ=1)bands

Quantum dynamics of ∞-Square well and Bohr rotor: What makes that "dipole"spectra?

Quantum dynamics of Double-well tunneling: Cheap models of NH_3 inversion doublet

Quantum "blasts" of strongly localized ∞-well or rotor waves: A lesson in quantum interference

Wavepacket explodes! (Then revives). . . . .*some xtra stuff on Farey-Ford wave resonance*

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

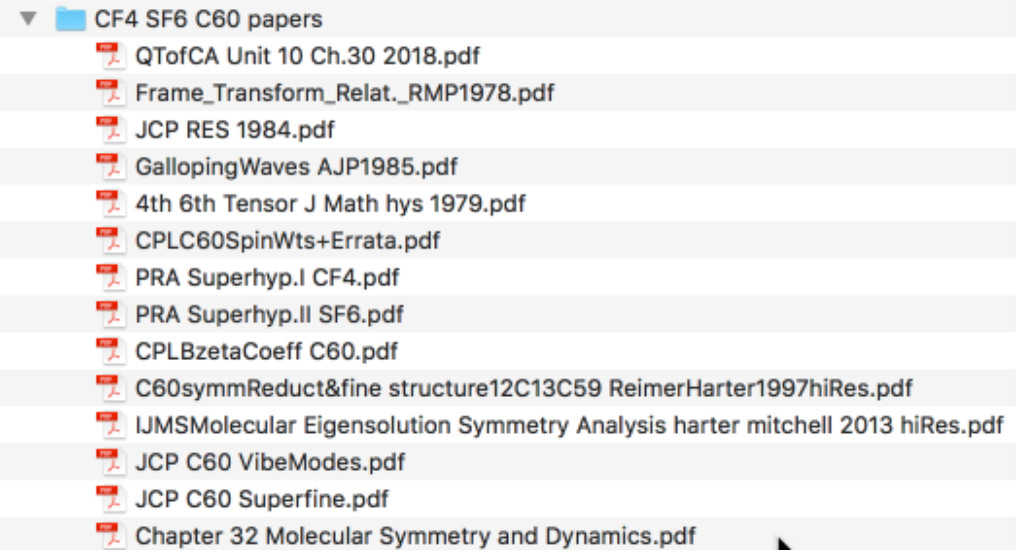
QTCA Unit 10 Ch 30 - 2013
Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978 (Alt Scanned version)
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - ajp-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)
Theory of hyperfine and superfine levels in symmetric polyatomic molecules.
- **I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)**
- **II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)**

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013
Rotation–vibration spectra of icosahedral molecules.
- **I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989**
- **II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989**
- **III) Half-integral angular momentum - harter-reimer-jcp-1991**

AMOP Ch 32 Molecular Symmetry and Dynamics - 2019
AMOP Ch 0 Space-Time Symmetry - 2019

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

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


CF4 SF6 C60 papers
QTofCA Unit 10 Ch.30 2018.pdf
Frame_Transform_Relat._RMP1978.pdf
JCP RES 1984.pdf
GallopingWaves AJP1985.pdf
4th 6th Tensor J Math hys 1979.pdf
CPLC60SpinWts+Errata.pdf
PRA Superhyp.I CF4.pdf
PRA Superhyp.II SF6.pdf
CPLBzetaCoeff C60.pdf
C60symmReduct&fine structure12C13C59 ReimerHarter1997hiRes.pdf
IJMSMolecular Eigensolution Symmetry Analysis harter mitchell 2013 hiRes.pdf
JCP C60 VibeModes.pdf
JCP C60 Superfine.pdf
Chapter 32 Molecular Symmetry and Dynamics.pdf

Website front page

2014 AMOP front page

2017 Group Theory for QM   UAF Physics UTube channel

2018 AMOP front page

Spectral hierarchy of Born-Openheimer approximations to *AMOP*

➡ Sketch of modern molecular spectroscopy

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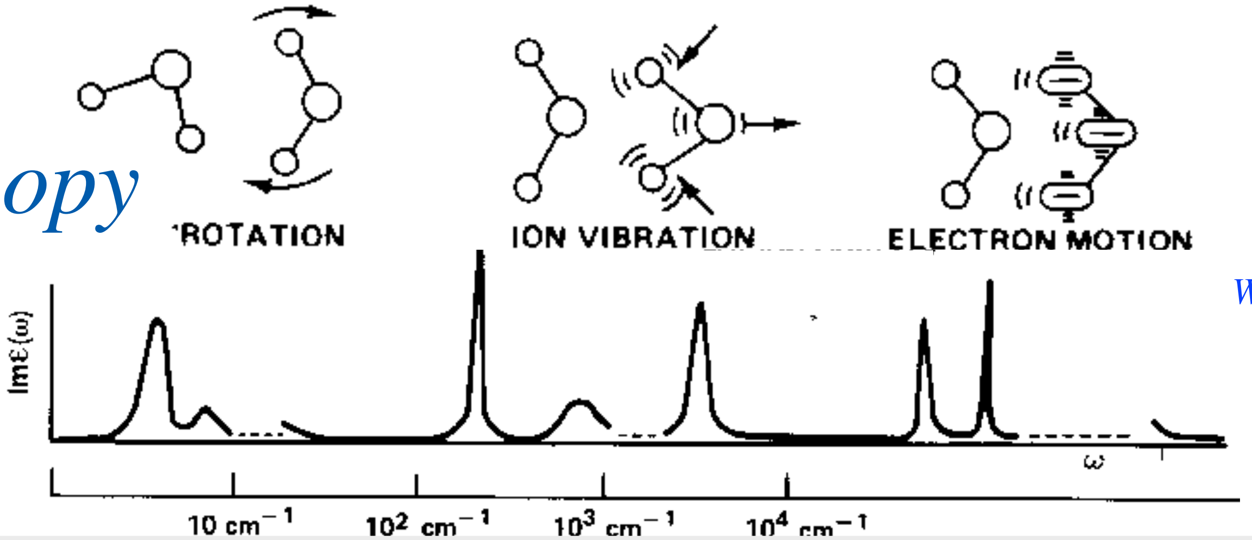
2005 AMOP Handbook

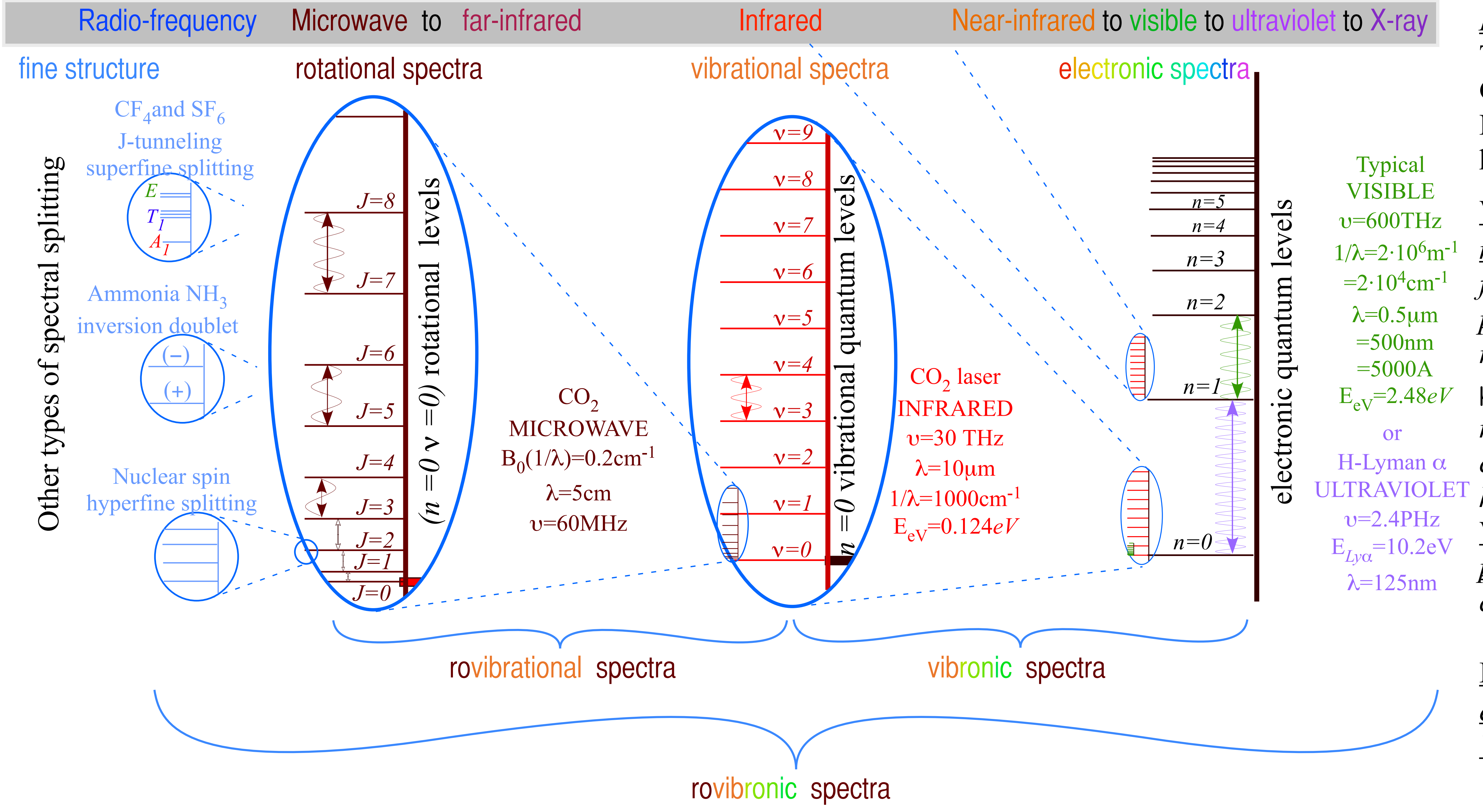
Example of16μm spectra of SF_6 *2018?AMOP Handbook*

A sketch of modern molecular spectroscopy

Frequency hierarchy



From Fig. 6.5.5.
Principles of Symmetry, Dynamics, and Spectroscopy
W. G. Harter, Wiley Interscience, NY (1993)



Radio-frequency Microwave to far-infrared Infrared Near-infrared to visible to ultraviolet to X-ray

fine structure

rotational spectra

vibrational spectra

electronic spectra

Other types of spectral splitting

CF_4 and SF_6
J-tunneling
superfine splitting

Ammonia NH_3
inversion doublet

Nuclear spin
hyperfine splitting

(n =0 v =0) rotational levels

CO_2
MICROWAVE
$B_0(1/\lambda)=0.2cm^{-1}$
λ=5cm
υ=60MHz

n =0 vibrational quantum levels

CO_2 laser
INFRARED
υ=30 THz
λ=10μm
$1/\lambda=1000cm^{-1}$
$E_{eV}=0.124eV$

electronic quantum levels

Typical
VISIBLE
υ=600THz
$1/\lambda=2\cdot10^6m^{-1}$
$=2\cdot10^4cm^{-1}$
λ=0.5μm
=500nm
=5000A
$E_{eV}=2.48eV$

or

H-Lyman α
ULTRAVIOLET
υ=2.4PHz
$E_{Ly\alpha}=10.2eV$
λ=125nm

rovibrational spectra

vibronic spectra

rovibronic spectra

Spectral
Quantities

Frequency υ
Hertz(sec^{-1})

THz	$10^{12}s^{-1}$
GHz	10^9s^{-1}
MHz	10^6s^{-1}
kHz	10^3s^{-1}

Wavelength λ
meters(*m*)

fm	$10^{-15}m$
pm	$10^{-12}m$
nm	$10^{-9}m$
μ*m*	$10^{-6}m$
mm	$10^{-3}m$
cm	$10^{-2}m$
km	10^3m

Wavenumber
per meter(m^{-1})

cm^{-1}	10^2m^{-1}

Energy *ehυ*
electonVolts(*eV*)

A sketch of modern molecular spectroscopy

Frequency hierarchy

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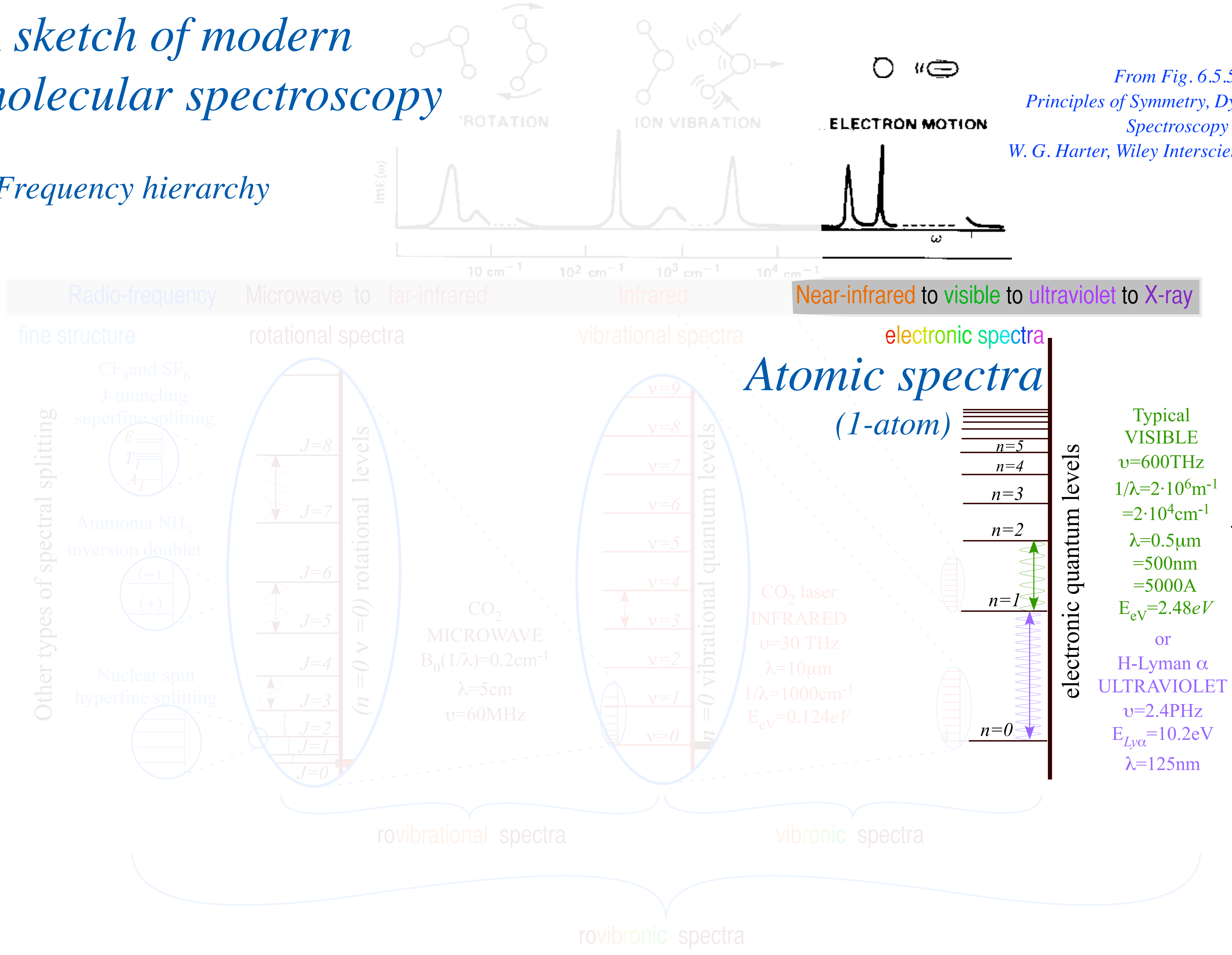

Atomic spectra

(1-atom)

Typical
VISIBLE
υ=600THz
$1/\lambda=2\cdot10^6\text{m}^{-1}$
$=2\cdot10^4\text{cm}^{-1}$
$\lambda=0.5\mu\text{m}$
=500nm
=5000A
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Spectral Quantities

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km $10^{3}m$
Wavenumber
per meter(m^{-1})
cm^{-1} $10^{2}m^{-1}$

Energy $eh\upsilon$
electonVolts(eV)

A sketch of modern molecular spectroscopy

Frequency hierarchy

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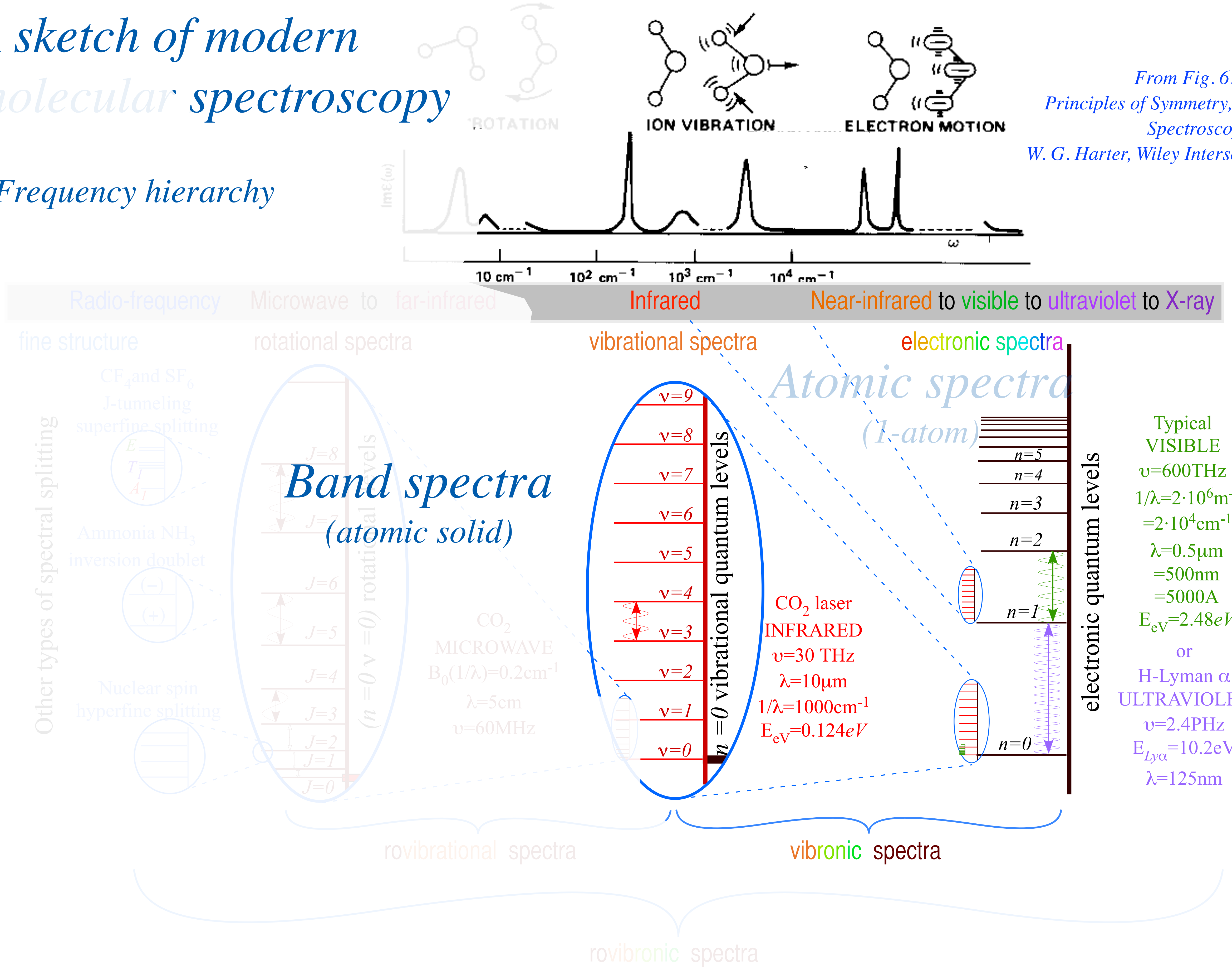

CO$_2$
MICROWAVE
$B_0(1/\lambda)=0.2\text{cm}^{-1}$
$\lambda=5\text{cm}$
$\upsilon=60\text{MHz}$

CO$_2$ laser
INFRARED
$\upsilon=30$ THz
$\lambda=10\mu\text{m}$
$1/\lambda=1000\text{cm}^{-1}$
$E_{eV}=0.124eV$

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$\upsilon=600\text{THz}$
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Spectral
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<u>*Hertz(sec*$^{-1}$)</u>
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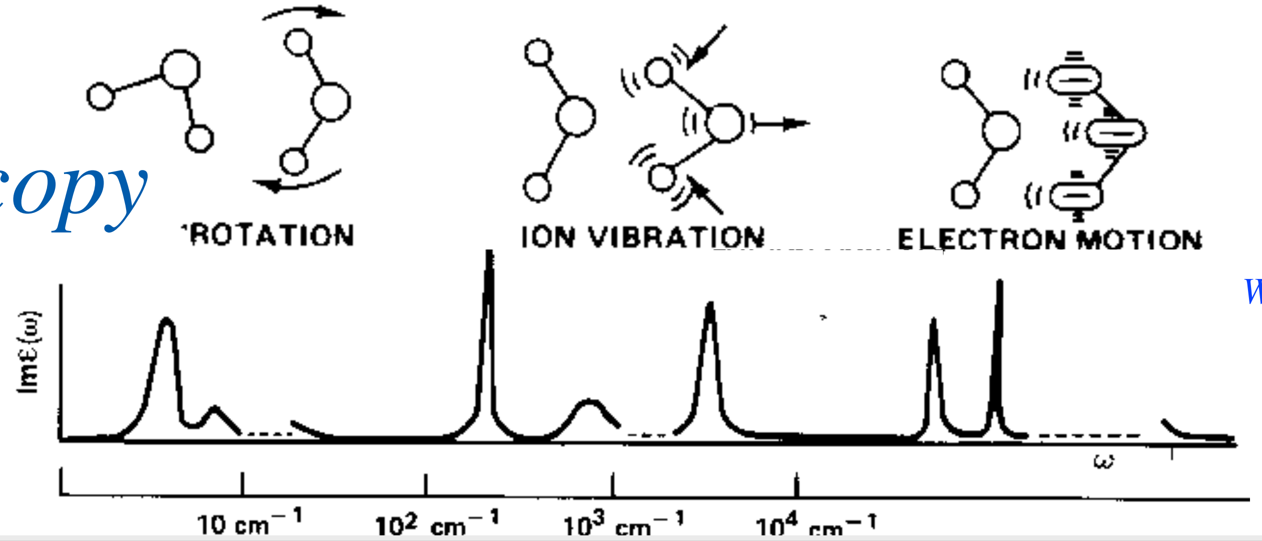
<u>Wavenumber</u>
<u>*per meter*(m^{-1})</u>
cm^{-1} $10^{2}m^{-1}$

<u>Energy *ehυ*</u>
<u>*electonVolts(eV)*</u>

A sketch of modern molecular spectroscopy

Frequency hierarchy



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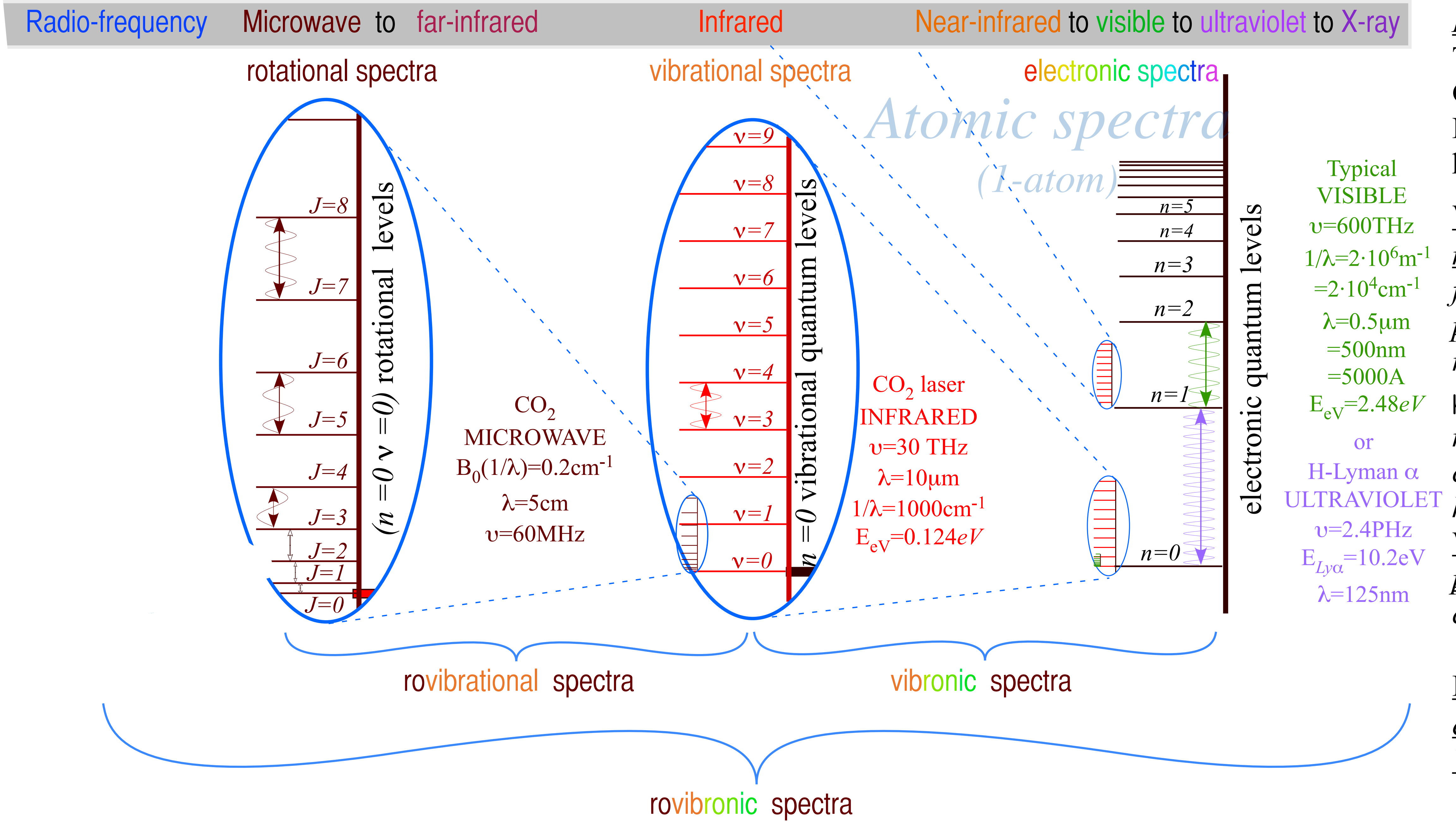
Radio-frequency Microwave to far-infrared Infrared Near-infrared to visible to ultraviolet to X-ray

rotational spectra

vibrational spectra

electronic spectra

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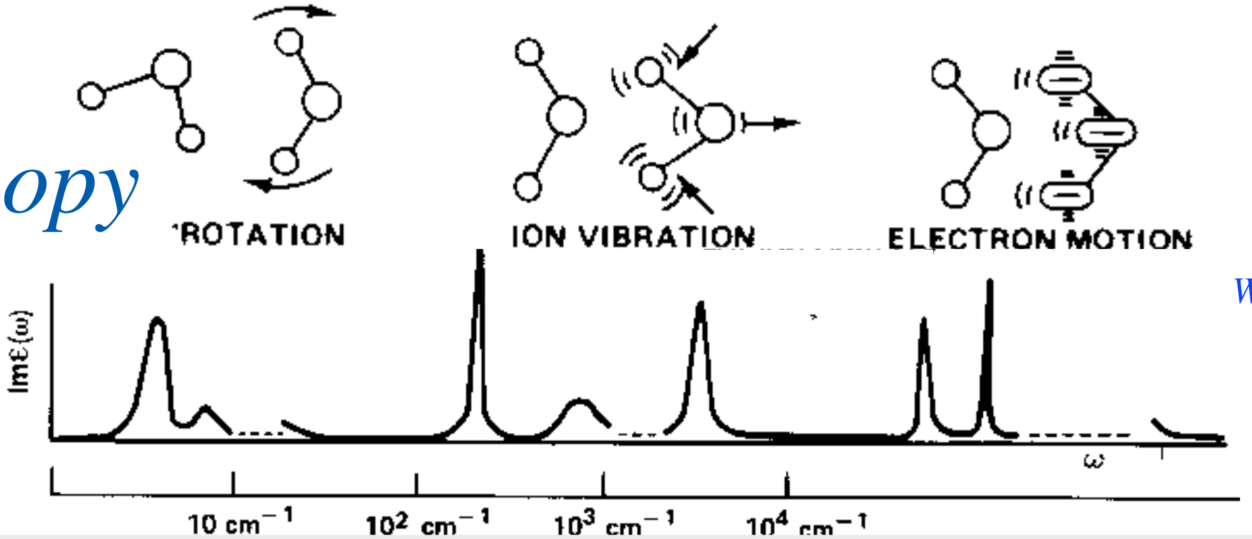
Energy *ehυ*
electonVolts(eV)

A sketch of modern molecular spectroscopy

Frequency hierarchy



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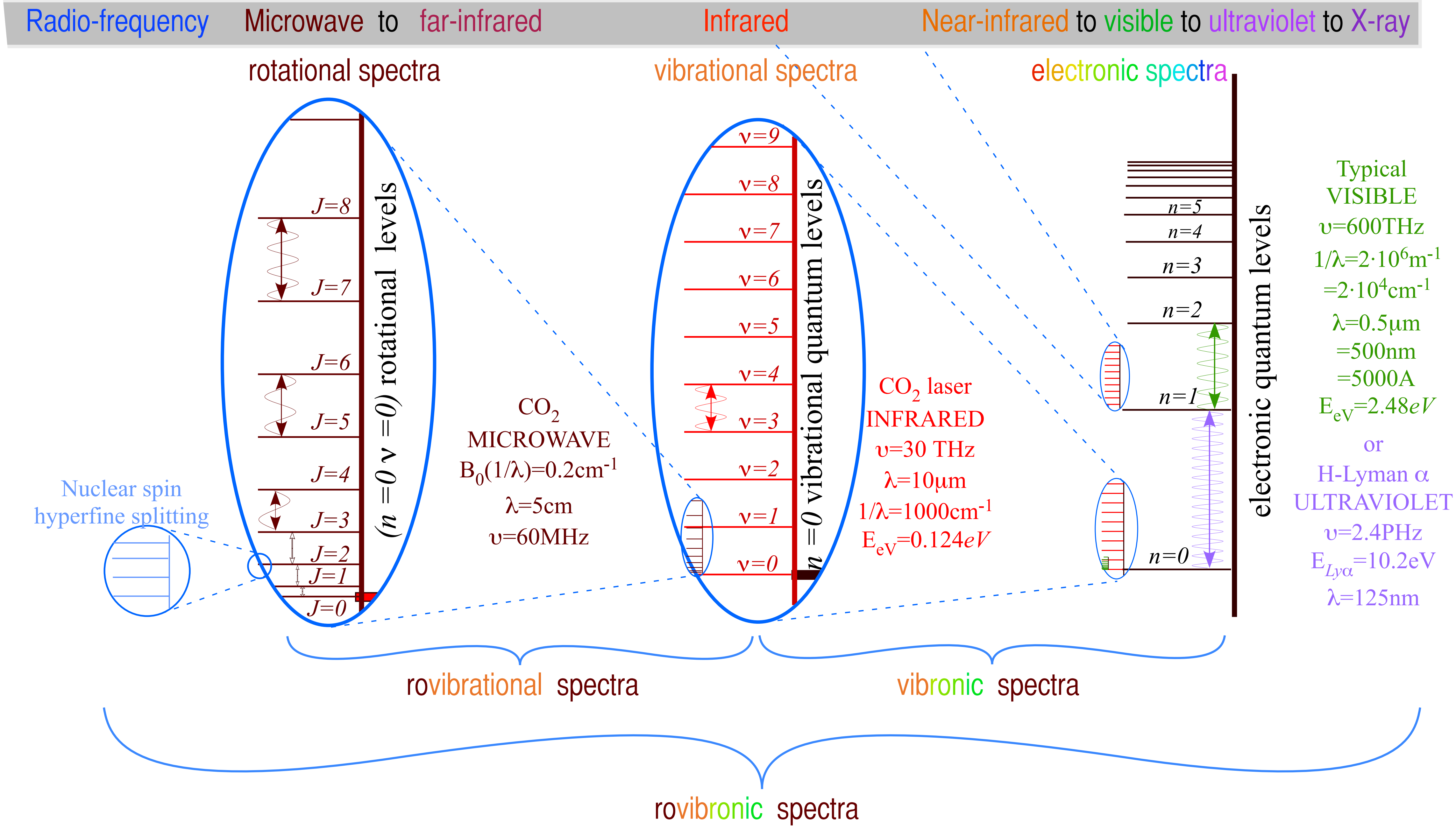

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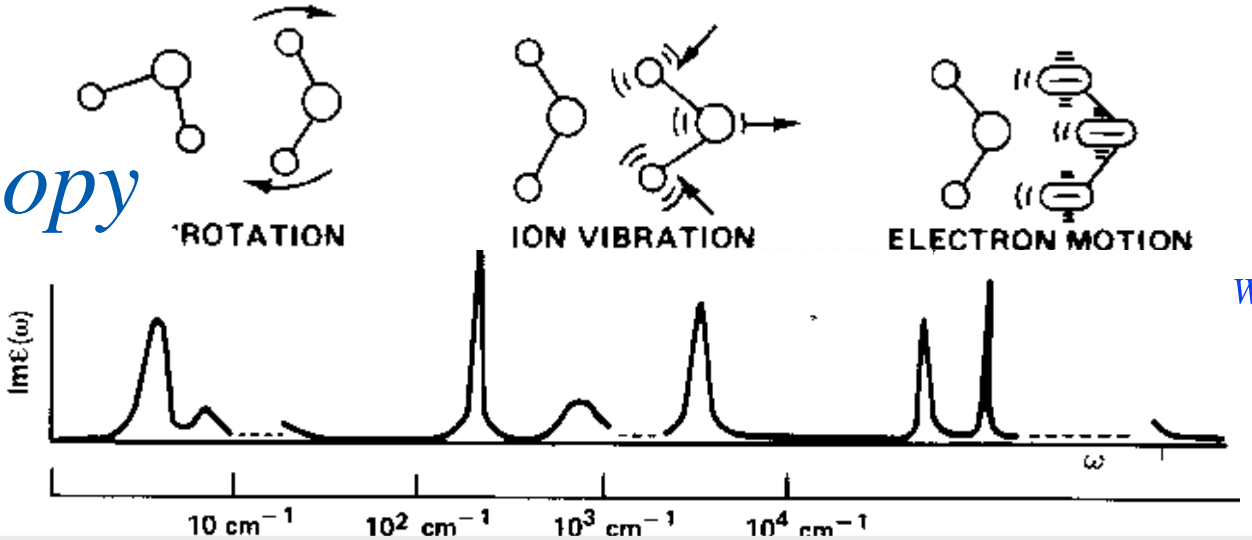
Wavenumber
per meter(m^{-1})

cm^{-1}	$10^{2}m^{-1}$

Energy $eh\upsilon$
electonVolts(eV)

A sketch of modern molecular spectroscopy

Frequency hierarchy



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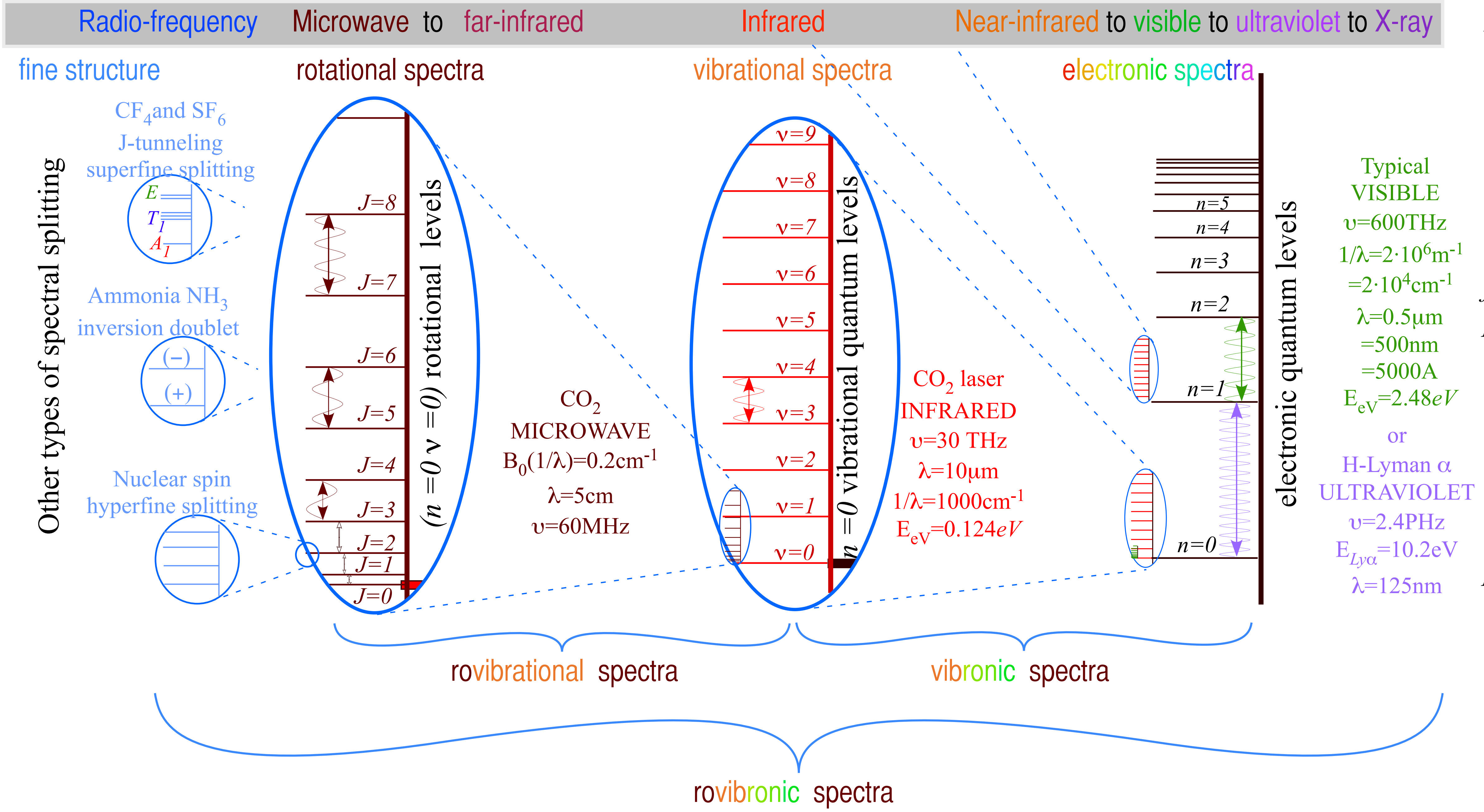

Radio-frequency | Microwave to far-infrared | Infrared | Near-infrared to visible to ultraviolet to X-ray

fine structure | rotational spectra | vibrational spectra | electronic spectra

Other types of spectral splitting

CF$_4$ and SF$_6$
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superfine splitting

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rovibrational spectra | vibronic spectra

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<u>Wavenumber</u>
<u>*per meter*(*m*$^{-1}$)</u>
cm^{-1} $10^{2}m^{-1}$

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<u>*electonVolts*(*eV*)</u>

Spectral hierarchy of Born-Openheimer approximations to *AMOP*

Sketch of modern molecular spectroscopy

➡ *Example of16μm spectra of* CF_4 *1996 AMOP Handbook*

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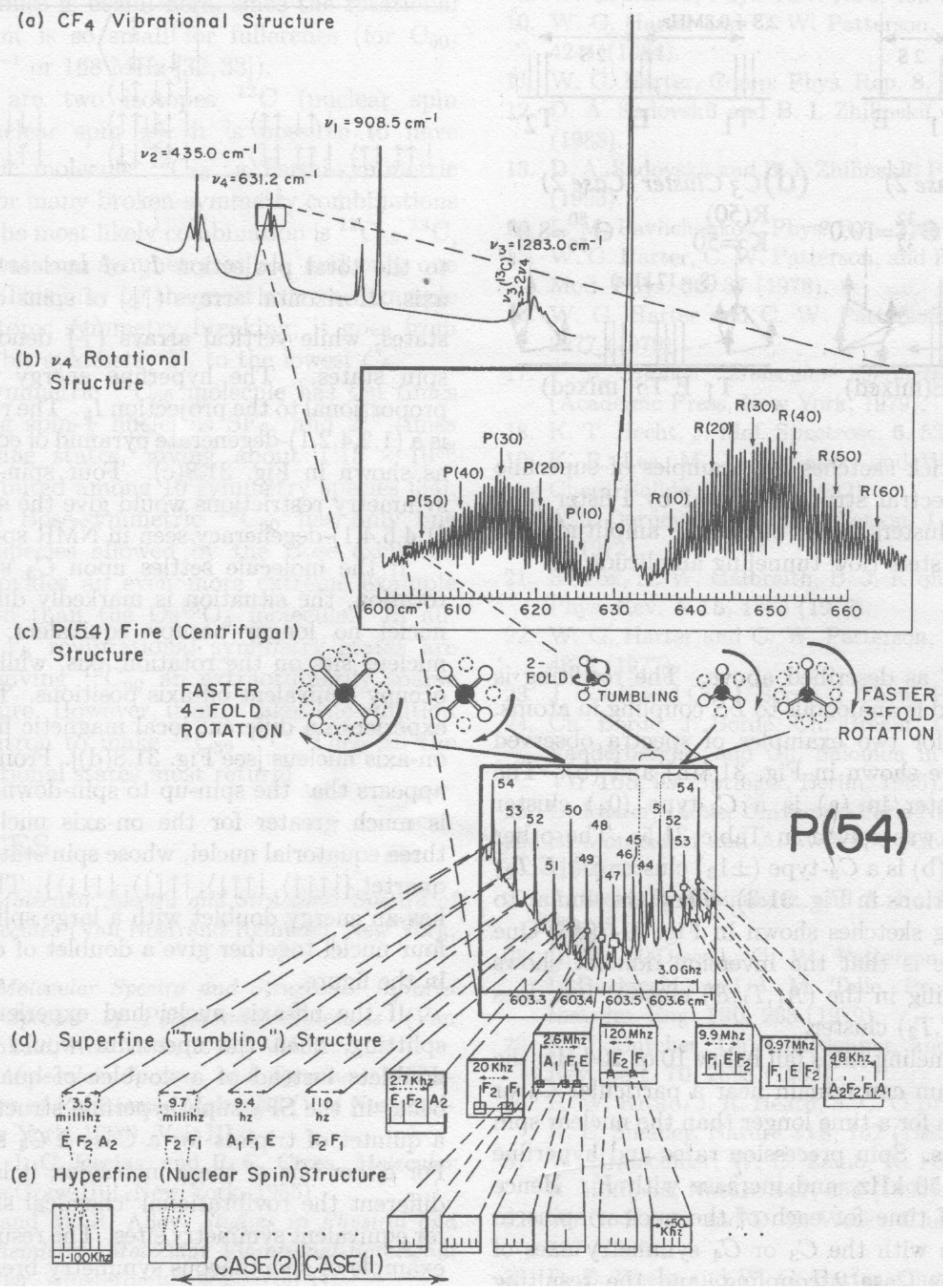
Example of frequency hierarchy
for 16μm spectra
of CF_4
(Freon-14)

W.G.Harter
Ch. 31
Atomic, Molecular, &
Optical Physics Handbook
Am. Int. of Physics
Gordon Drake Editor
(1996)



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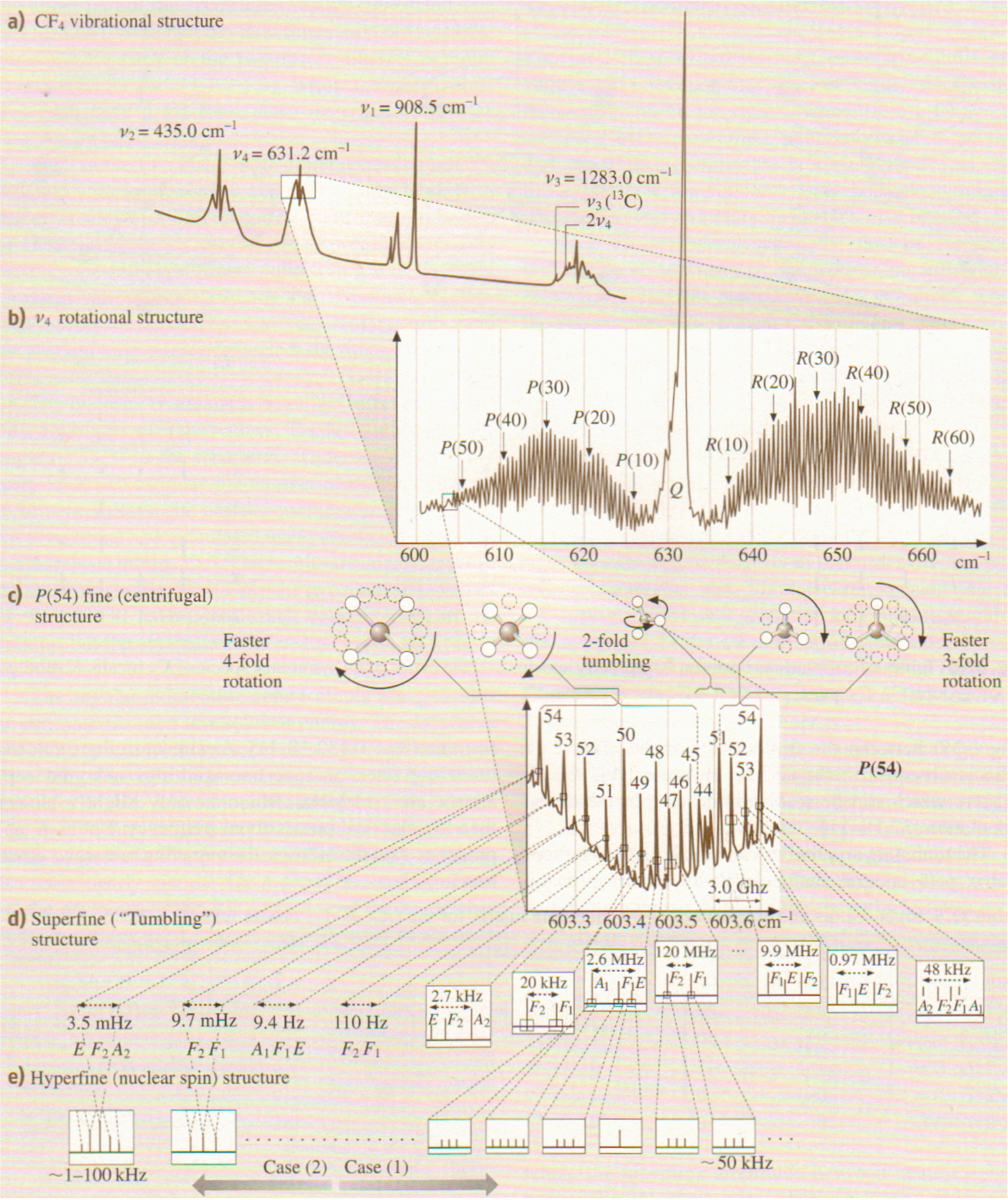
W.G.Harter
Fig. 32.7
Springer Handbook of
Atomic, Molecular, &
Optical Physics
Gordon Drake Editor
(2005)



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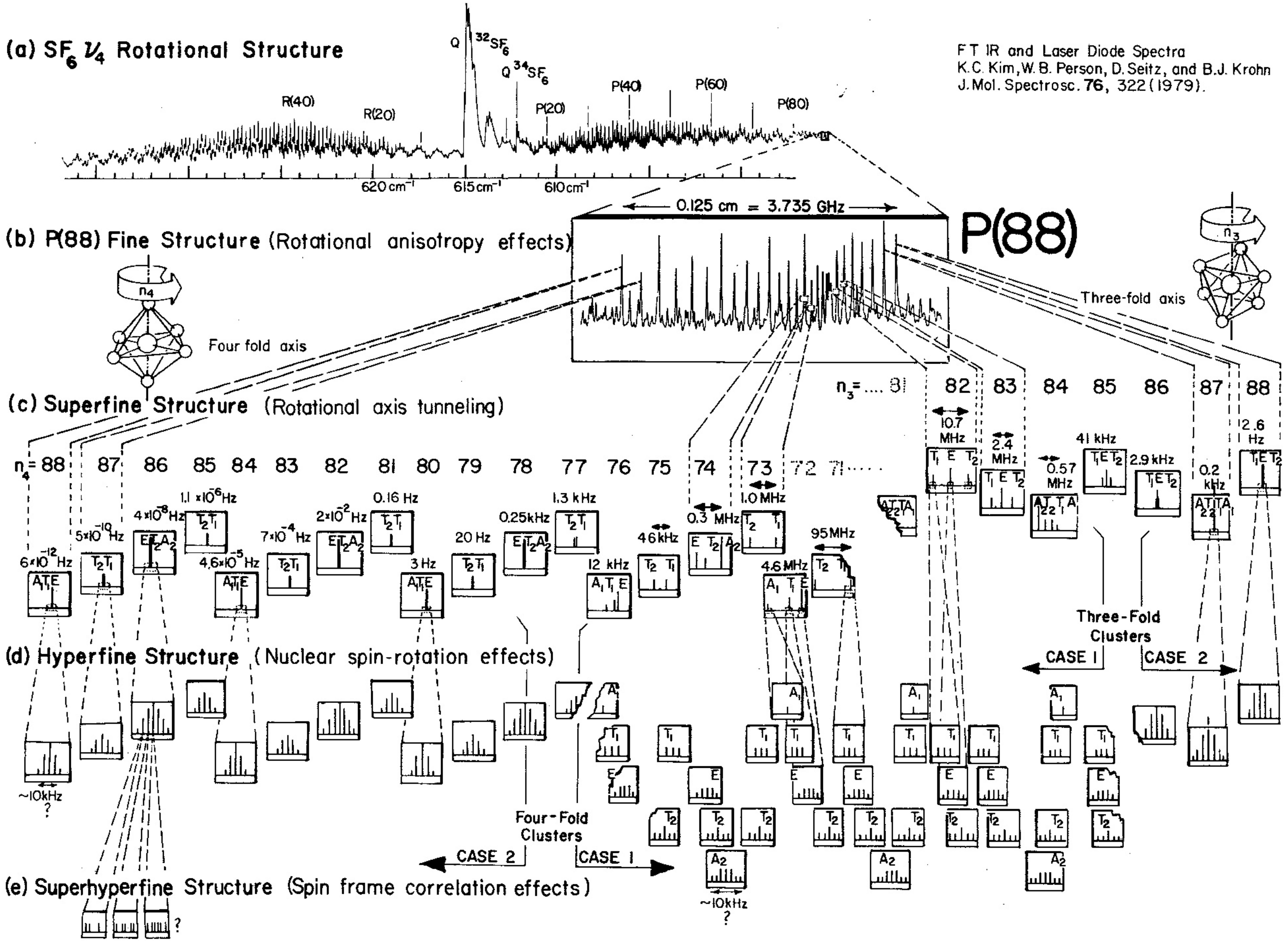
Example of ??μm spectra of C_{60} *?*



FT IR and Laser Diode Spectra
K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. **76**, 322 (1979).

I) <u>Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981</u>

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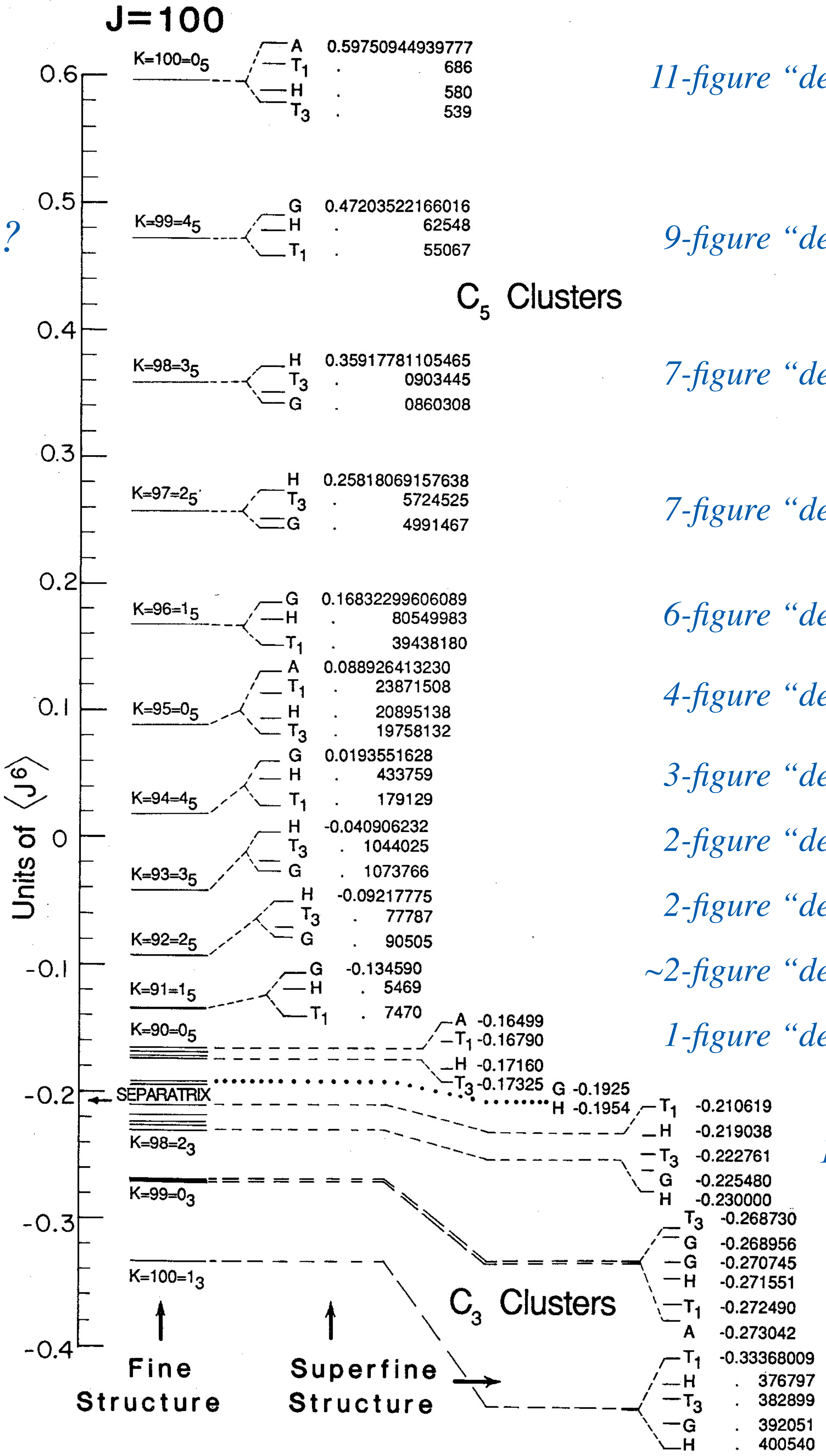
Spectral windows in atmosphere due to molecules

Example of ??μm spectra of C_{60} ?



11-figure "degeneracy"

9-figure "degeneracy"

7-figure "degeneracy"

7-figure "degeneracy"

6-figure "degeneracy"

4-figure "degeneracy"

3-figure "degeneracy"

2-figure "degeneracy"

2-figure "degeneracy"

~2-figure "degeneracy"

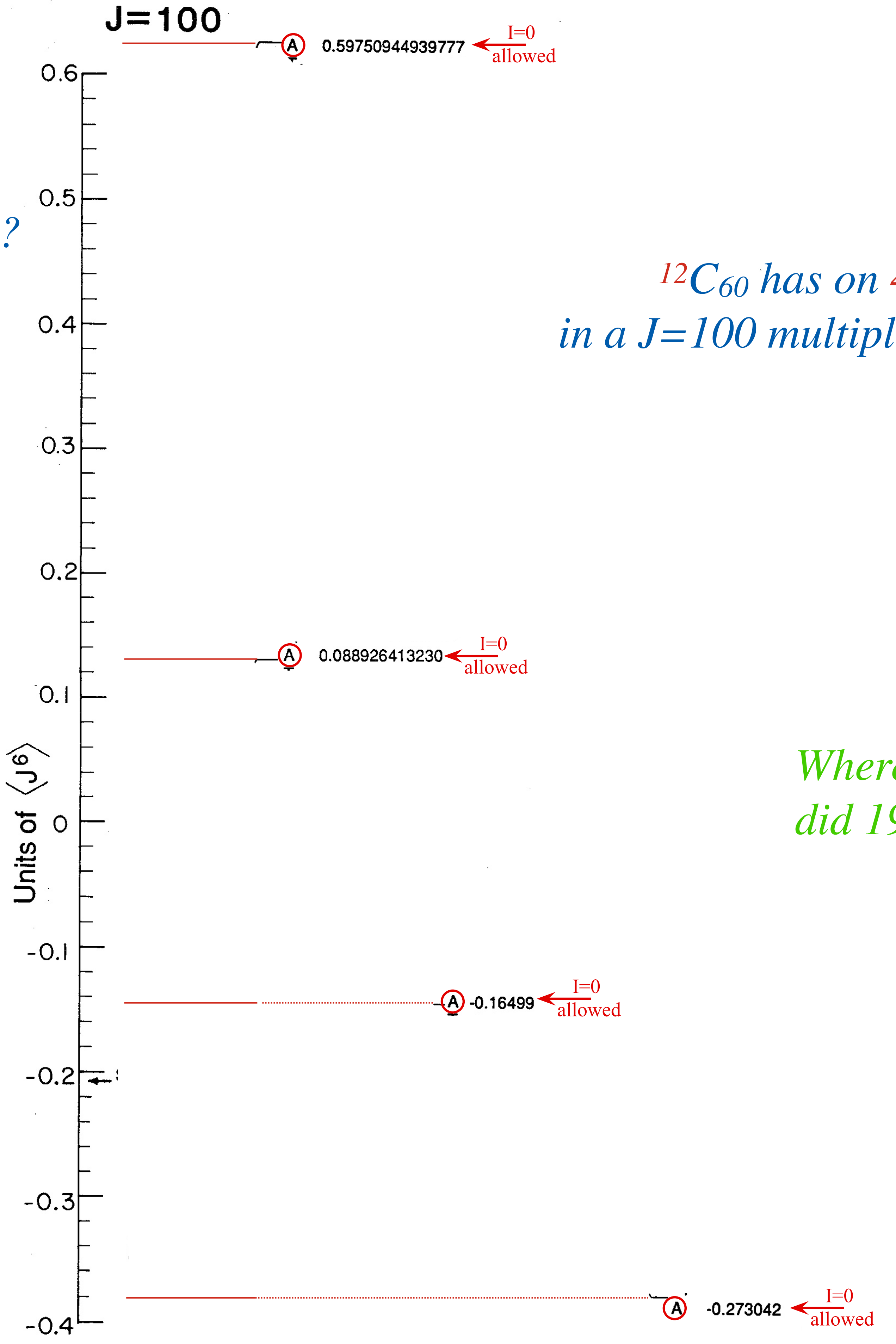
1-figure "degeneracy"

1-figure "degeneracy"

2-figure "degeneracy"

~3-figure "degeneracy"

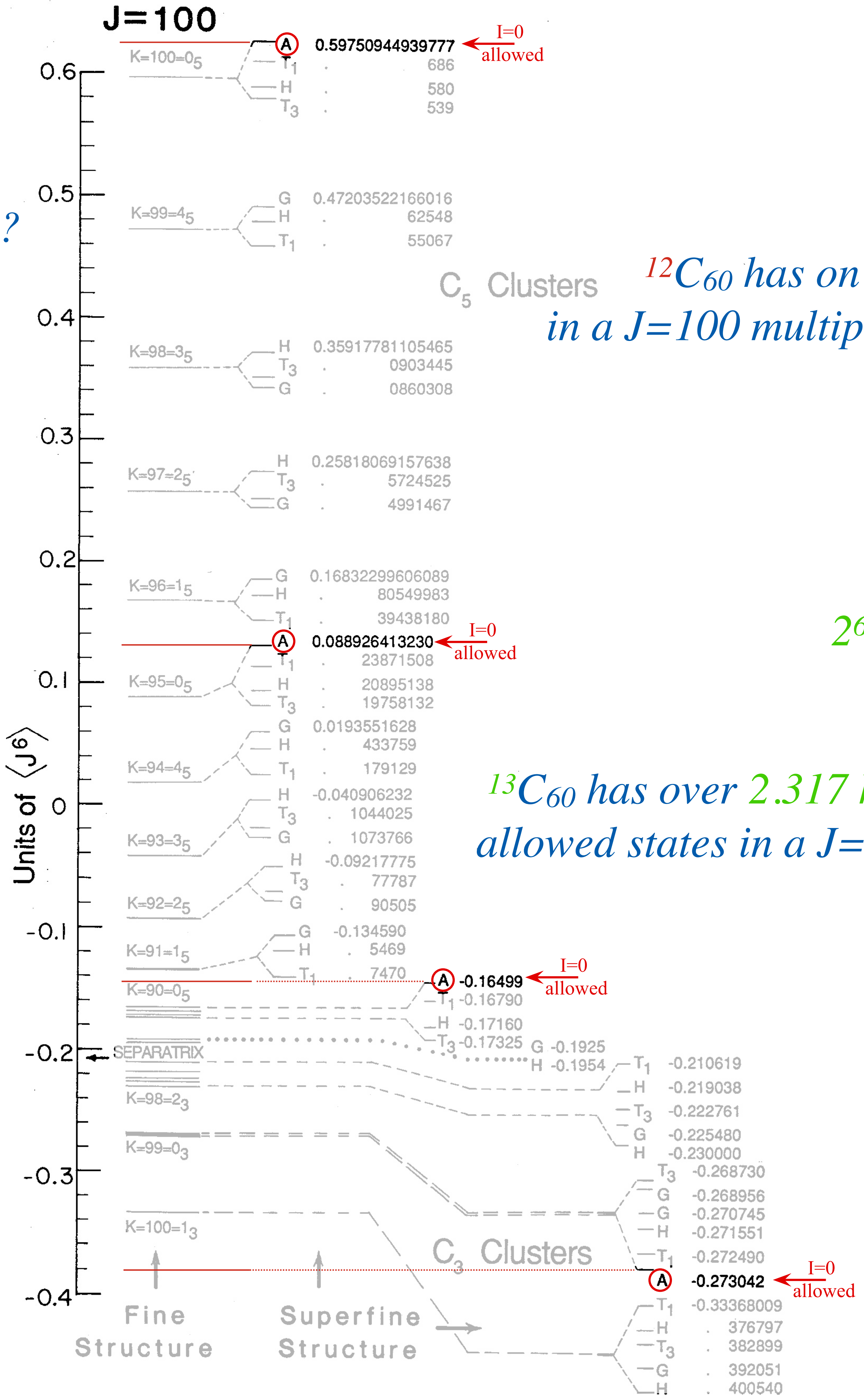
Example of ??µm spectra of $^{12}C_{60}$?



$^{12}C_{60}$ has on 4 allowed states
in a J=100 multiplet of 201=2J+1

Where the !#@$%
did 197 states go??!!

Example of ??μm spectra of $^{12}C_{60}$?



$^{12}C_{60}$ has on 4 allowed states
in a J=100 multiplet of 201=2J+1

$2^{60}=1.5292 \cdot 10^{18}$

$^{13}C_{60}$ has over 2.317 hundred octillion
allowed states in a J=100 multiplet of 201

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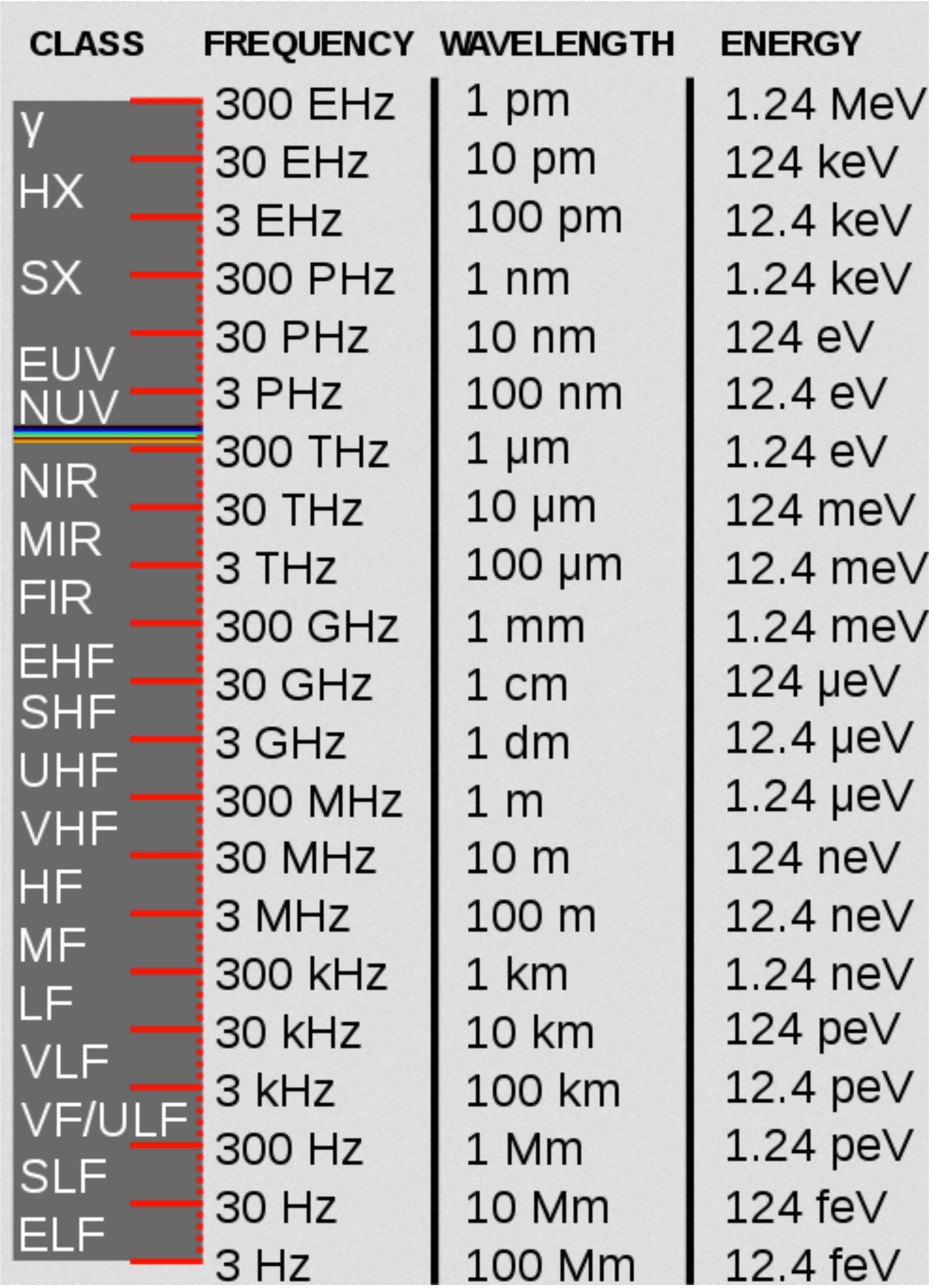
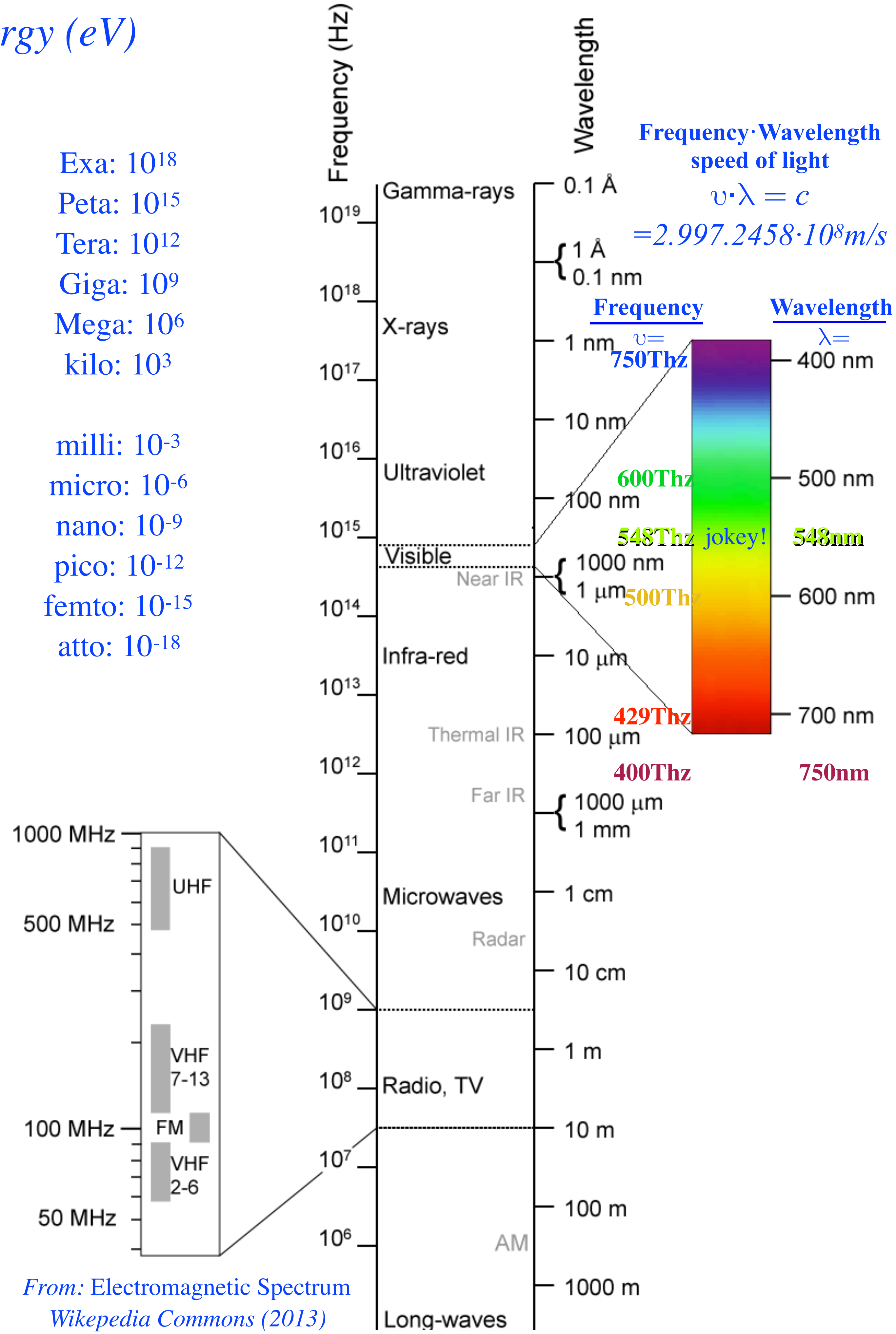


CLASS	FREQUENCY	WAVELENGTH	ENERGY
	300 EHz	1 pm	1.24 MeV
γ			
	30 EHz	10 pm	124 keV
HX			
	3 EHz	100 pm	12.4 keV
SX			
	300 PHz	1 nm	1.24 keV
	30 PHz	10 nm	124 eV
EUV			
	3 PHz	100 nm	12.4 eV
NUV			
	300 THz	1 μm	1.24 eV
NIR			
	30 THz	10 μm	124 meV
MIR			
	3 THz	100 μm	12.4 meV
FIR			
	300 GHz	1 mm	1.24 meV
EHF			
	30 GHz	1 cm	124 μeV
SHF			
	3 GHz	1 dm	12.4 μeV
UHF			
	300 MHz	1 m	1.24 μeV
VHF			
	30 MHz	10 m	124 neV
HF			
	3 MHz	100 m	12.4 neV
MF			
	300 kHz	1 km	1.24 neV
LF			
	30 kHz	10 km	124 peV
VLF			
	3 kHz	100 km	12.4 peV
VF/ULF			
	300 Hz	1 Mm	1.24 peV
SLF			
	30 Hz	10 Mm	124 feV
ELF			
	3 Hz	100 Mm	12.4 feV

From: Electromagnetic Spectrum
Wikepedia Commons (2013)

Exa: 10^{18}
Peta: 10^{15}
Tera: 10^{12}
Giga: 10^{9}
Mega: 10^{6}
kilo: 10^{3}

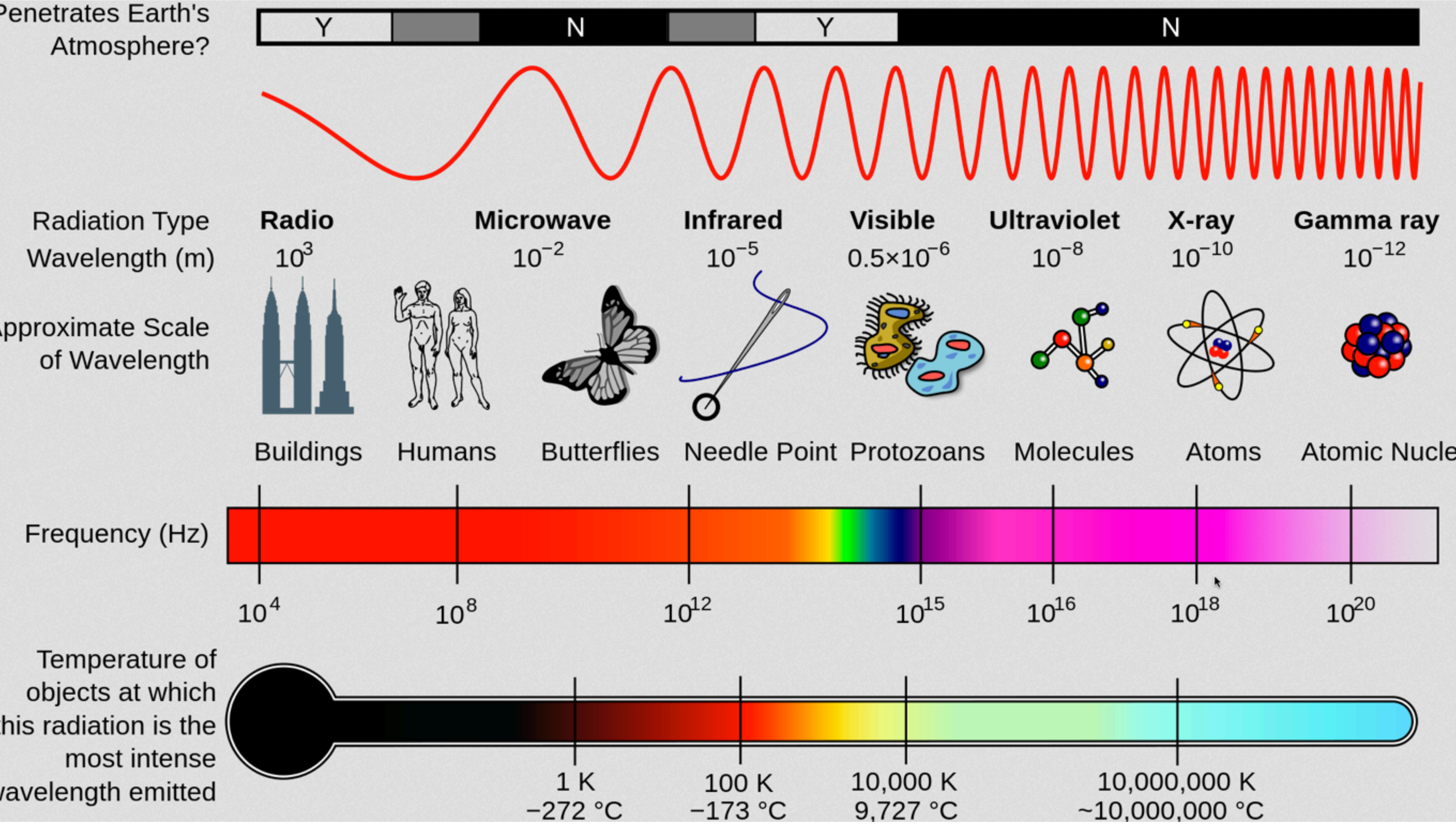
milli: 10^{-3}
micro: 10^{-6}
nano: 10^{-9}
pico: 10^{-12}
femto: 10^{-15}
atto: 10^{-18}



Frequency·Wavelength
speed of light
$\upsilon \cdot \lambda = c$
$= 2.997.2458 \cdot 10^8 m/s$

From: Electromagnetic Spectrum
Wikepedia Commons (2013)

Units of frequency (Hz), wavelength (m), and energy (eV)



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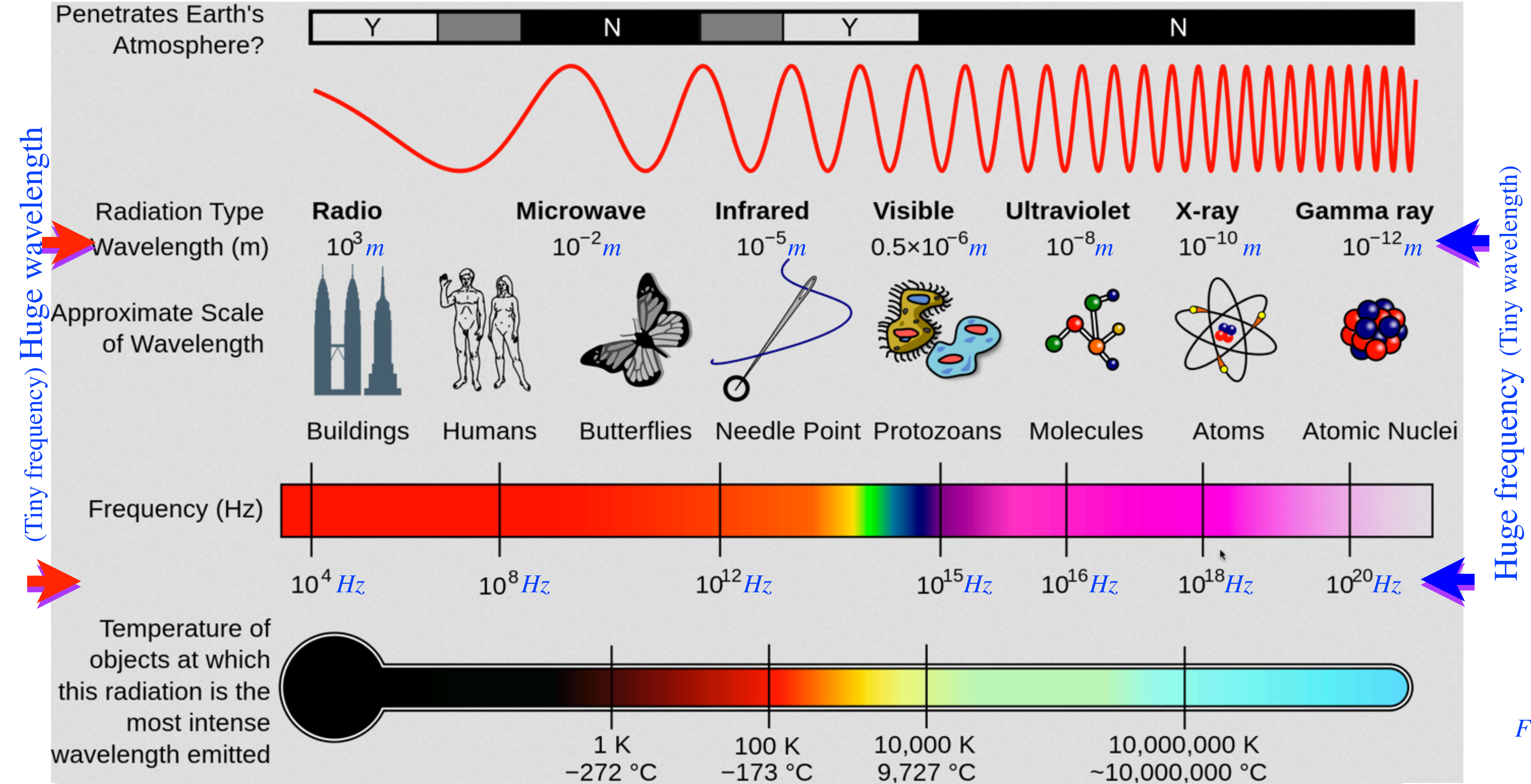
Spectral windows in atmosphere due to molecules



From: Electromagnetic Spectrum
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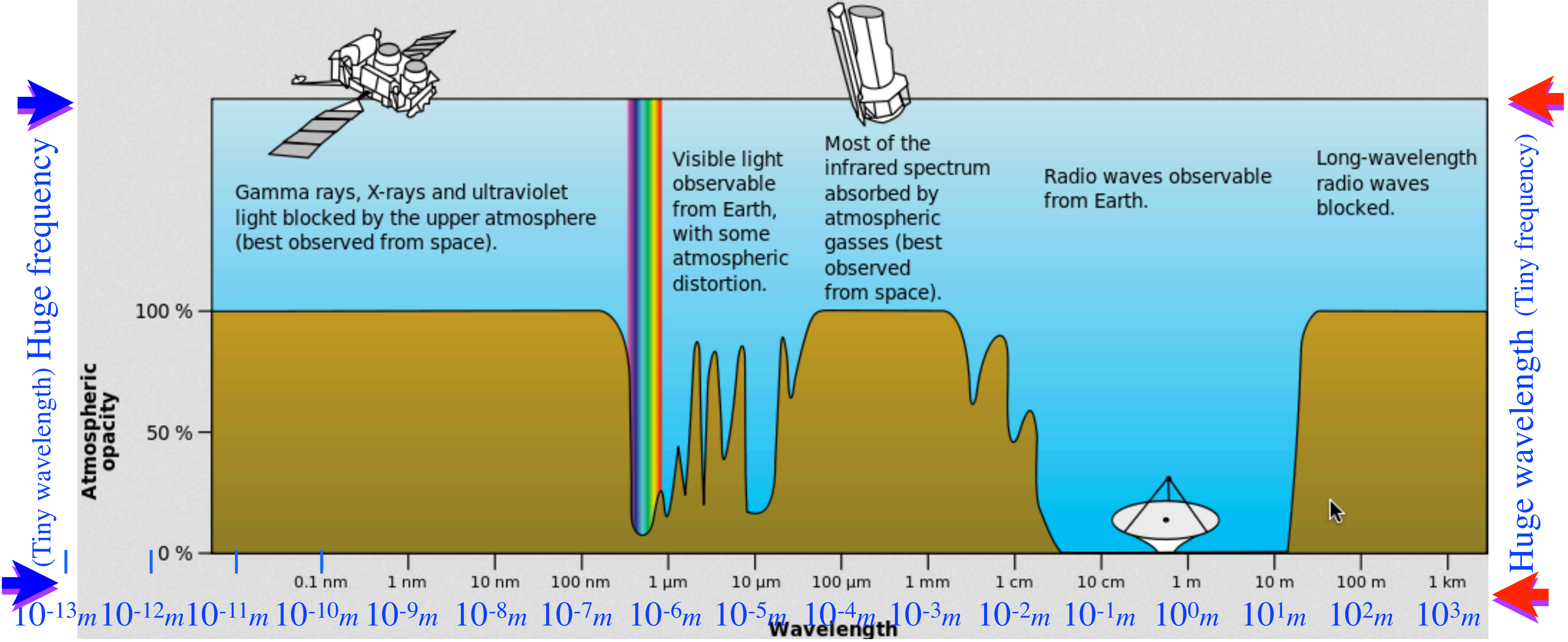
Spectral windows in Earth atmosphere



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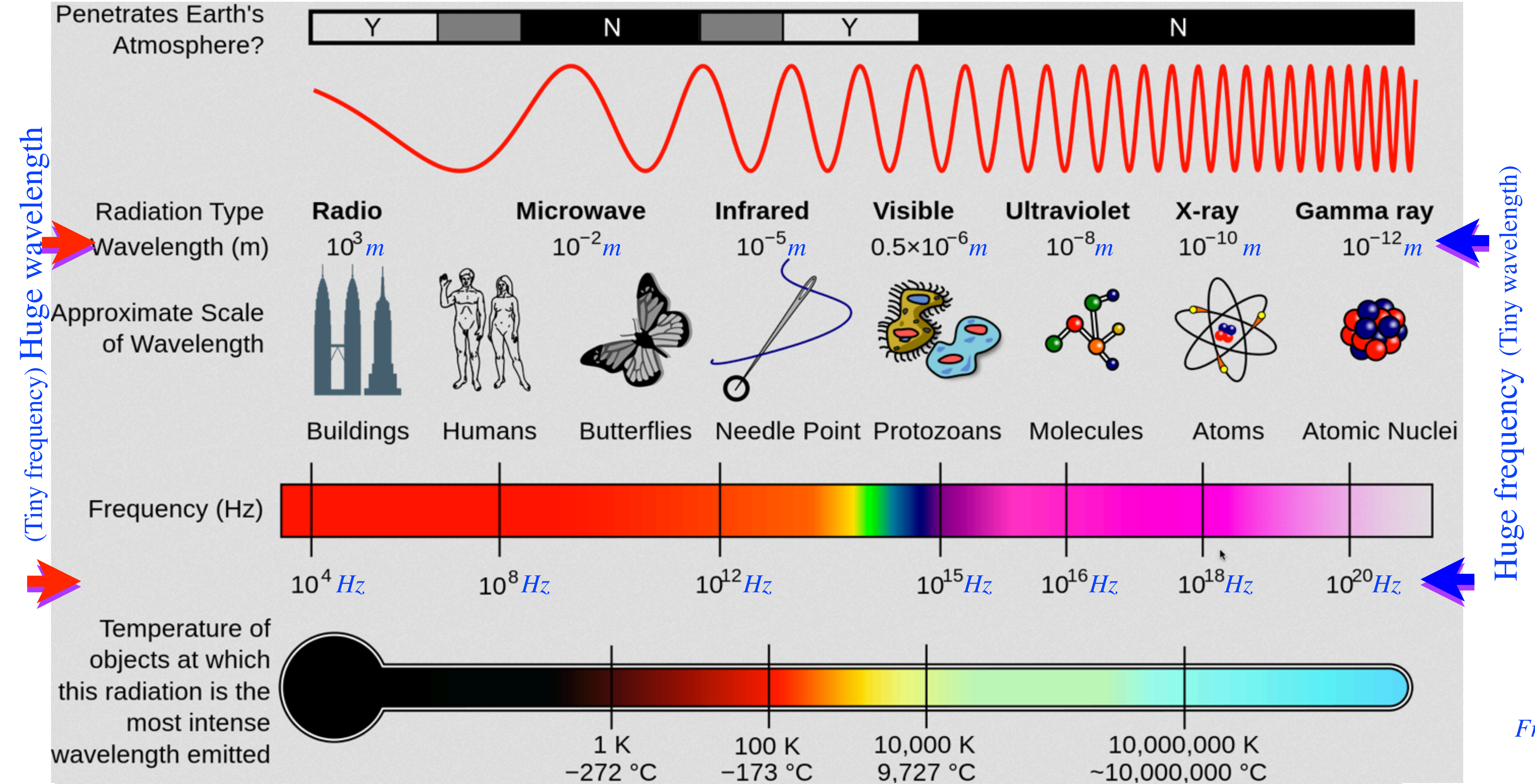

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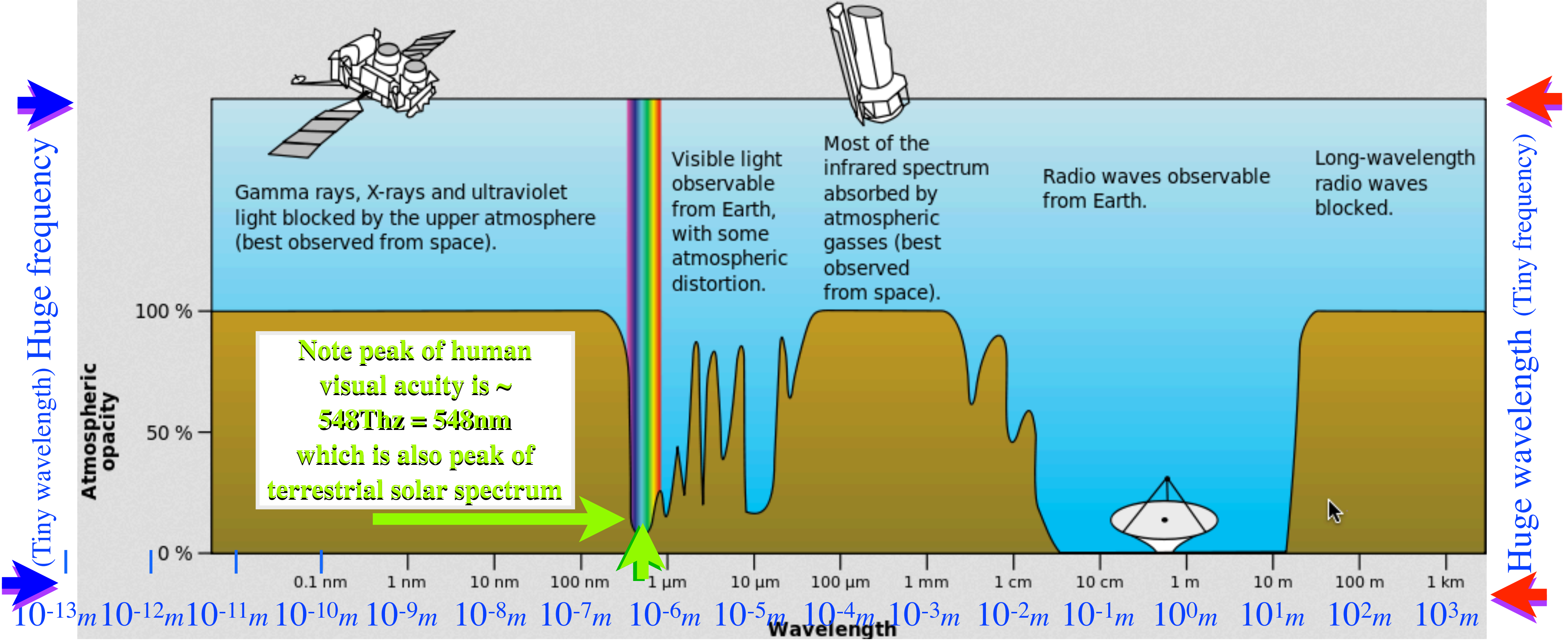

Note peak of human visual acuity is ~ 548Thz = 548nm which is also peak of terrestrial solar spectrum

Spectral windows in Earth atmosphere

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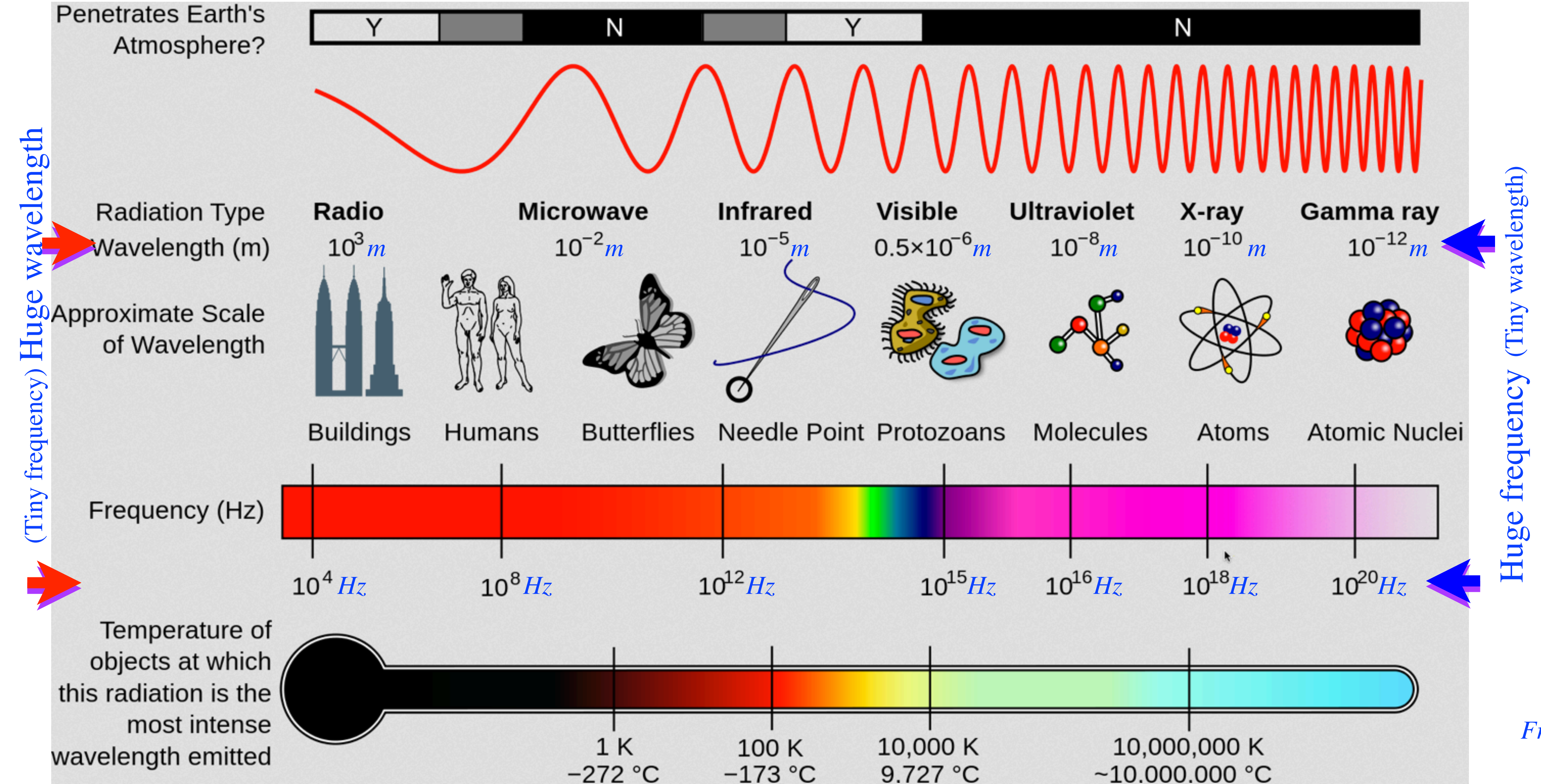
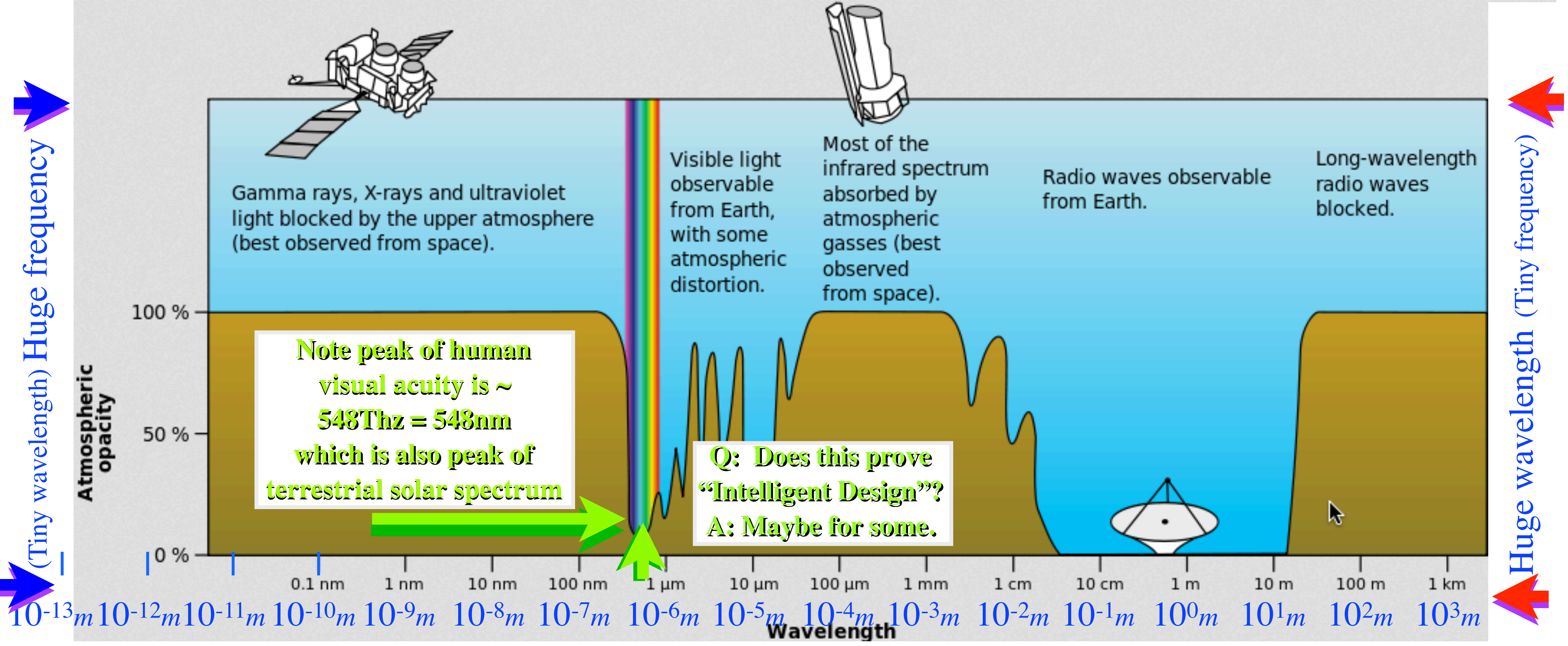
Wikepedia Commons (2013)



From: Electromagnetic Spectrum *Wikepedia Commons (2013)*



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Q: Does this prove "Intelligent Design"?
A: Maybe for some.

Spectral windows in Earth atmosphere

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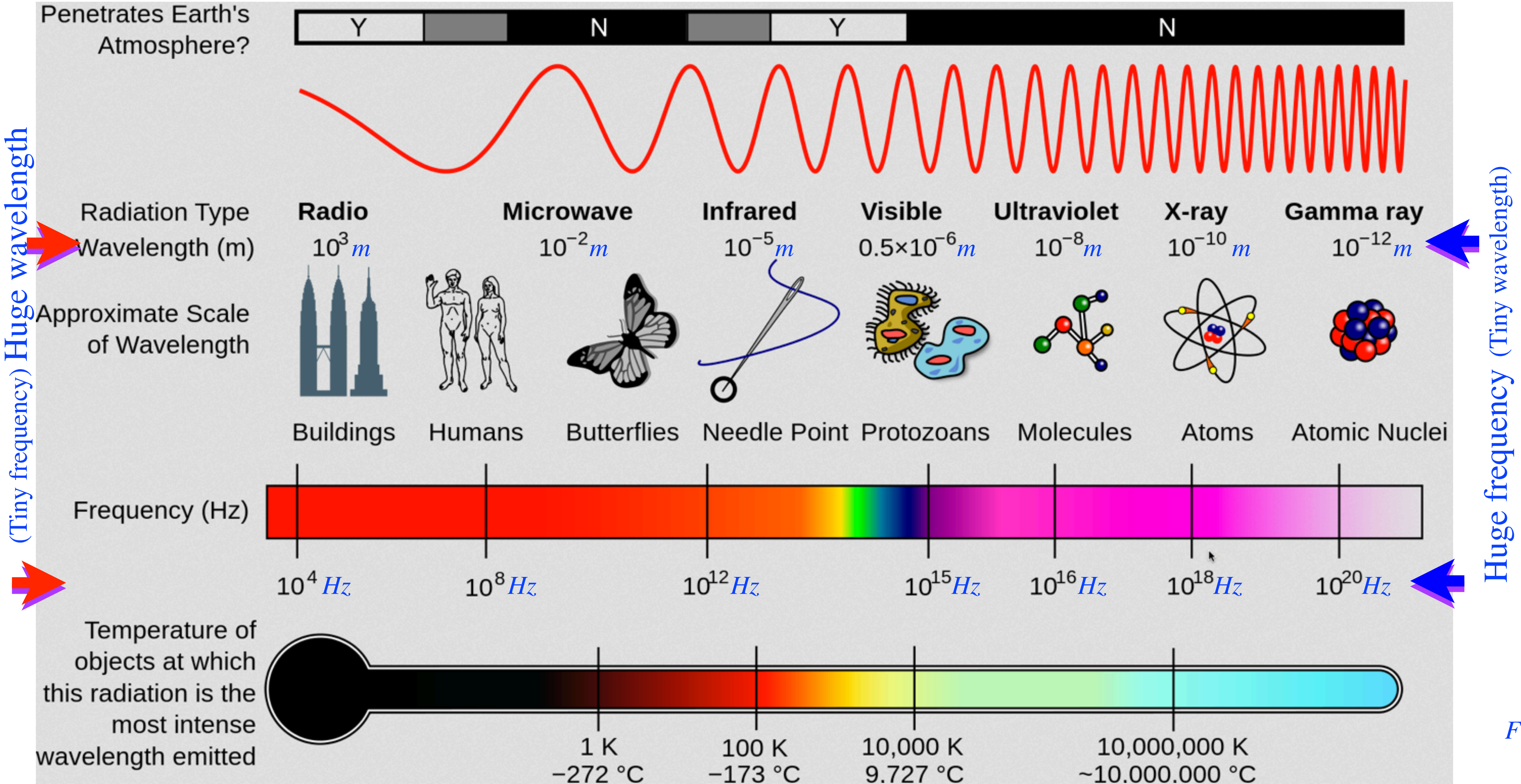

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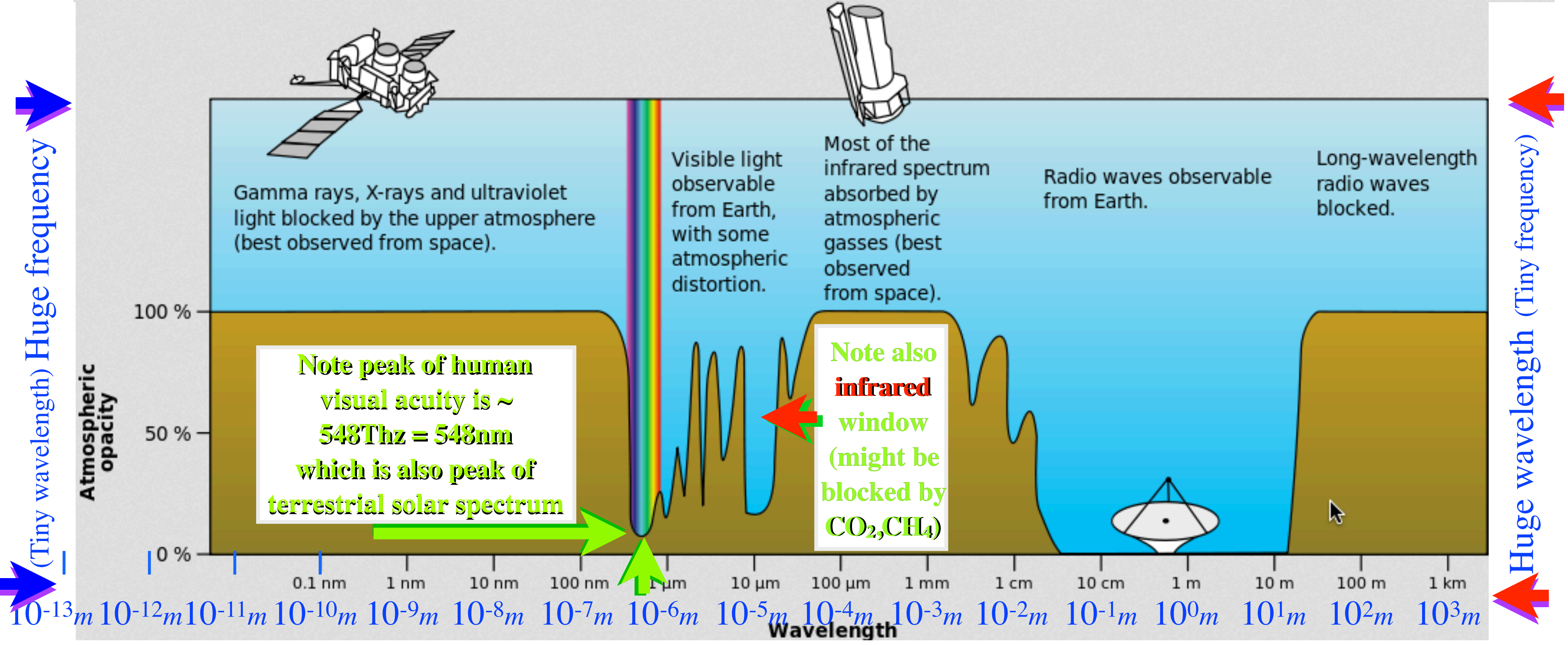

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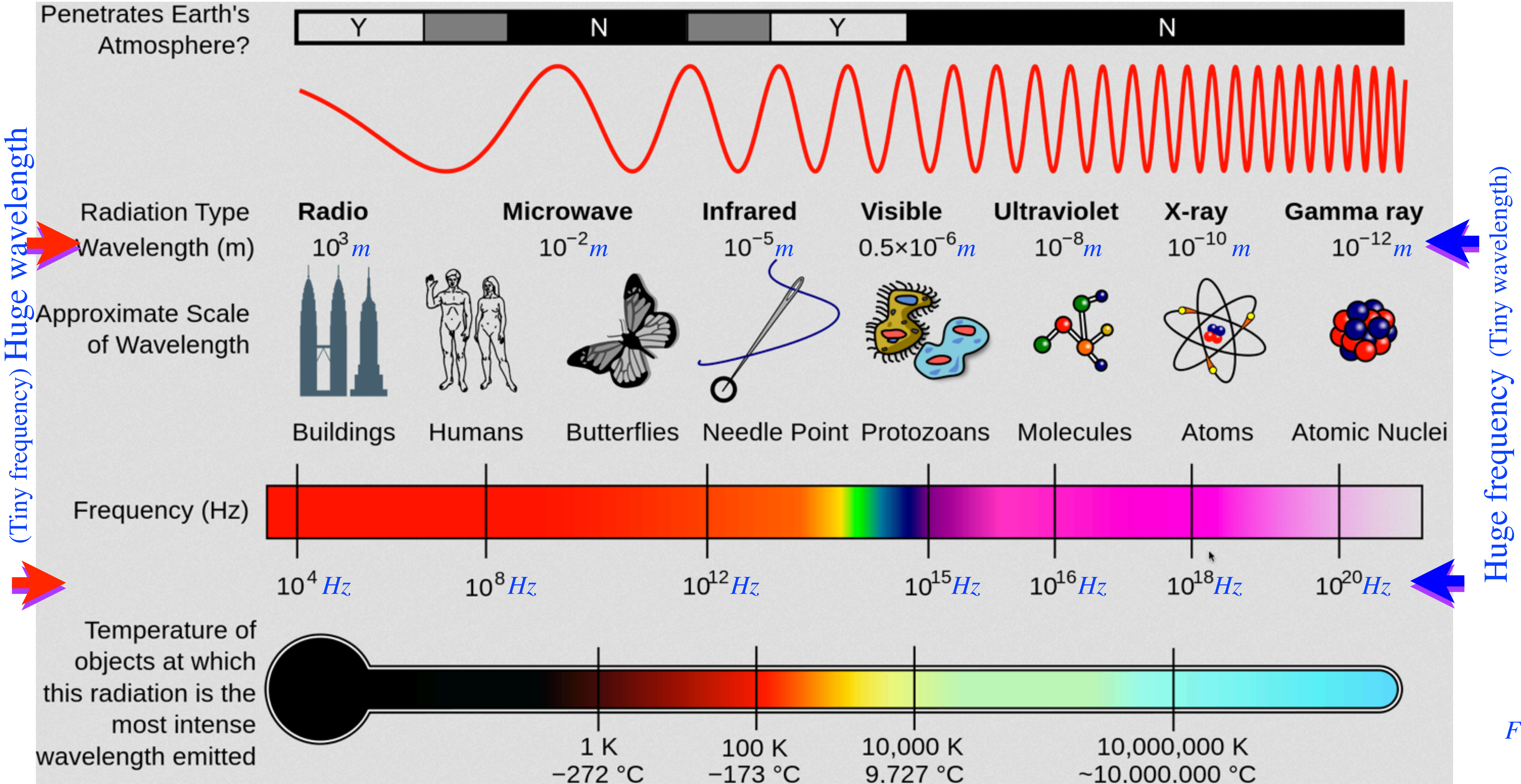

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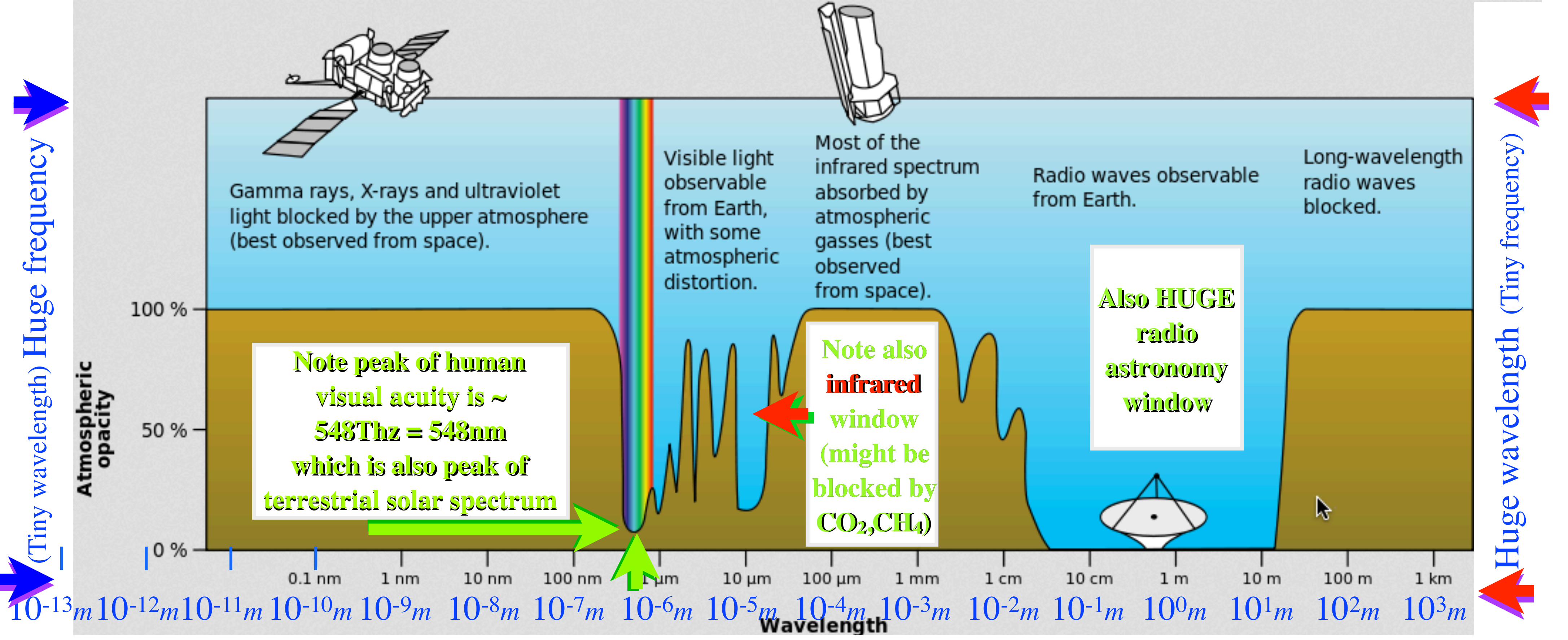

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Also HUGE radio astronomy window

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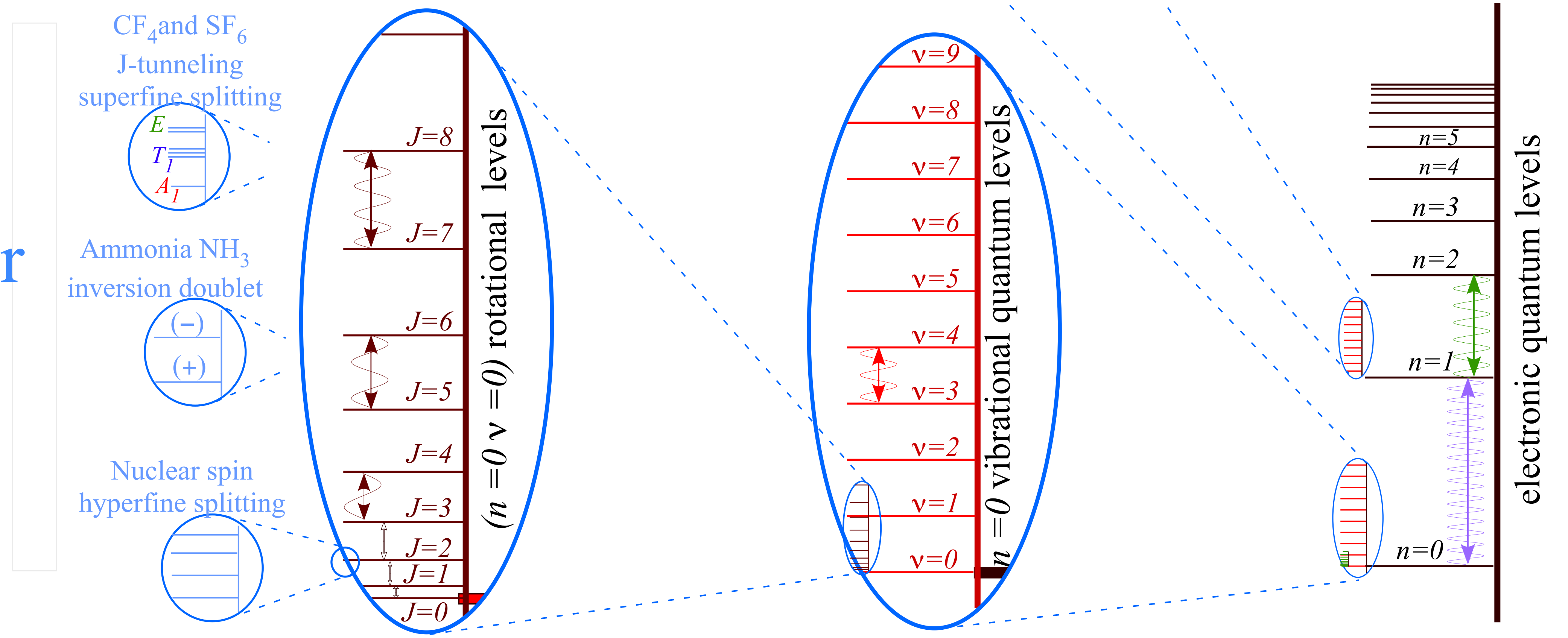
Simple Molecular Spectra Models



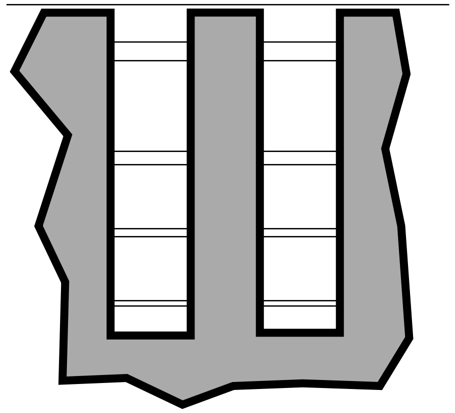
fine structure

rotational spectra

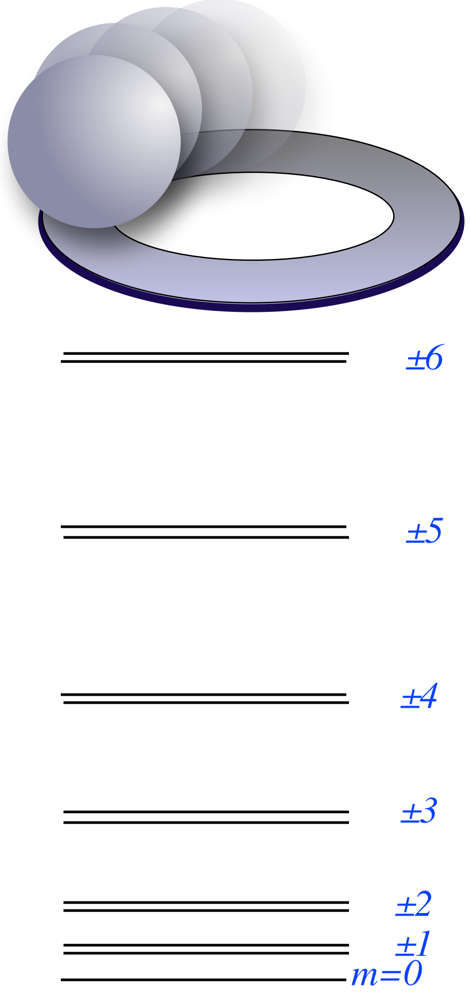
vibrational spectra

electronic spectra

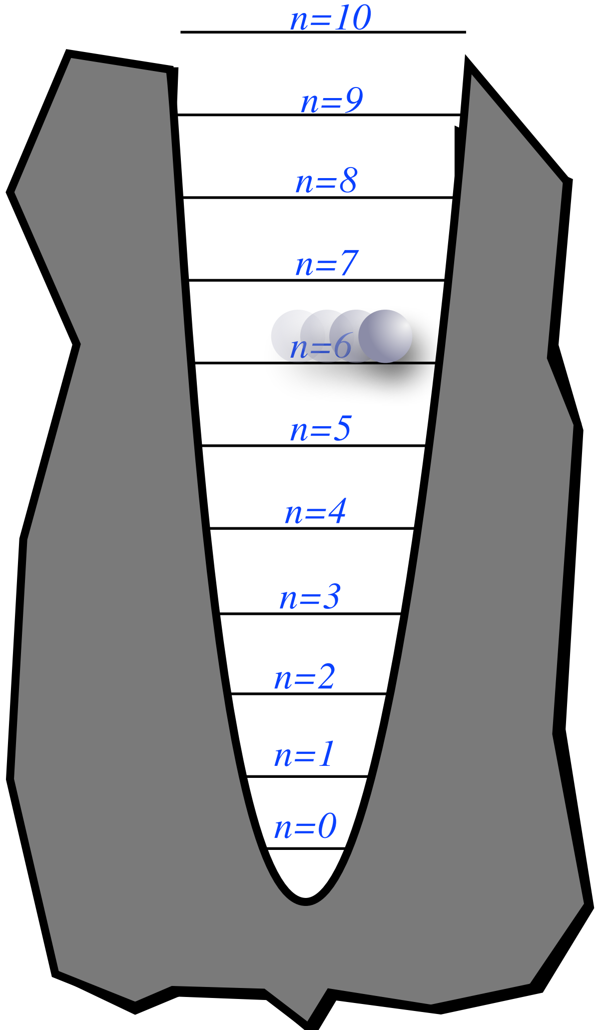
2-well tunneling



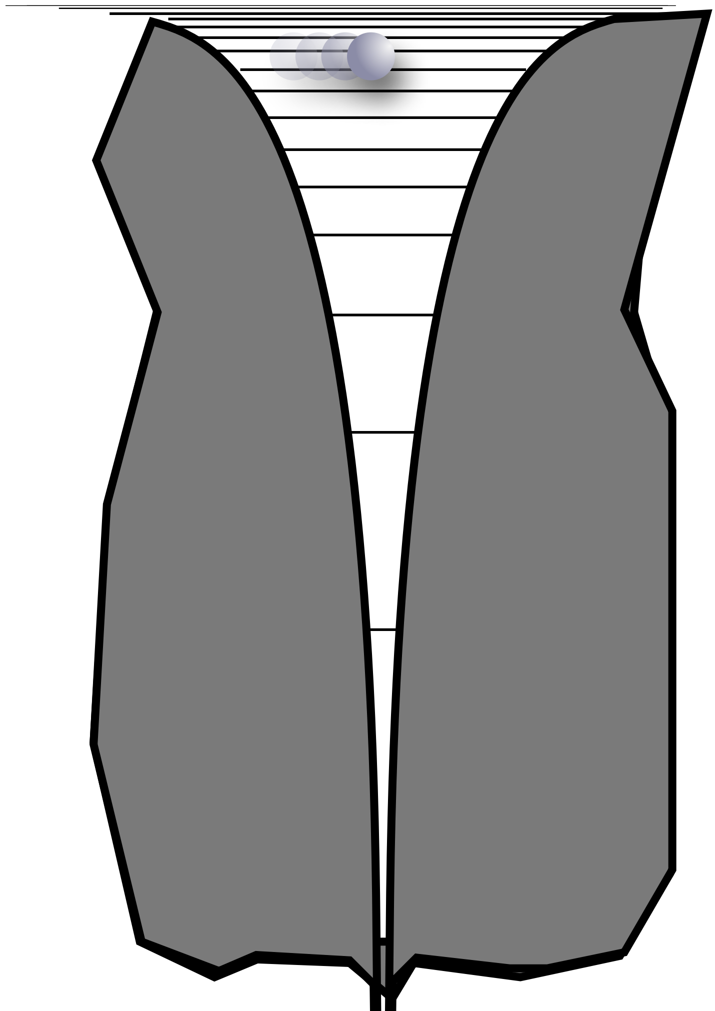
Bohr mass-on-ring



1D harmonic oscillator

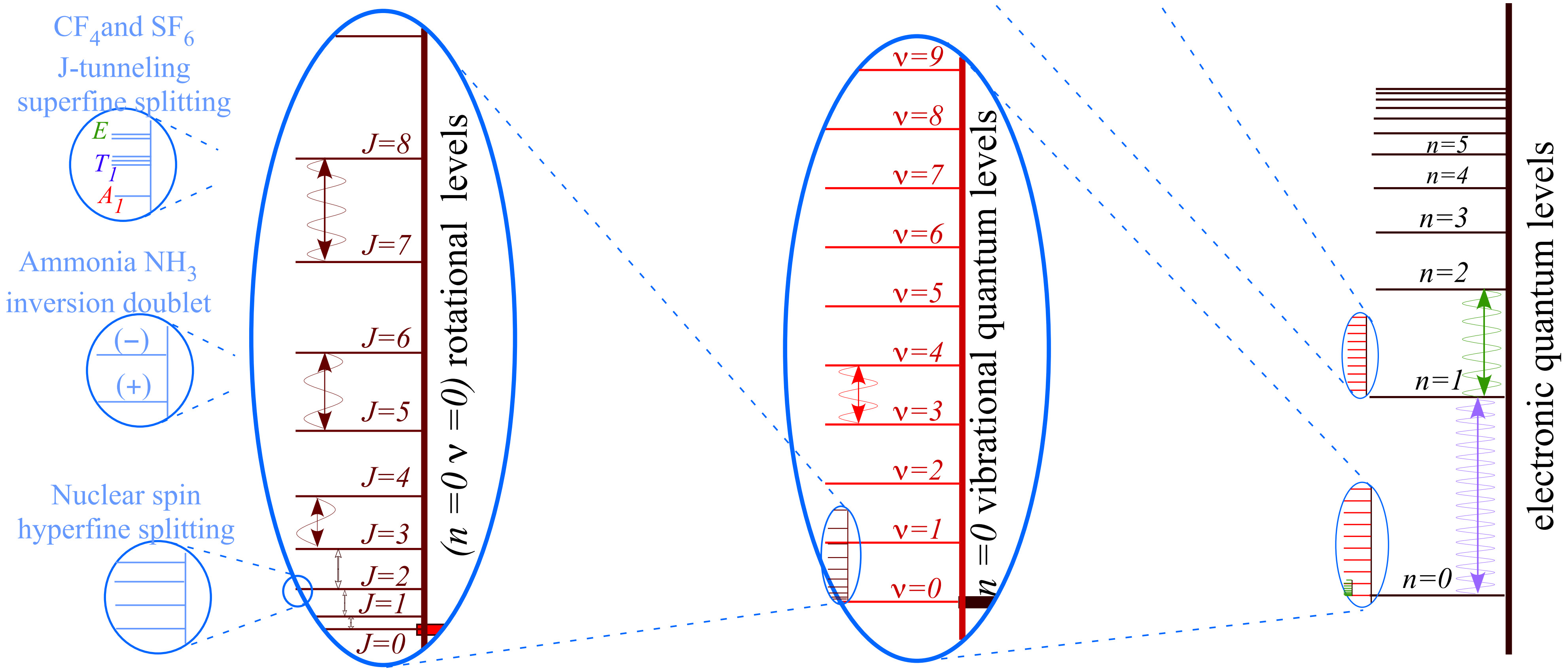


Coulomb PE models



More Advanced Molecular Spectra Models

(Use symmetry group theory)



fine structure

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electronic spectra

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Bohr mass-on-a-ring

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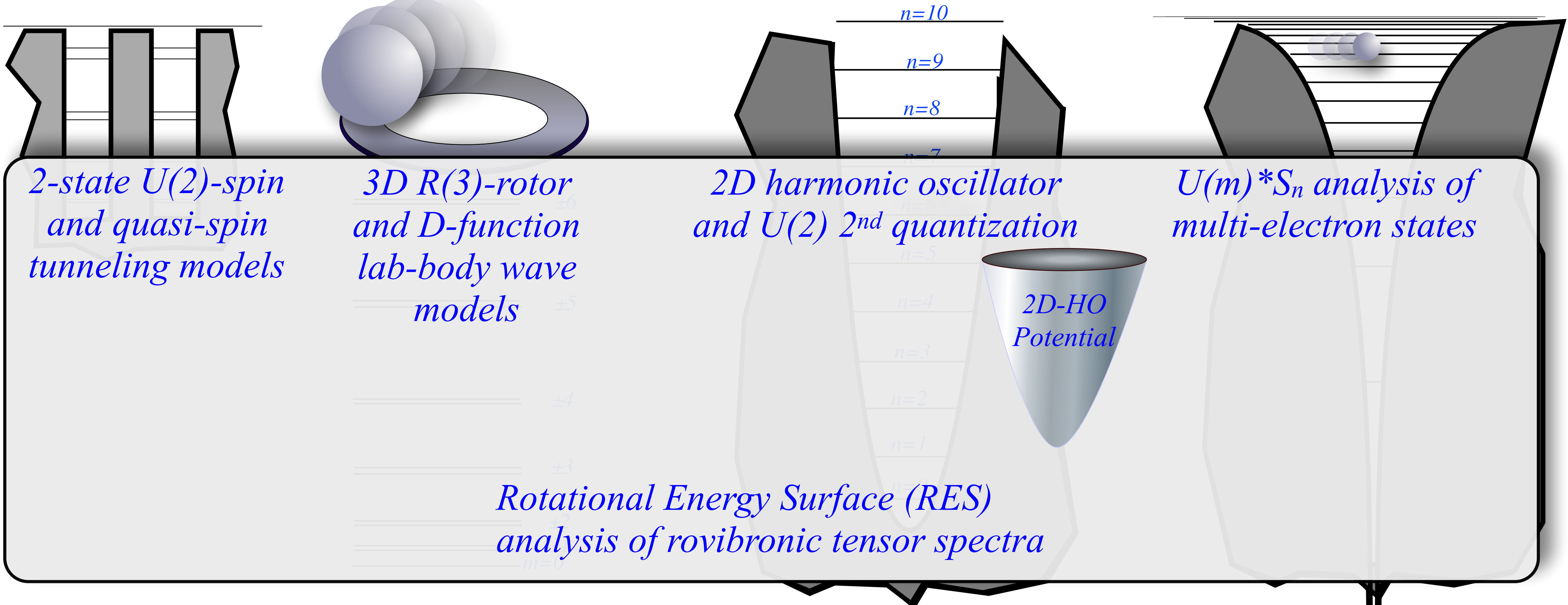

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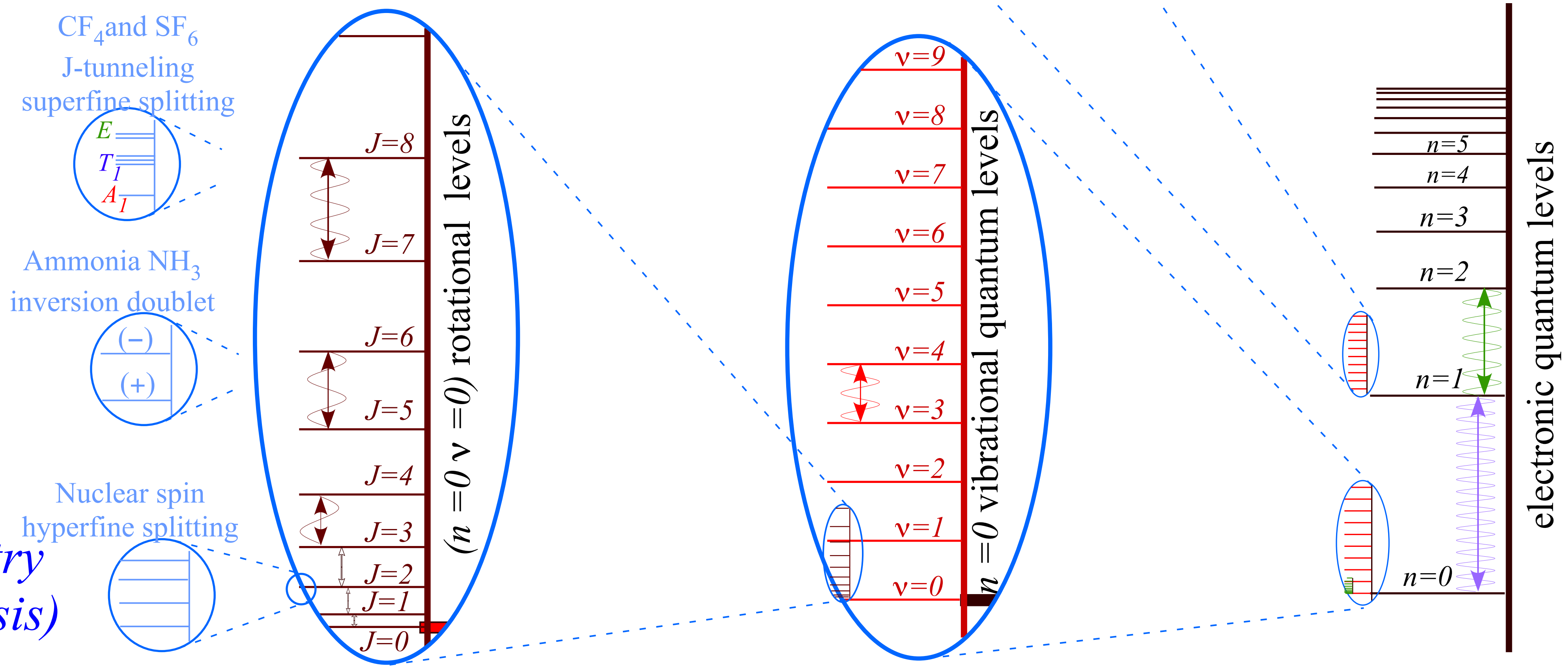
*U(m)*S$_n$ analysis of multi-electron states*

Rotational Energy Surface (RES) analysis of rovibronic tensor spectra

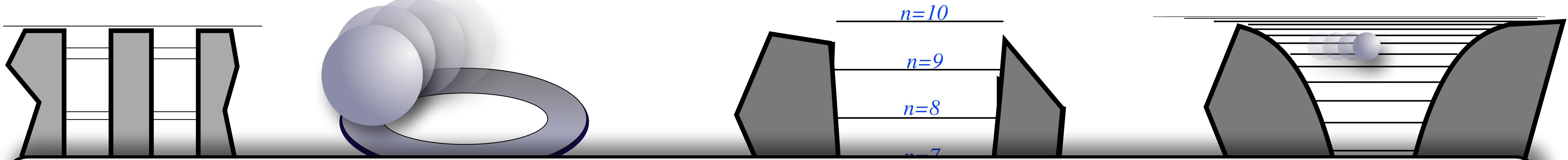
More Advanced Molecular Spectra Models

(Involve symmetry algebraic analysis)



fine structure | rotational spectra | vibrational spectra | electronic spectra

2-well tunneling | *Bohr mass-on-a-ring* | *1D harmonic oscillator* | *Coulomb PE models*



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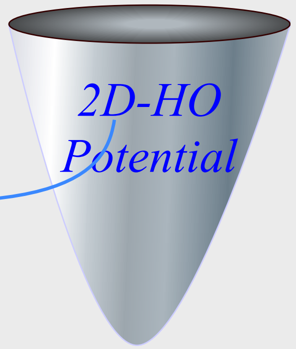
U(m)S_n analysis of multi-electron states*

(closely connected)



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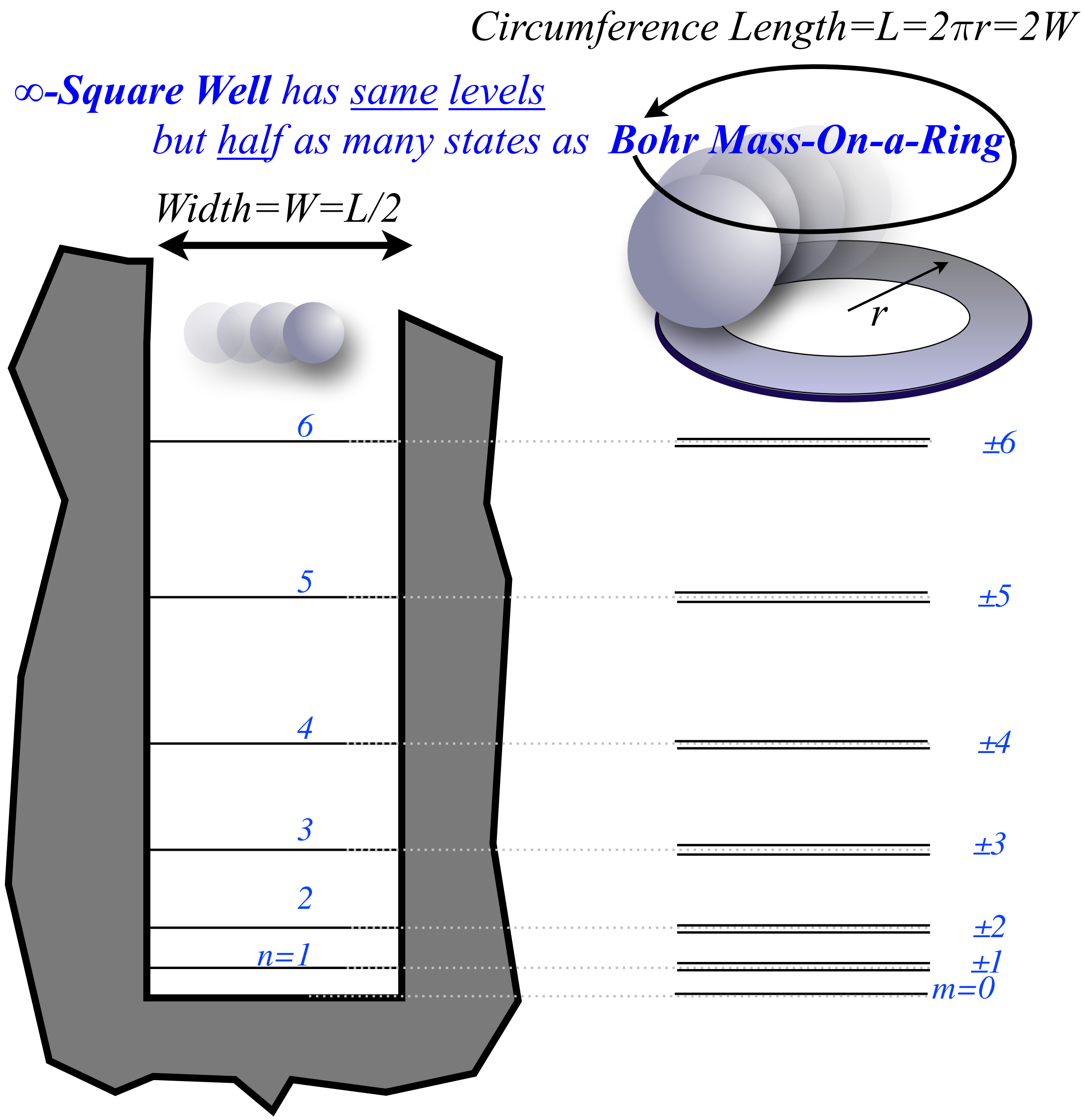

Circumference Length=L=2πr=2W

*∞-**Square Well** has same levels*
*but half as many states as **Bohr Mass-On-a-Ring***

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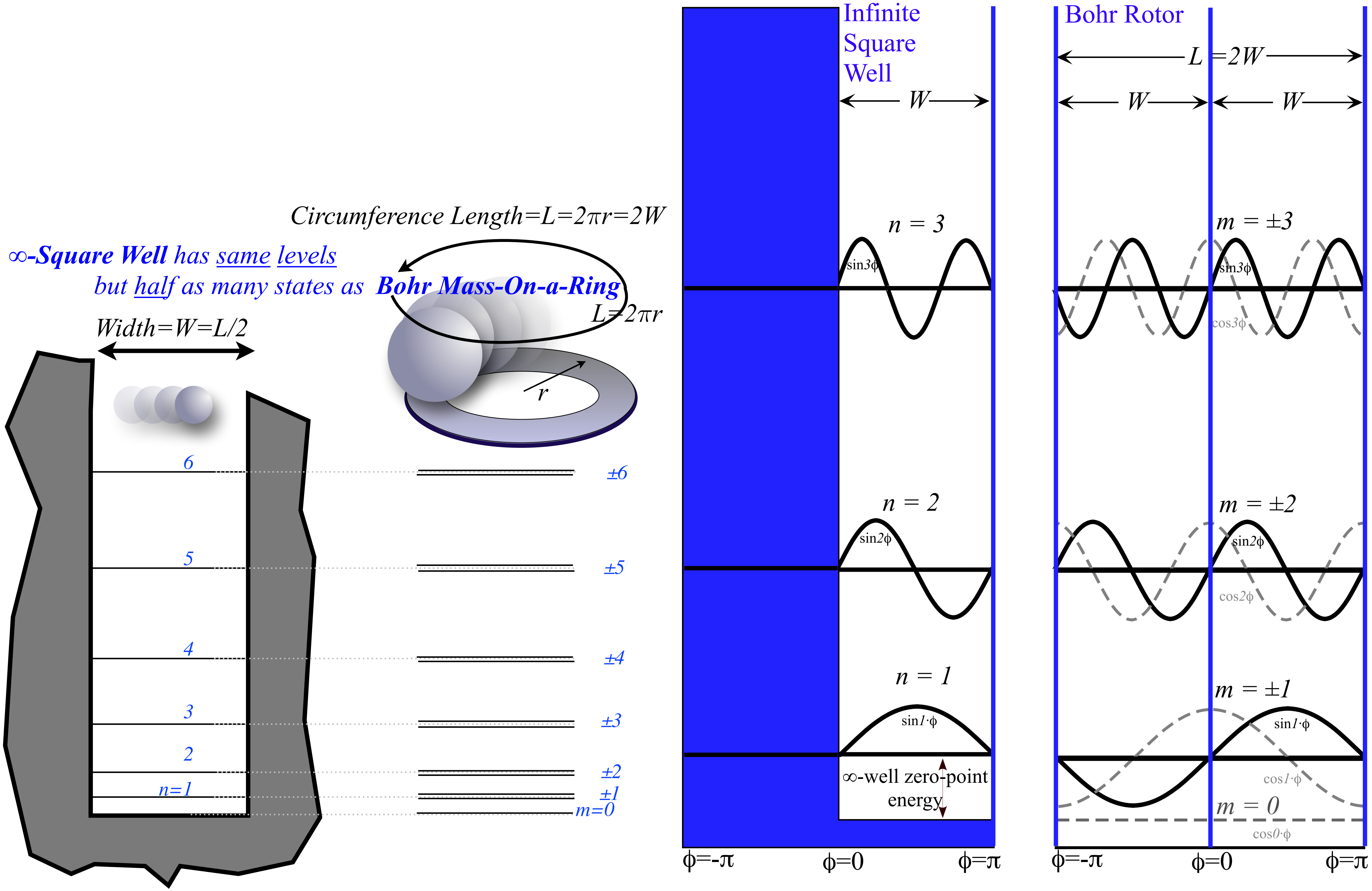

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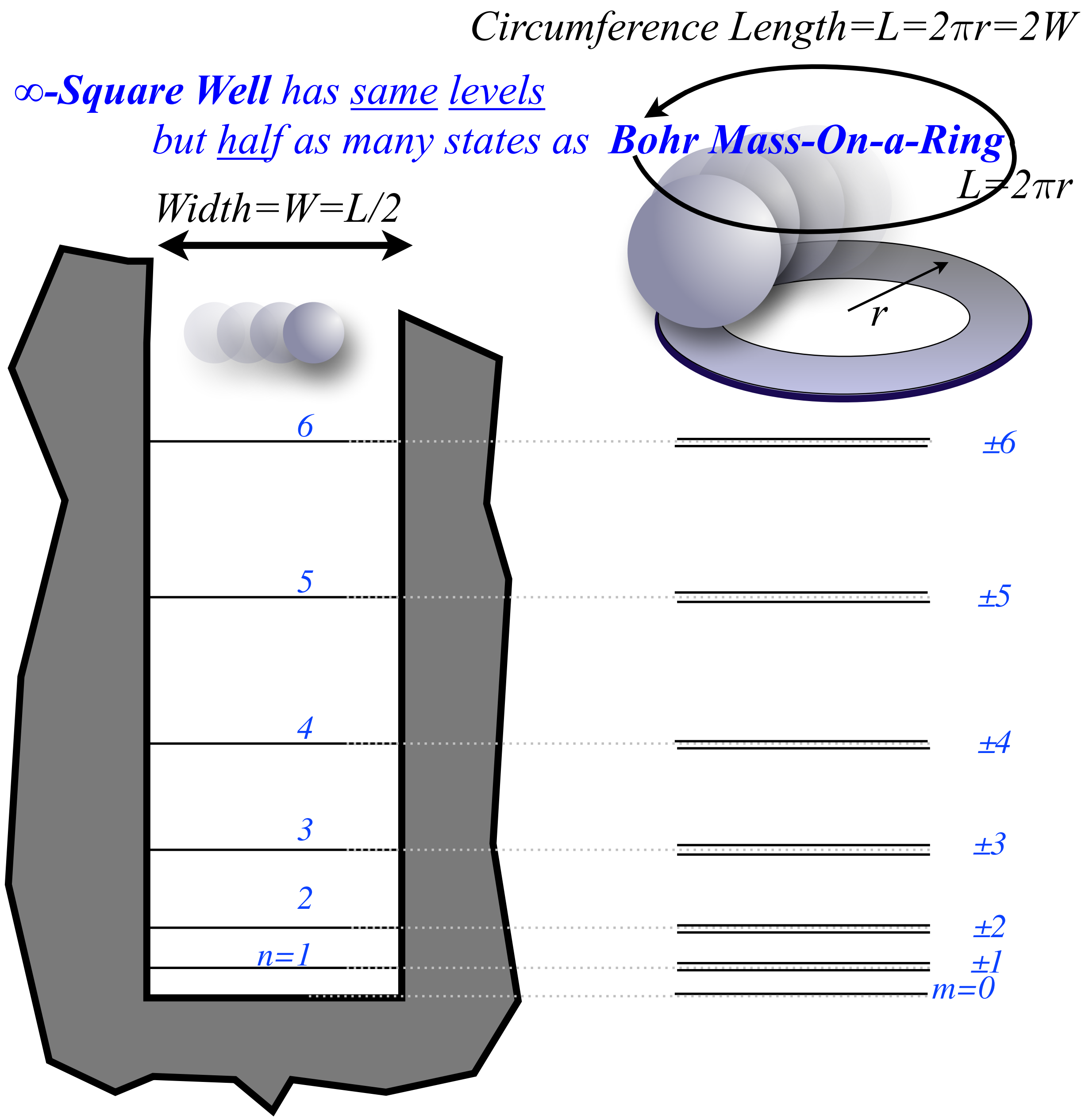
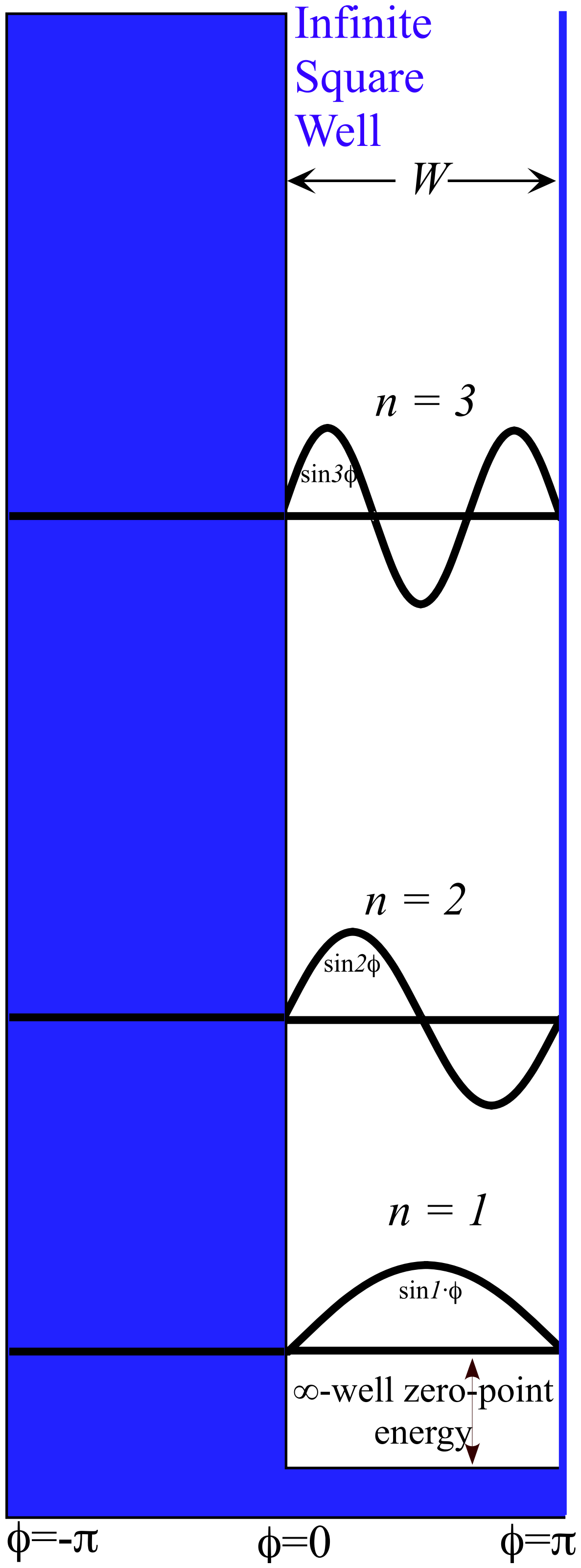
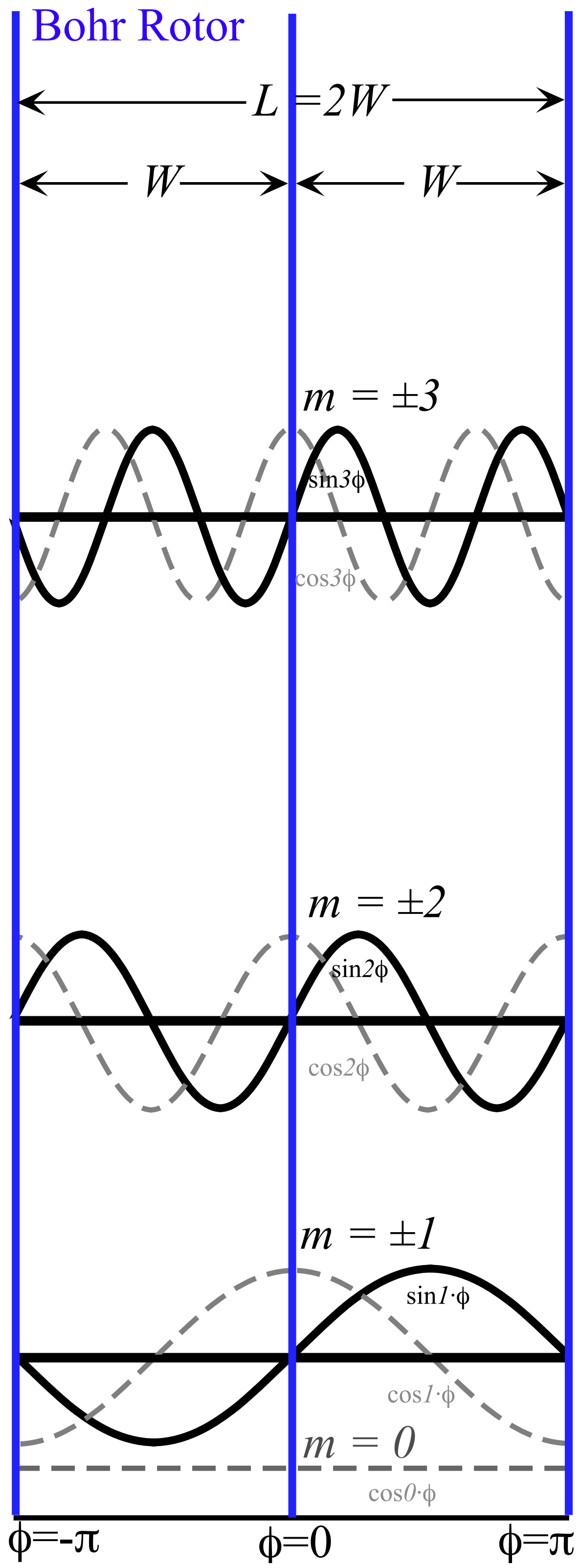


***∞-Square Well** has only sine standing waves* $\psi_n = A\sin n\phi$

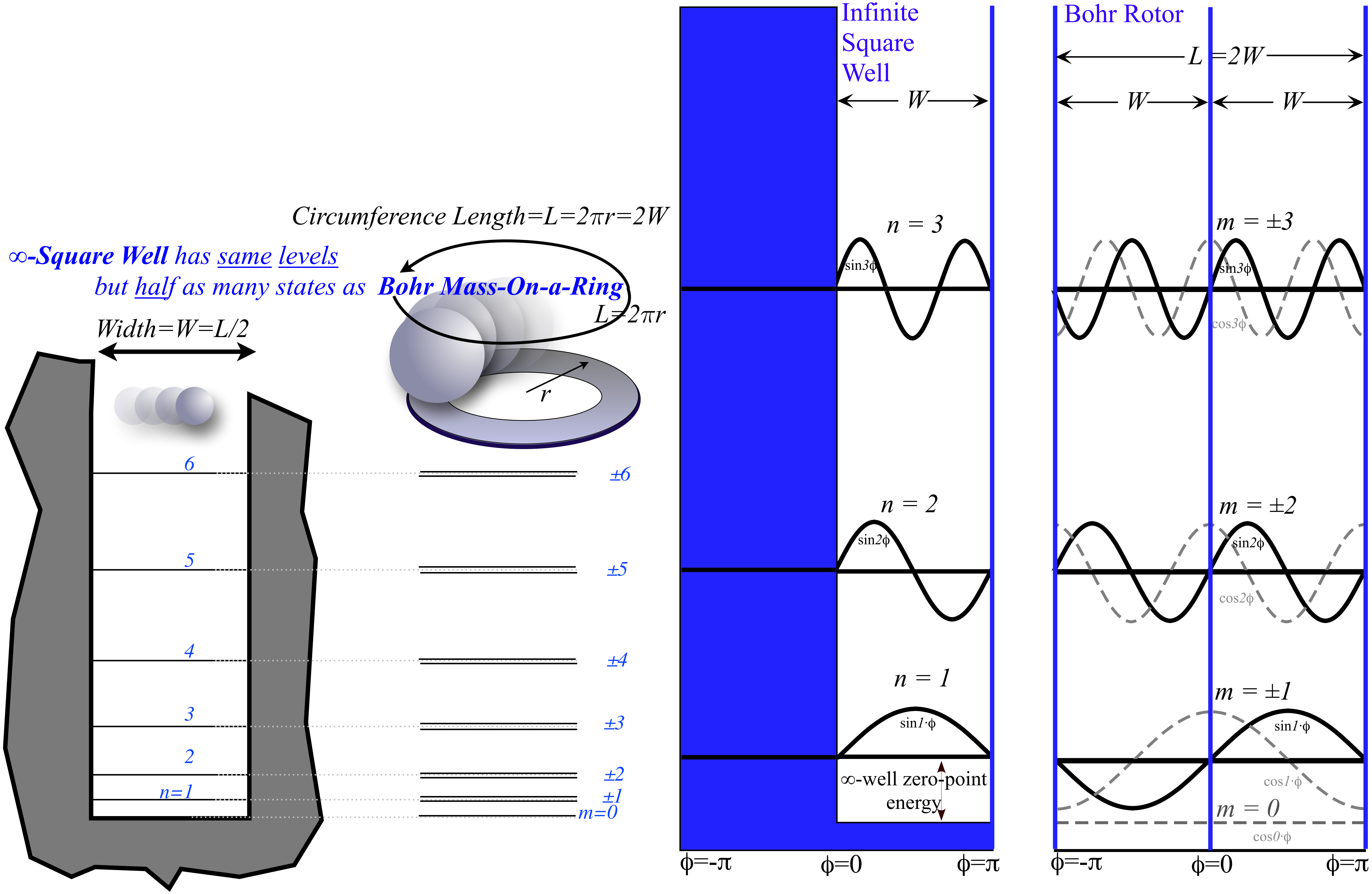




Bohr Mass-On-a-Ring *(model of rotation) and related* ***∞-Square Well*** *(model of quantum dots)*

∞-Square Well *has only* *<u>sine</u>* *<u>standing</u>* *waves* $\psi_n = A\sin n\phi$

Bohr Ring *has sine and cosine* *<u>standing</u>* *and* $e^{\pm im\phi}$ *<u>moving</u>* *waves* $\psi_{\pm m} = A(\cos m\phi \pm i\sin m\phi) = Ae^{\pm im\phi}$



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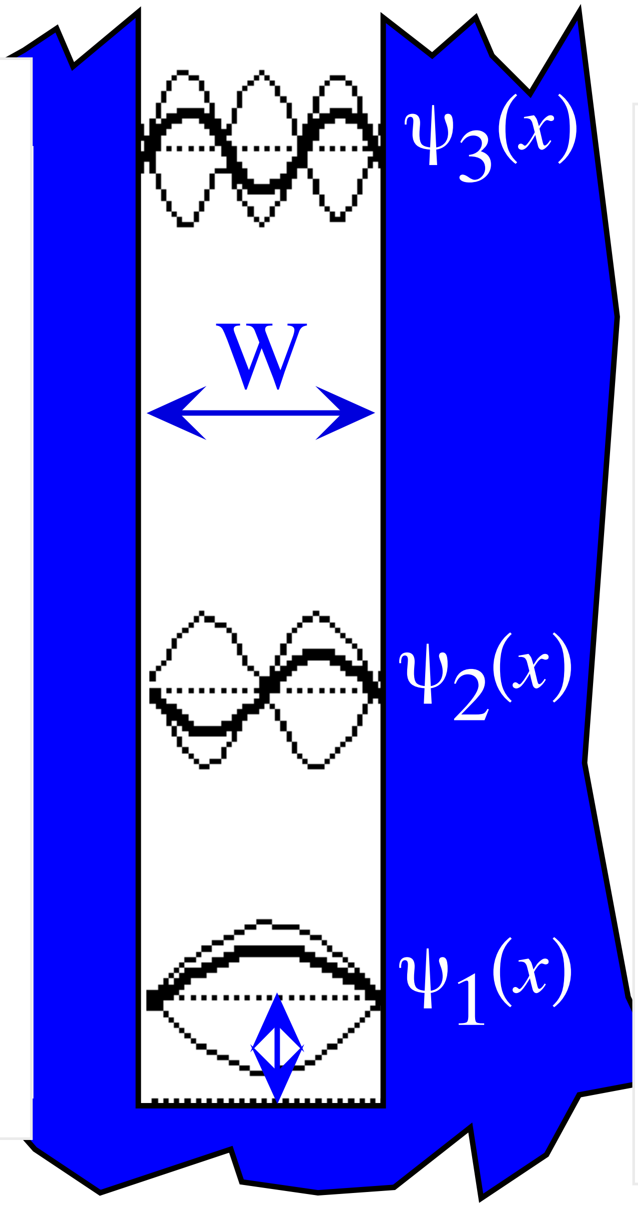
$$= A\sin\left(\frac{n\pi x}{W}\right) \quad (n=1,2,3,\ldots\infty)$$



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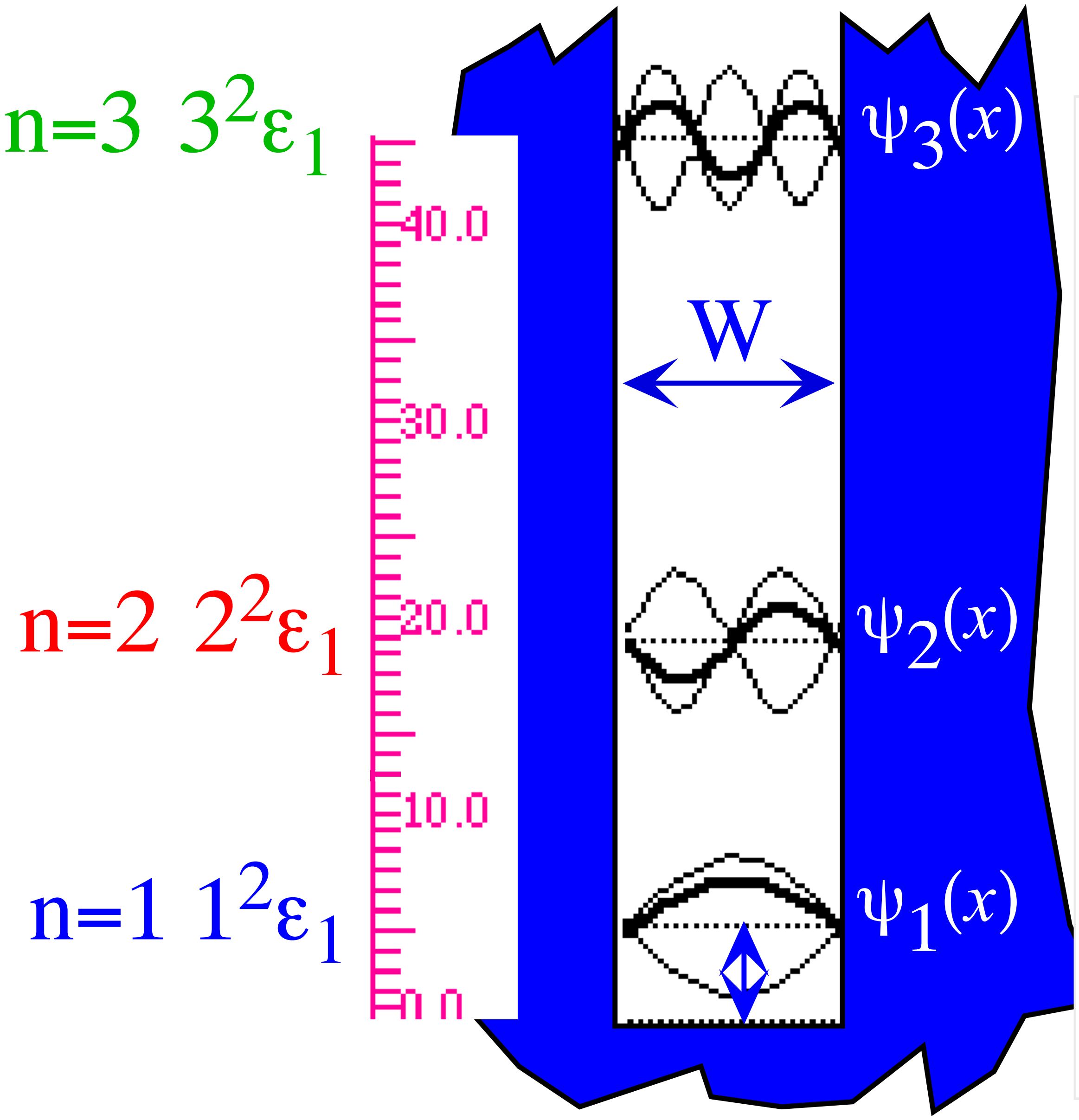
Gives energy levels:

$$\varepsilon_n=\frac{\hbar^2}{2M}k^2=\frac{\hbar^2n^2\pi^2}{2MW^2}=\left(1^2,\ 2^2,\ 3^2,\ldots\text{or } n^2\right)\frac{h^2}{8MW^2}$$



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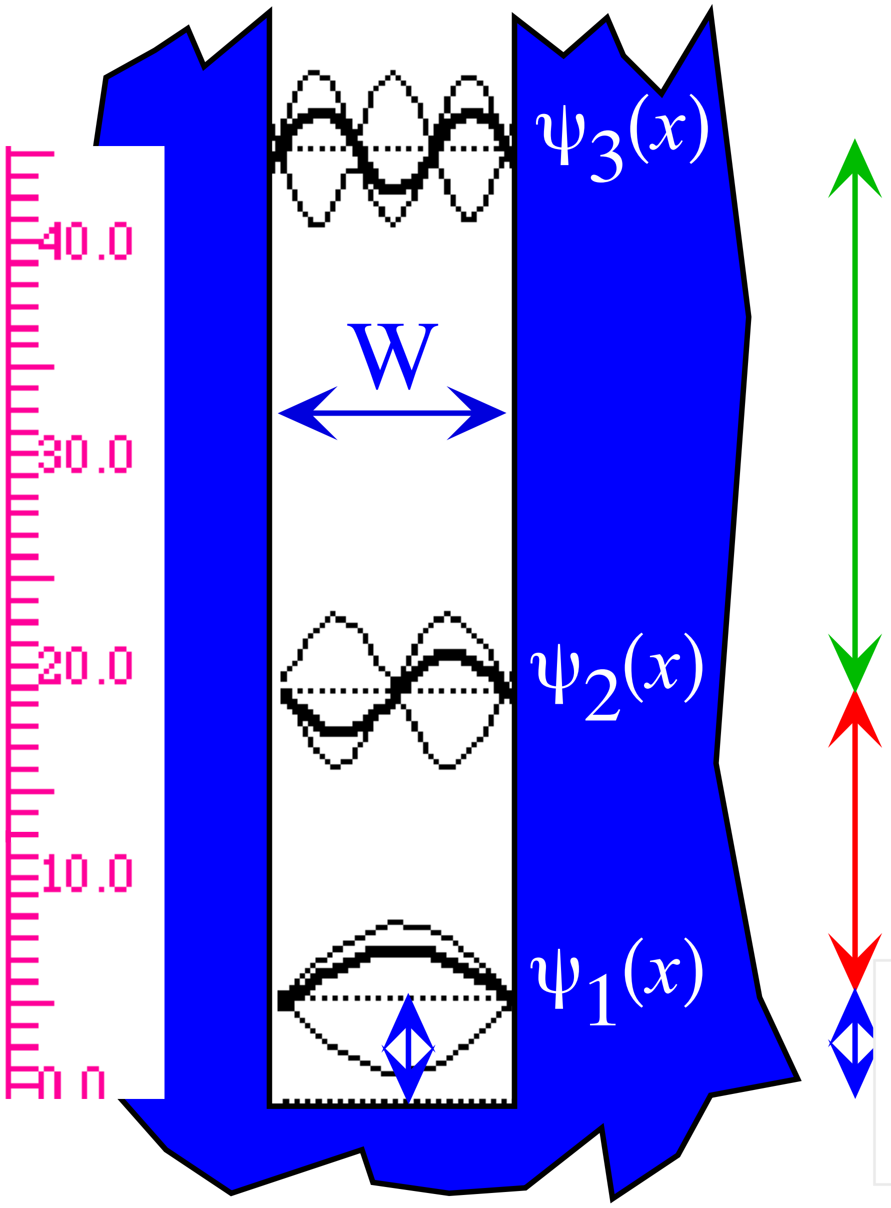

n=3 $3^2\varepsilon_1$

n=2 $2^2\varepsilon_1$

n=1 $1^2\varepsilon_1$

2nd transition

energy $5\varepsilon_1$

1st transition

("beat") energy $3\varepsilon_1$

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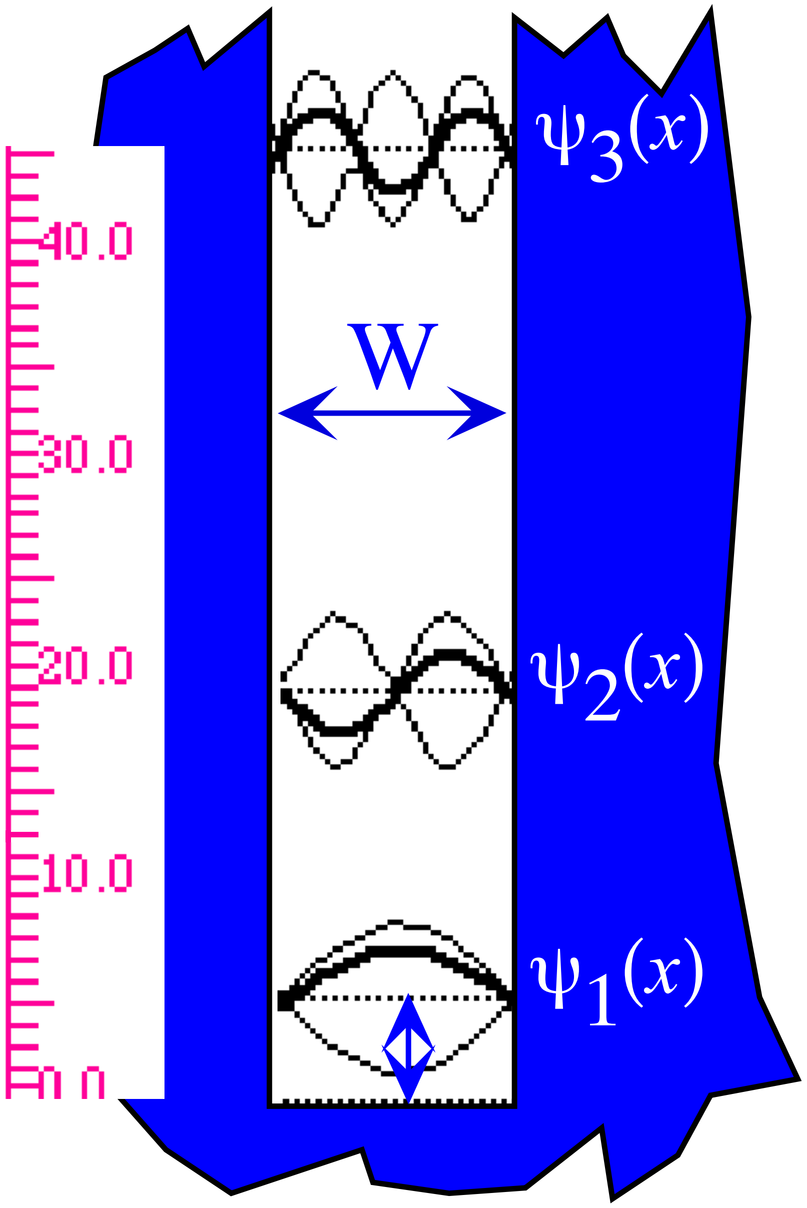
Set $W = \pi r$ *to get rotor energy:*



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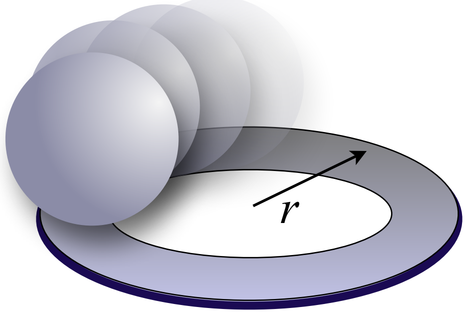
n=1 $1^2\varepsilon_1$

Zero-point energy $\varepsilon_1 = \frac{h^2}{8MW^2}$

(For ∞-Square well)



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$$= \frac{h^2}{8M\pi^2 r^2}n^2 = \frac{\hbar^2}{2Mr^2}n^2 = \frac{\hbar^2}{2I}n^2$$

rotor energy
for: $W = \pi r$

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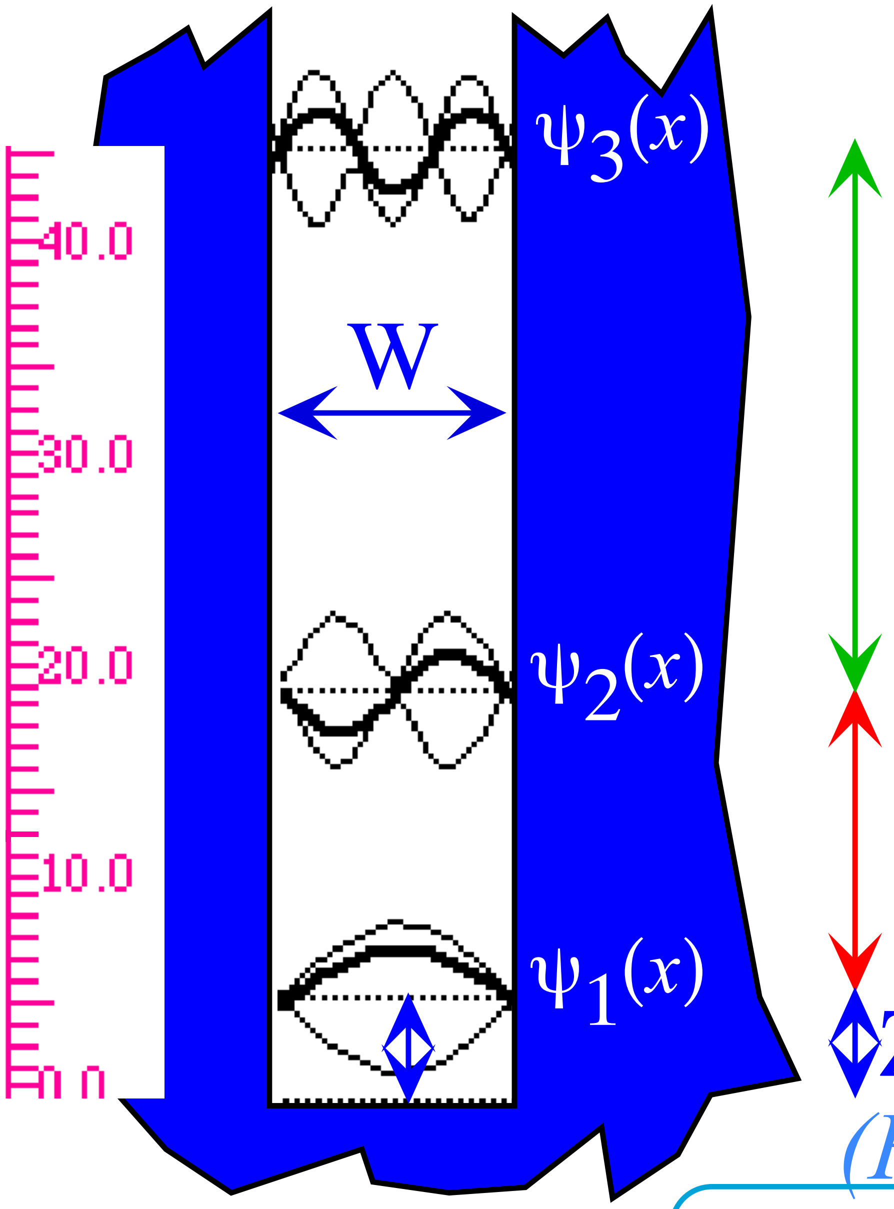

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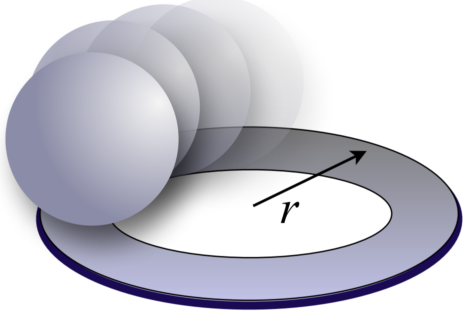

rotor energy B-constant: $= \frac{\hbar^2}{2I} = B$

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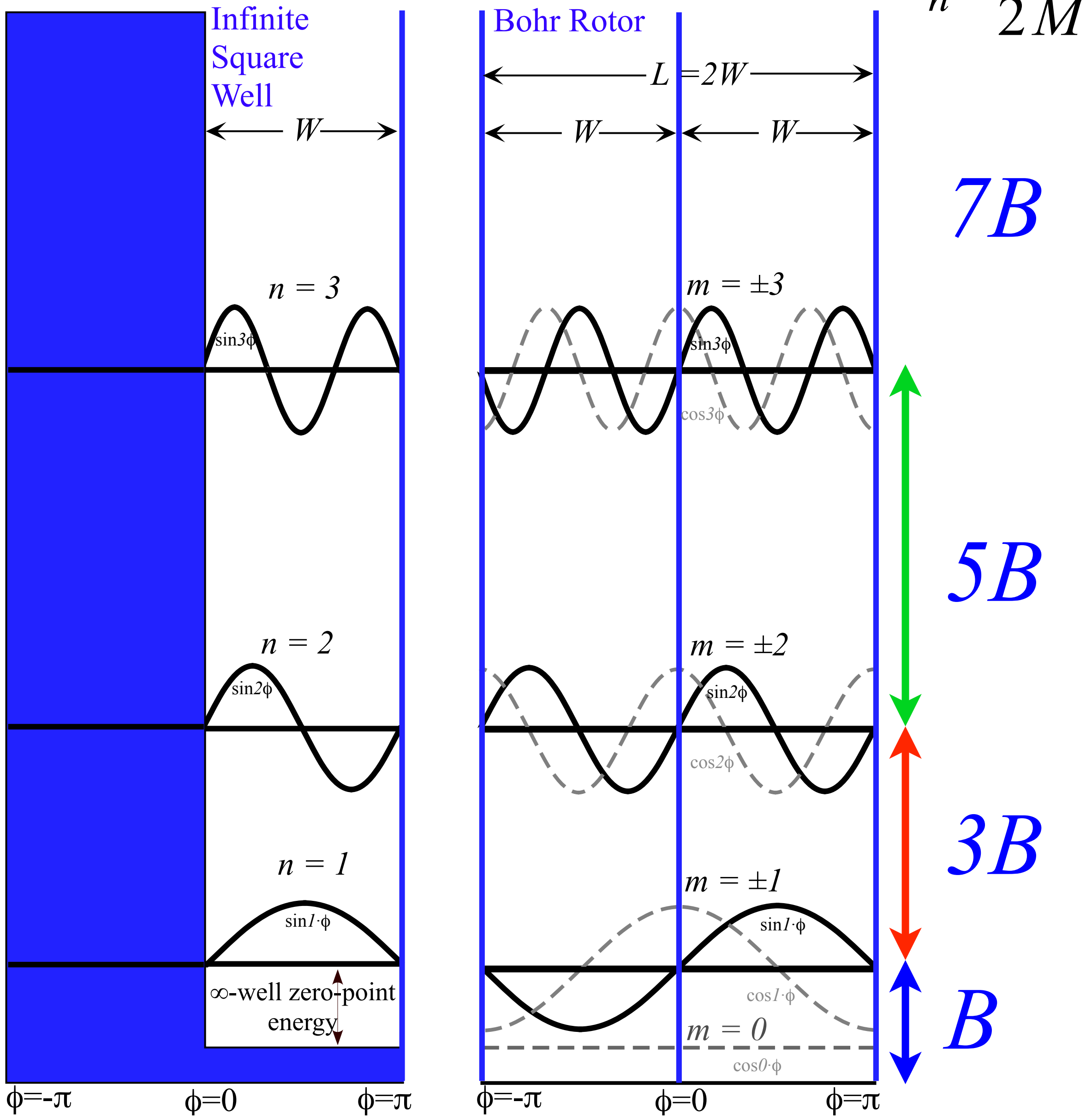
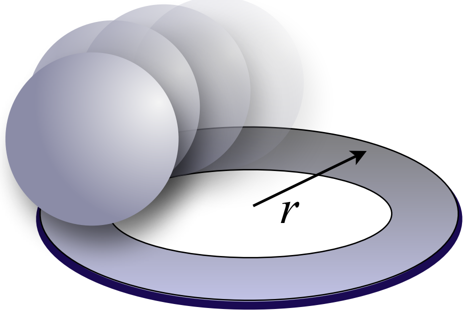
rotor energy for: $W=\pi r$





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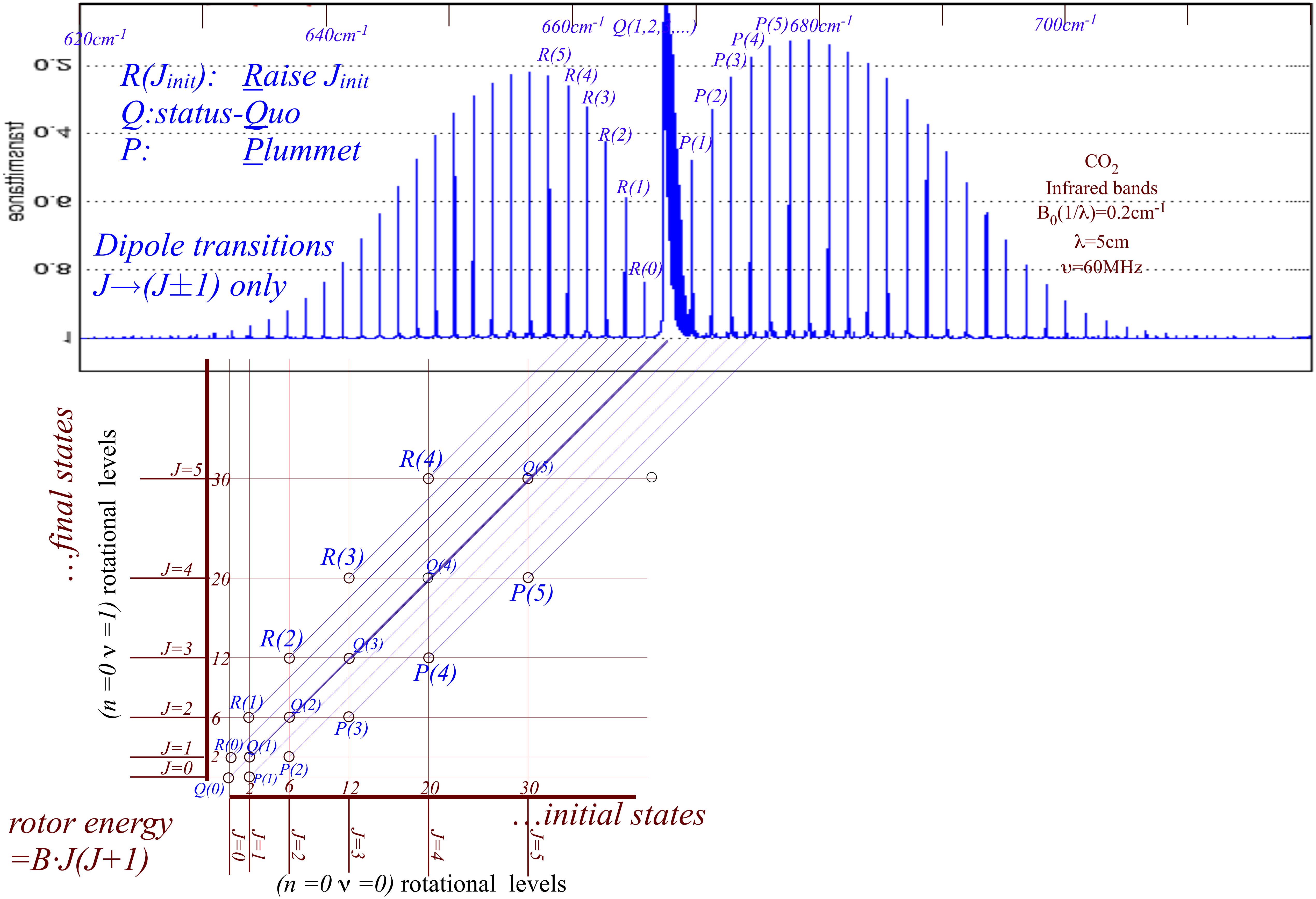
Example of CO_2 rotational (υ=0)⇔(υ=1)bands



R(J_{init}): Raise J_{init}

Q:status-Quo

P: Plummet

Dipole transitions

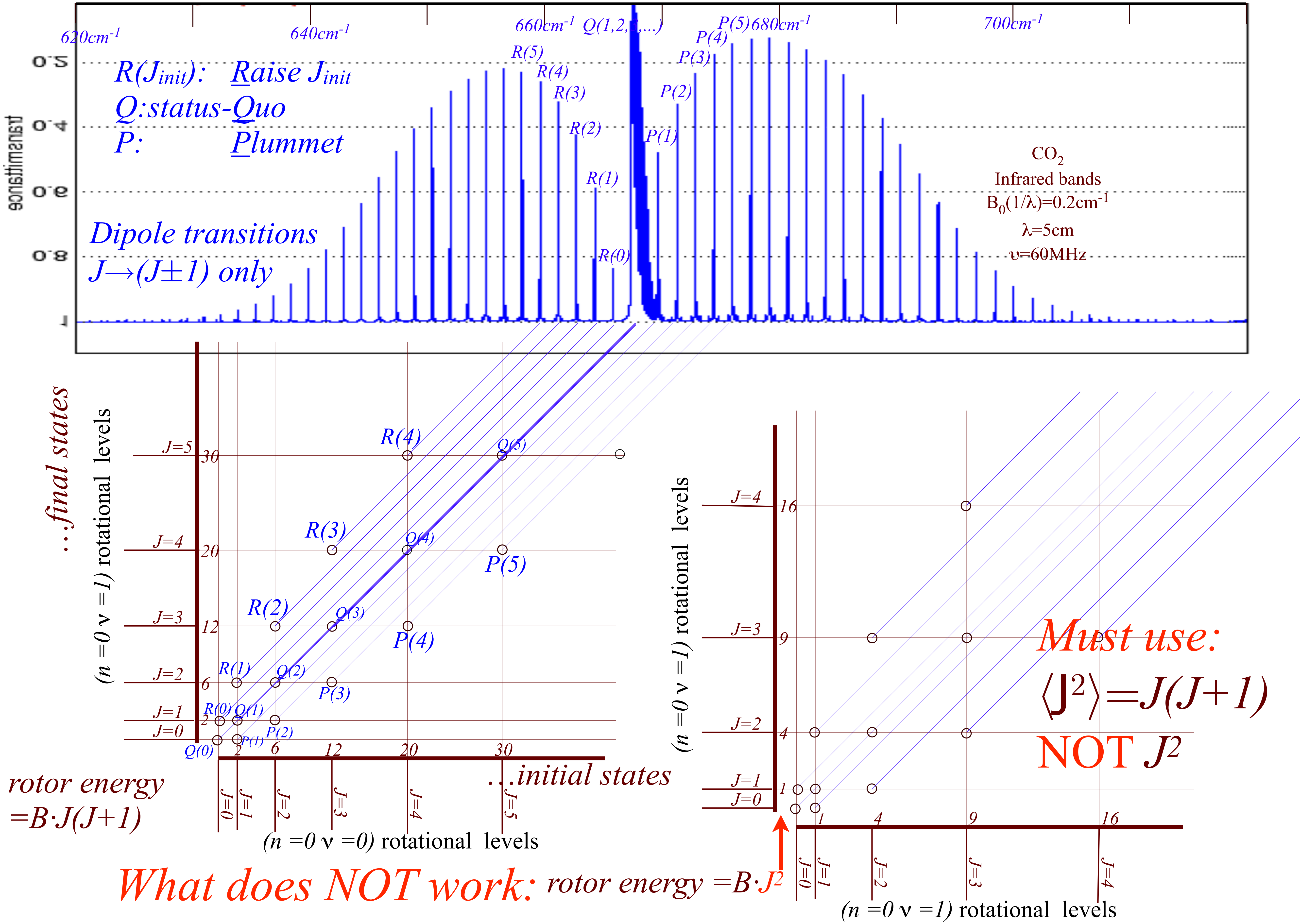
J→(J±1) only

rotor energy

=B·J(J+1)

B=(½)/rotor inertia (here assumed the same initially and finally)

Example of CO_2 rotational $(\upsilon=0)\Leftrightarrow(\upsilon=1)$ bands



$R(J_{init})$: <u>R</u>aise J_{init}

Q: status-<u>Quo</u>

P: <u>P</u>lummet

Dipole transitions

$J\rightarrow(J\pm1)$ only

CO_2

Infrared bands

$B_0(1/\lambda)=0.2\text{cm}^{-1}$

λ=5cm

υ=60MHz

...final states

...initial states

rotor energy $=B\cdot J(J+1)$

Must use:

$\langle J^2\rangle=J(J+1)$

NOT J^2

What does NOT work: rotor energy $=B\cdot J^2$

Spectral hierarchy of Born-Openheimer approximations to *AMOP*

Sketch of modern molecular spectroscopy

Example of16µm spectra of CF_4 1996 AMOP Handbook
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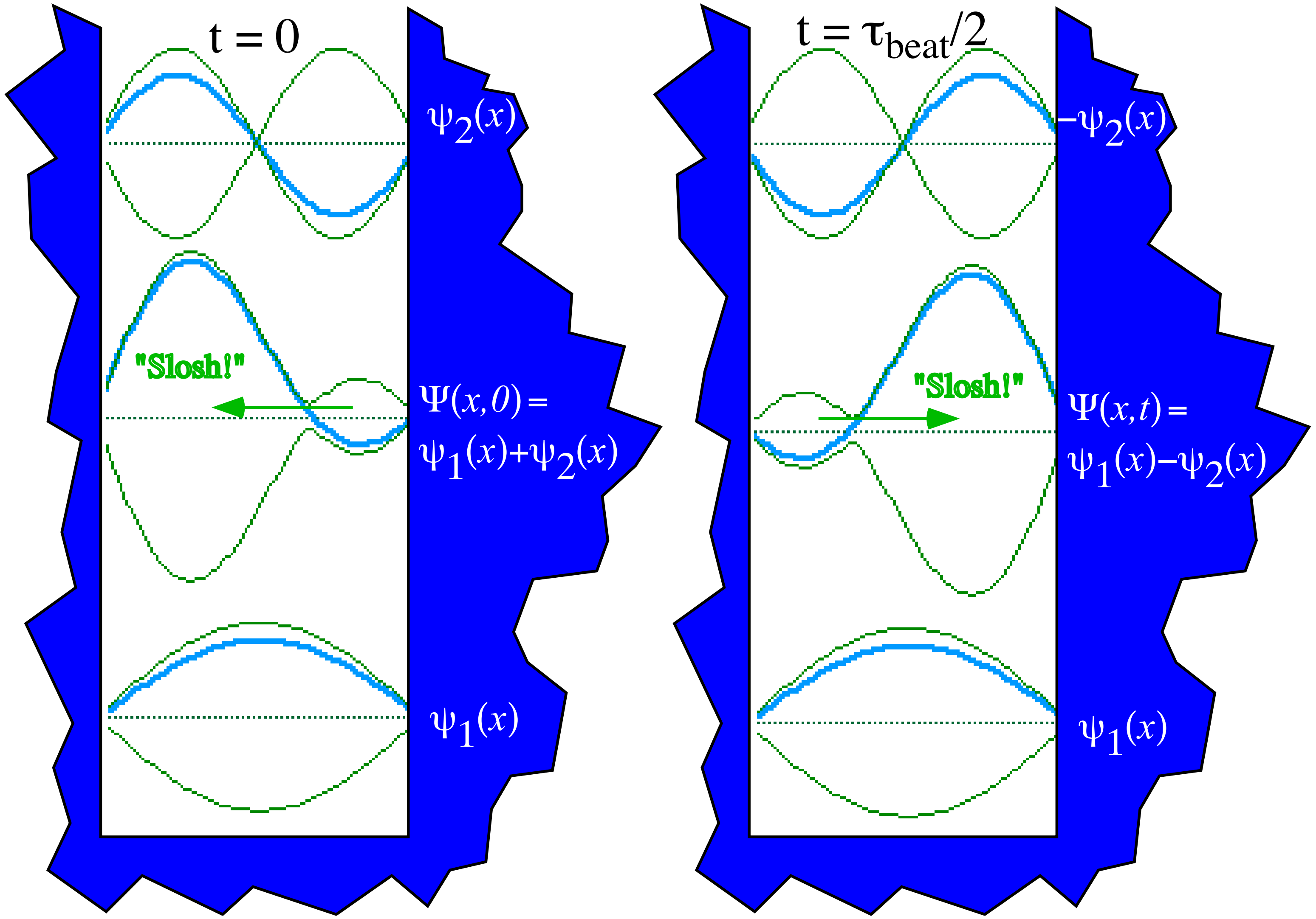
How and what makes that "dipole" spectra?

...in this case a non-quantized (½and½) state



"Sloshing" charge acts like dipole antenna broadcasting linear polarized radiation*

Fig. 12.1.2 Exercise in prison. Infinite square well eigensolution combination "sloshes" back and forth.

**Or receives (Depending on relative phase)*

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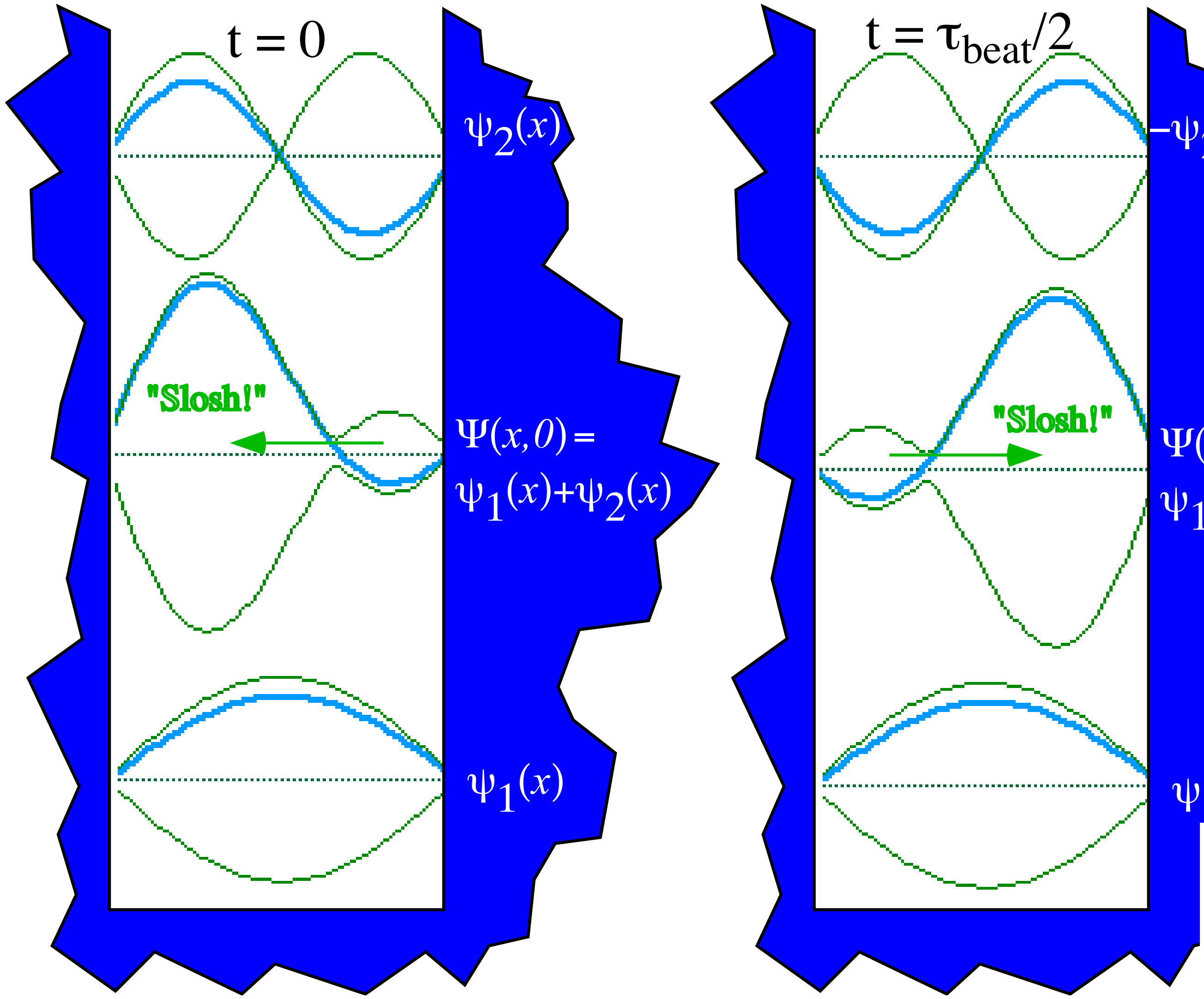
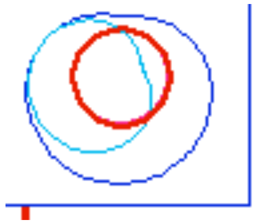
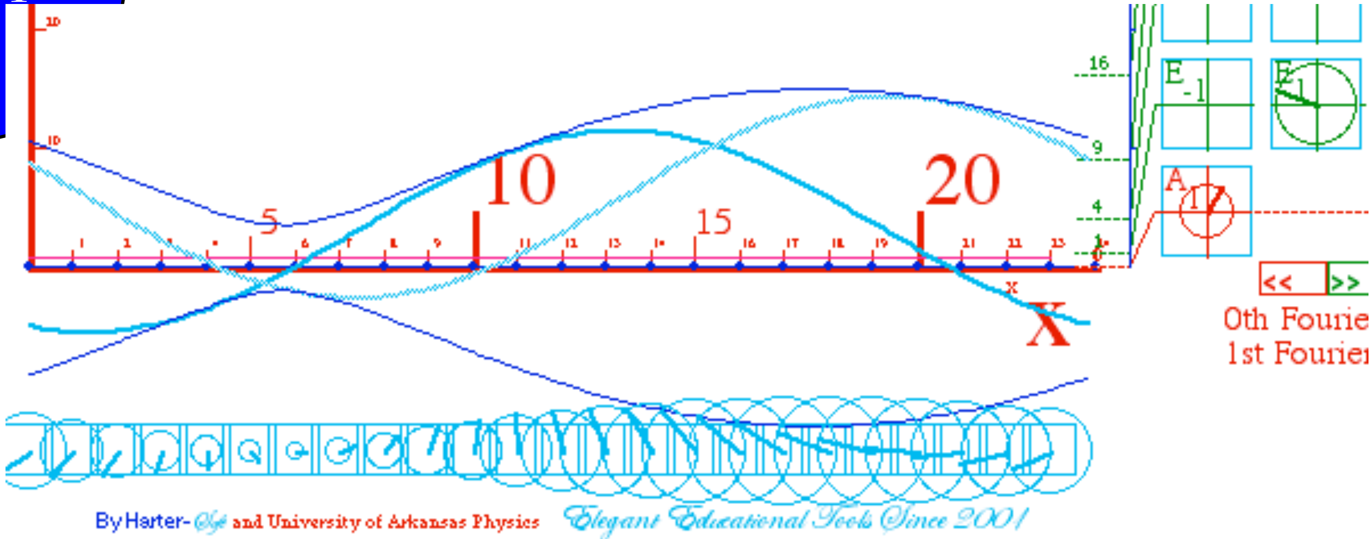


*Rotating charge broadcasts**
circularly polarized radiation





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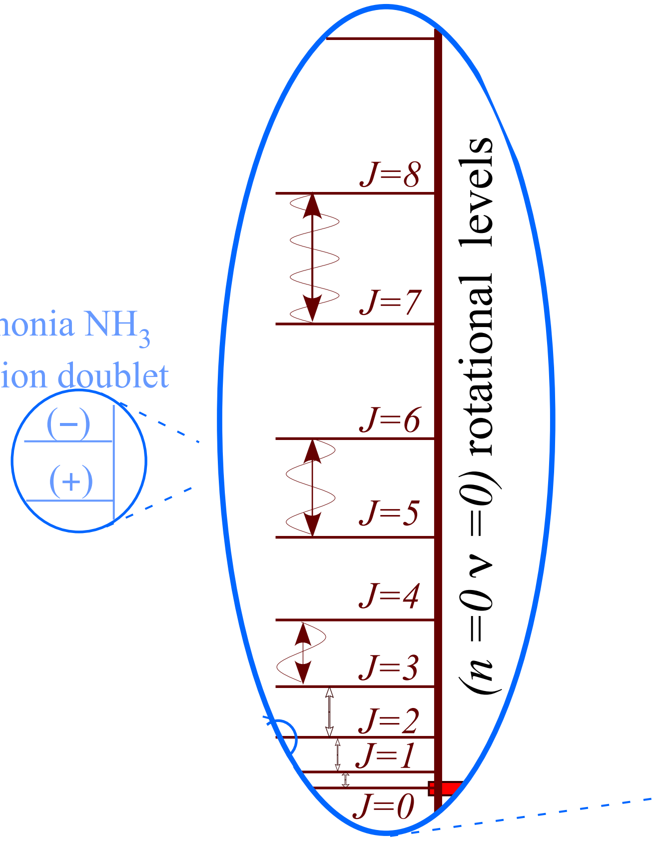
Quantum dynamics of Double-well tunneling

Cheap models of NH_3 inversion doublet and general 2-level quantum systems

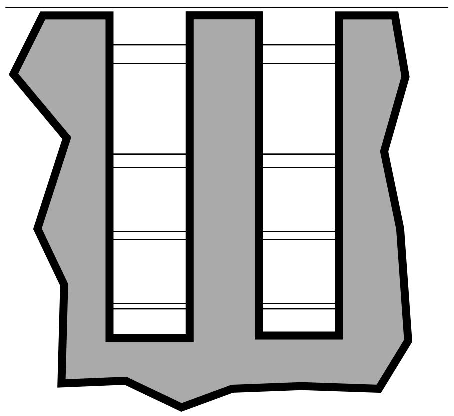
Other types of spectral splitting



fine structure

rotational spectra

2-well tunneling



Quantum dynamics of Double-well tunneling

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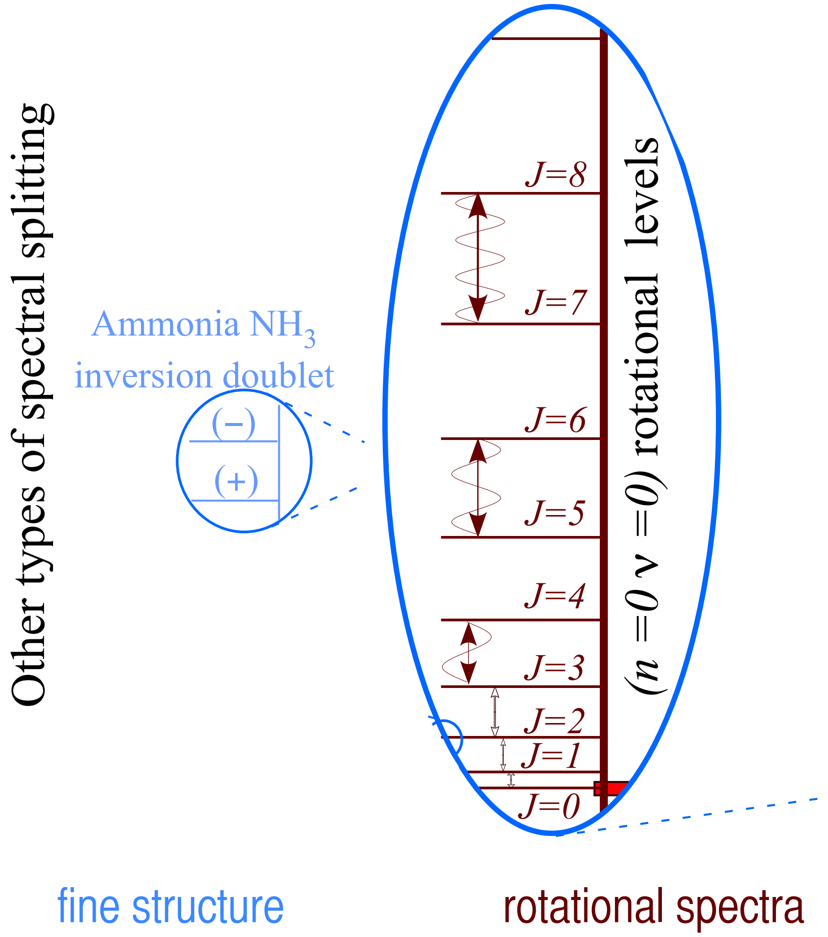
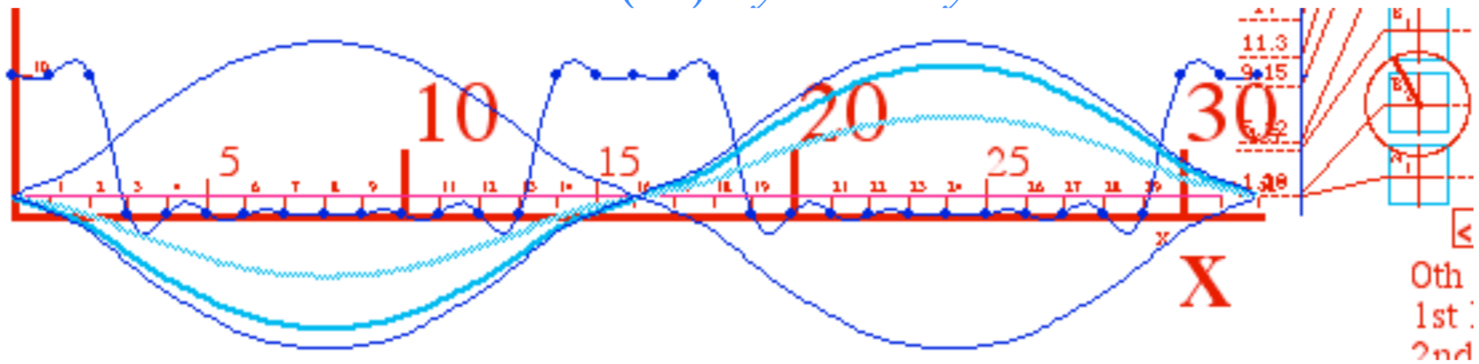


If you add some excited state (−)-symmetry wave...



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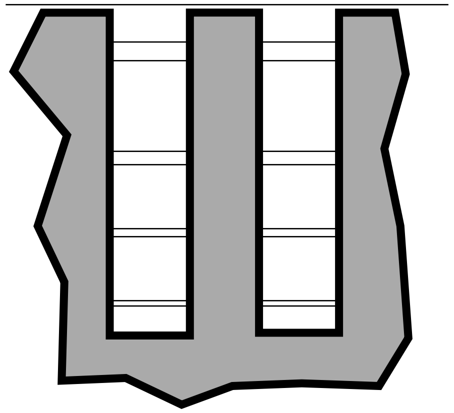

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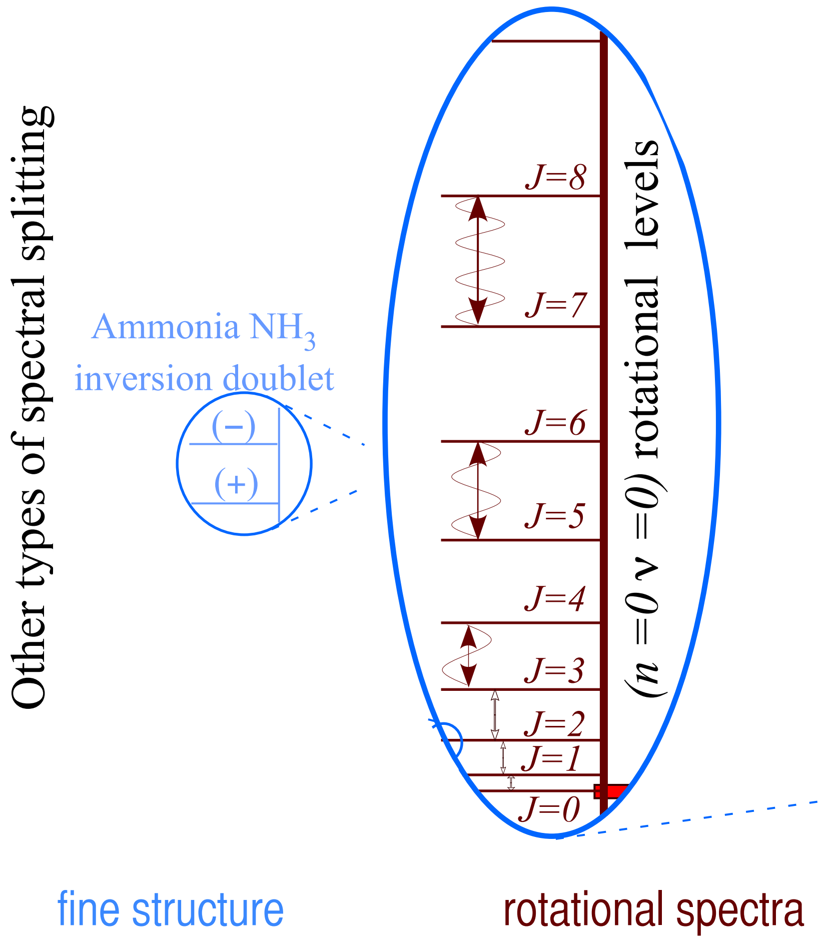

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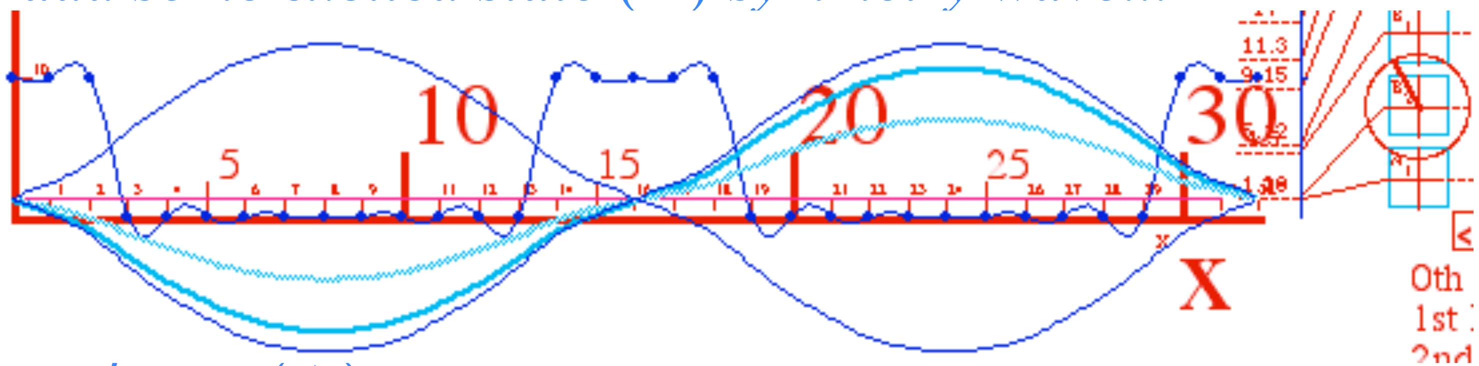
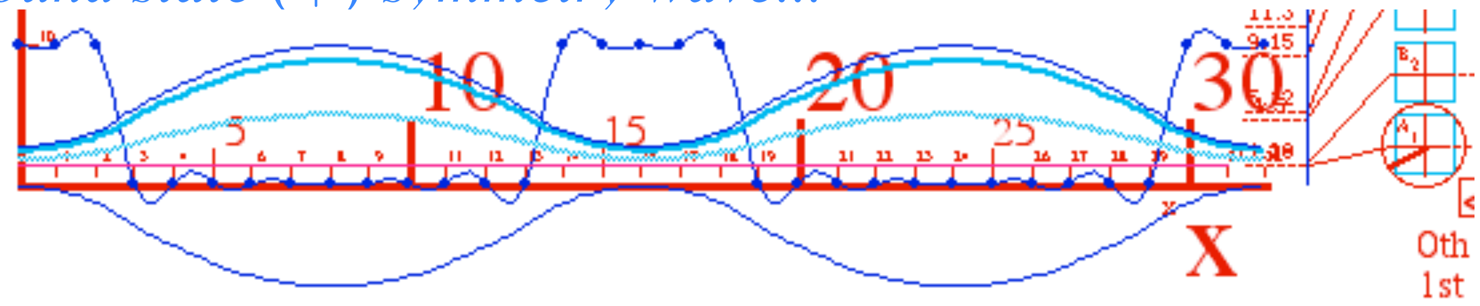
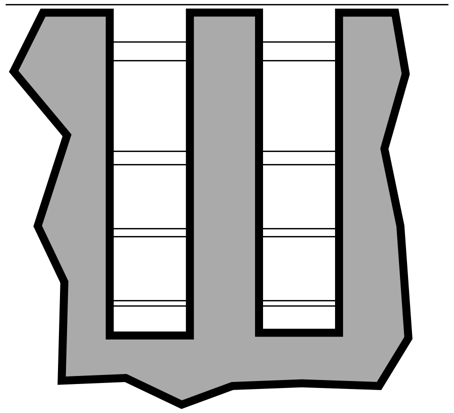


...to ground state (+)-symmetry wave...



2-well tunneling



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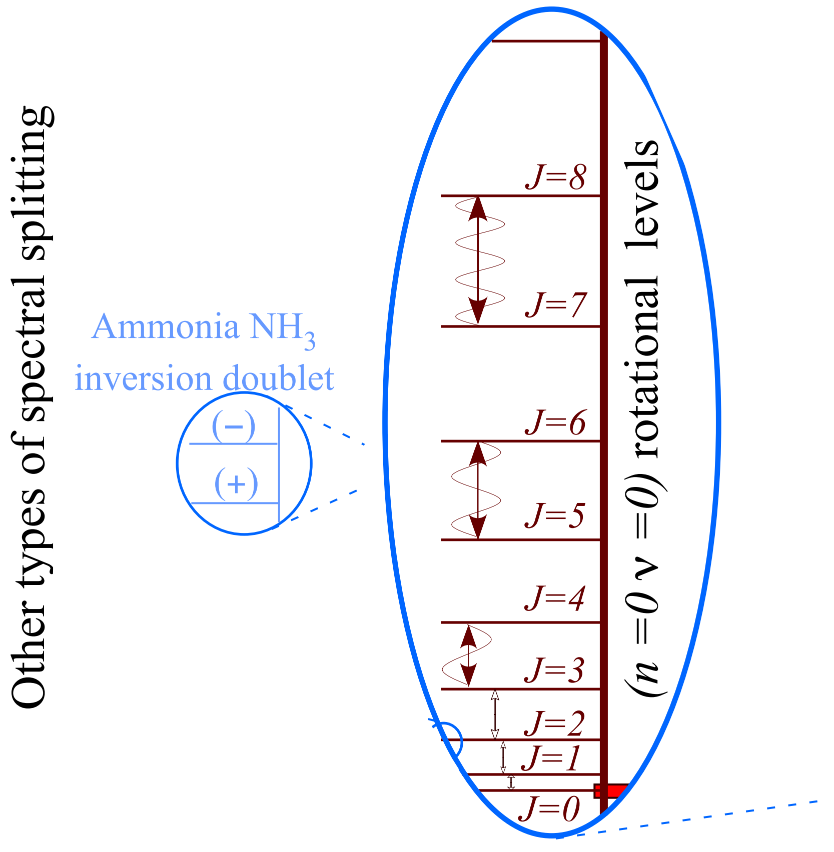


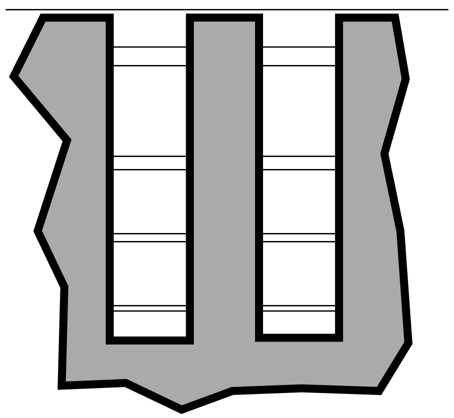
Other types of spectral splitting

Ammonia NH_3 inversion doublet

fine structure

rotational spectra

2-well tunneling



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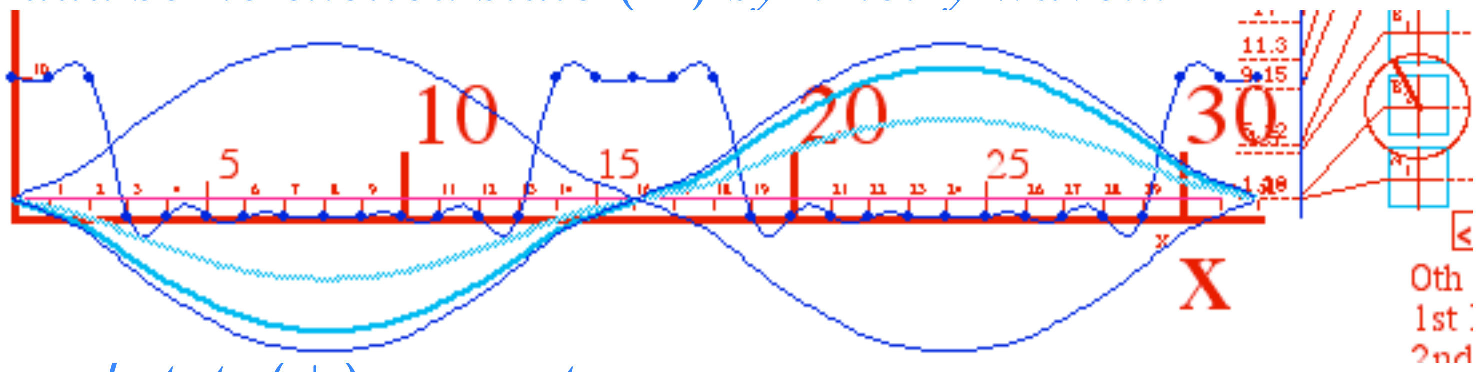

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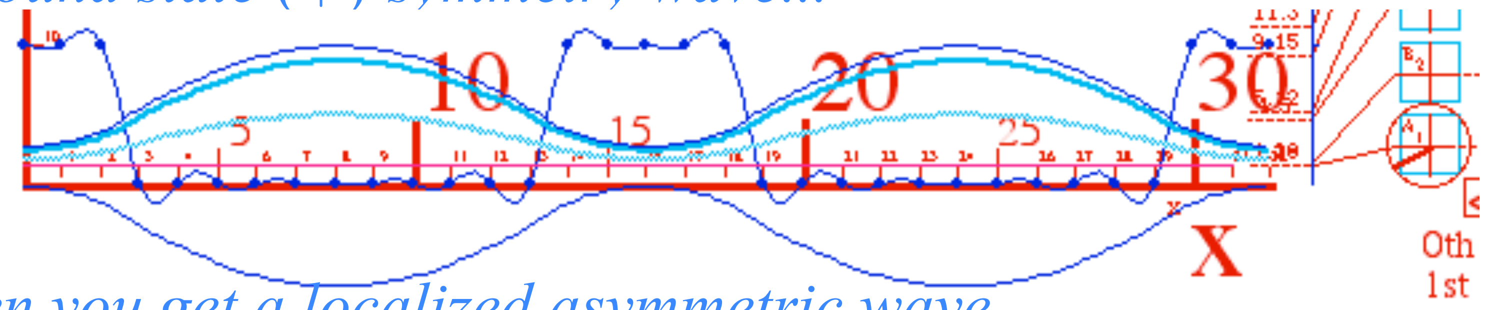
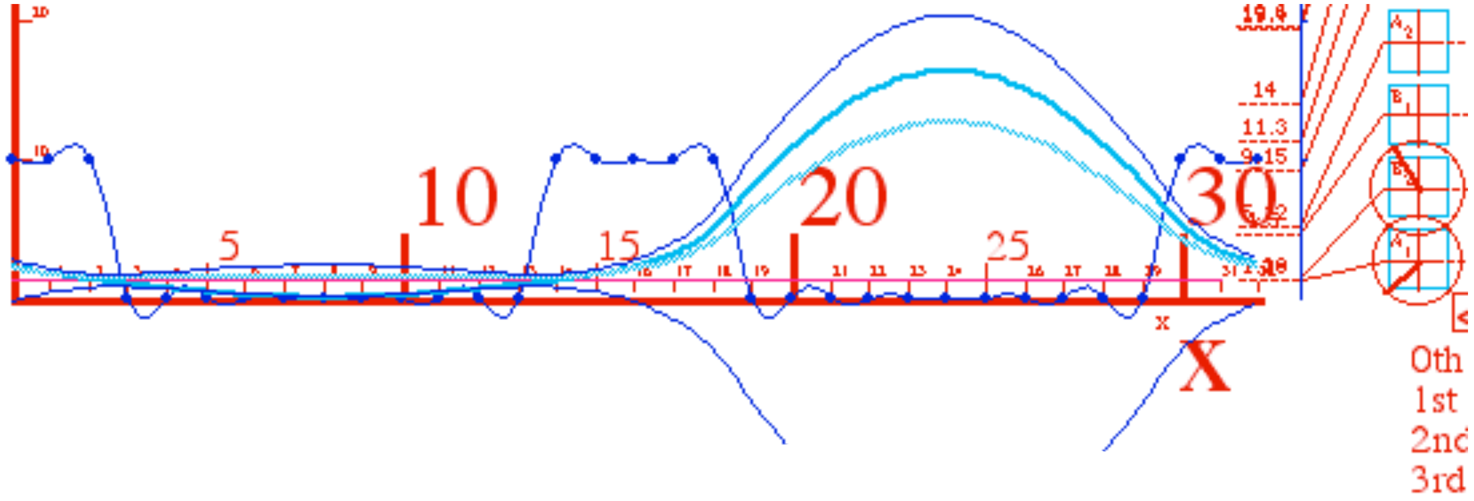


...then you get a localized asymmetric wave...



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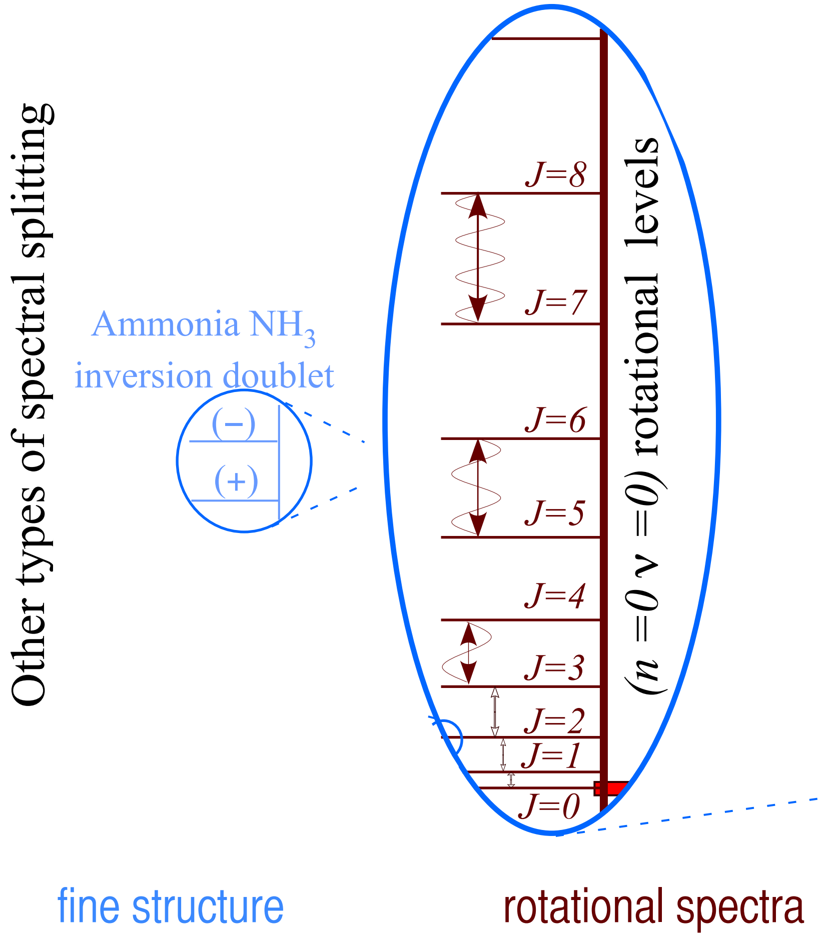
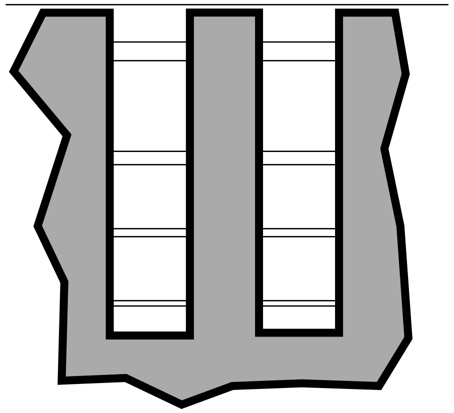


2-well tunneling



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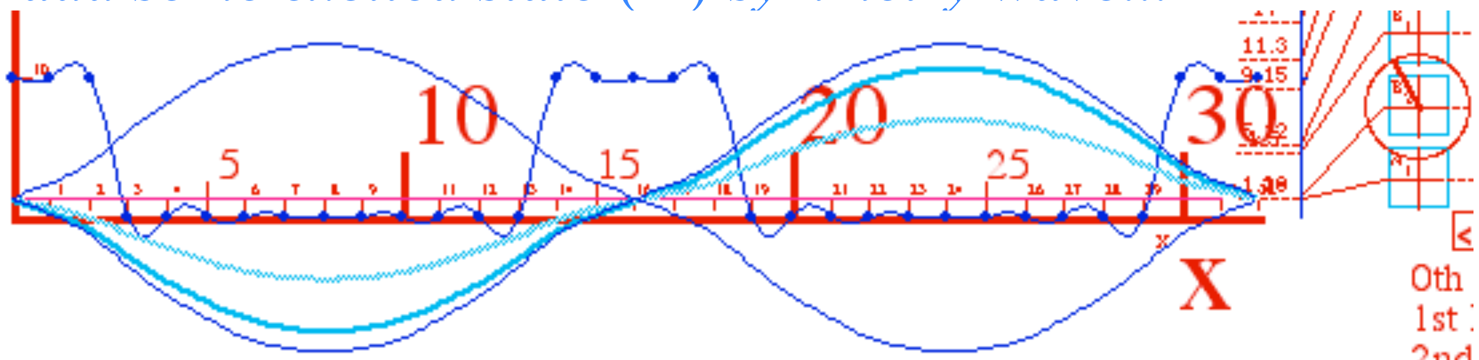

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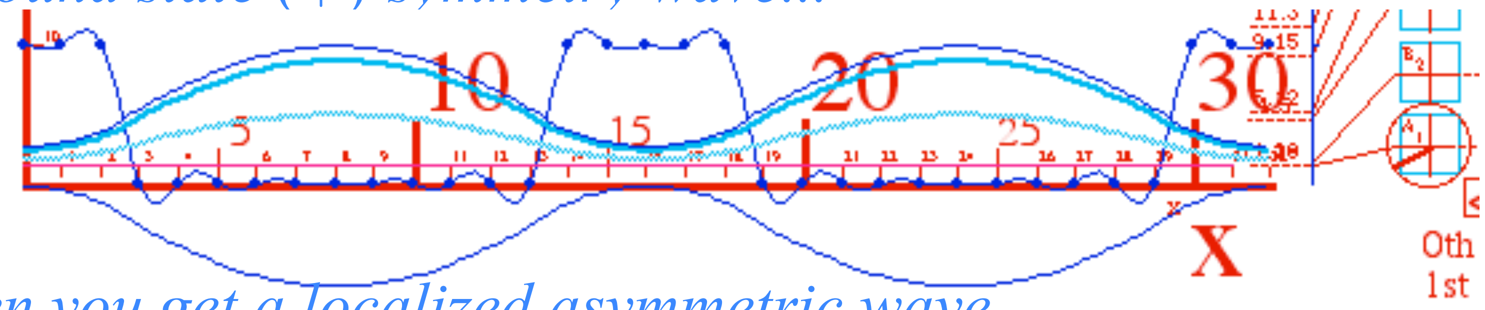

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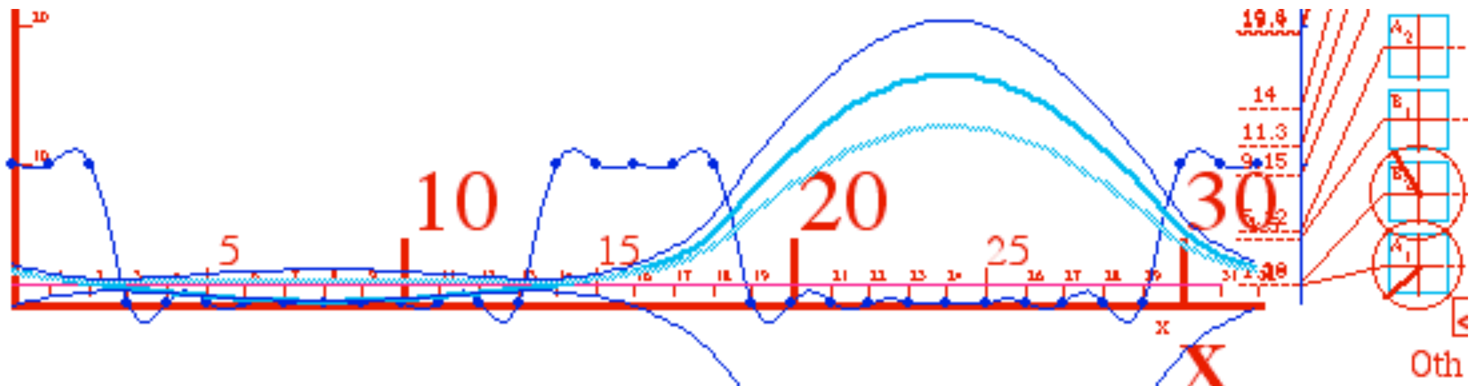
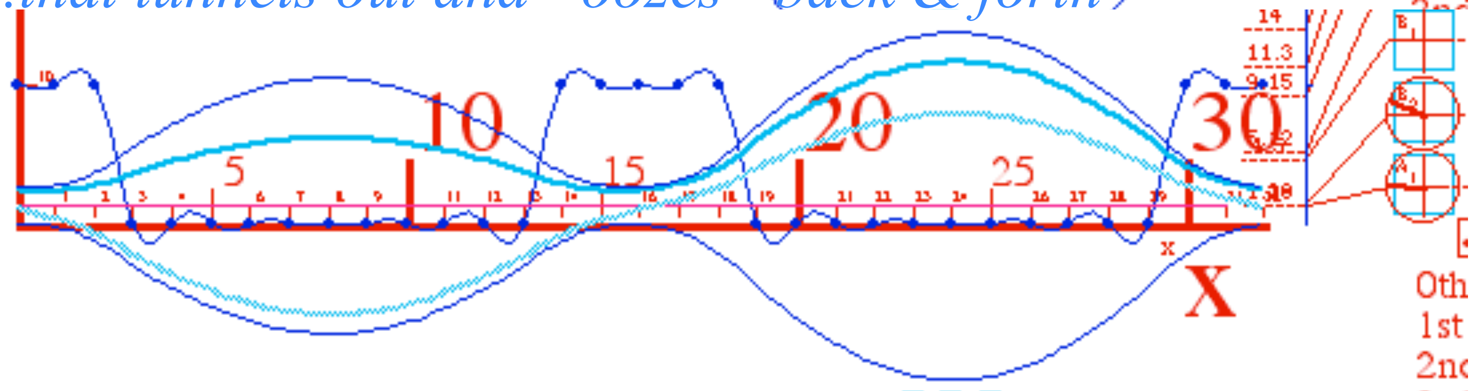


...that tunnels out and "oozes" back & forth



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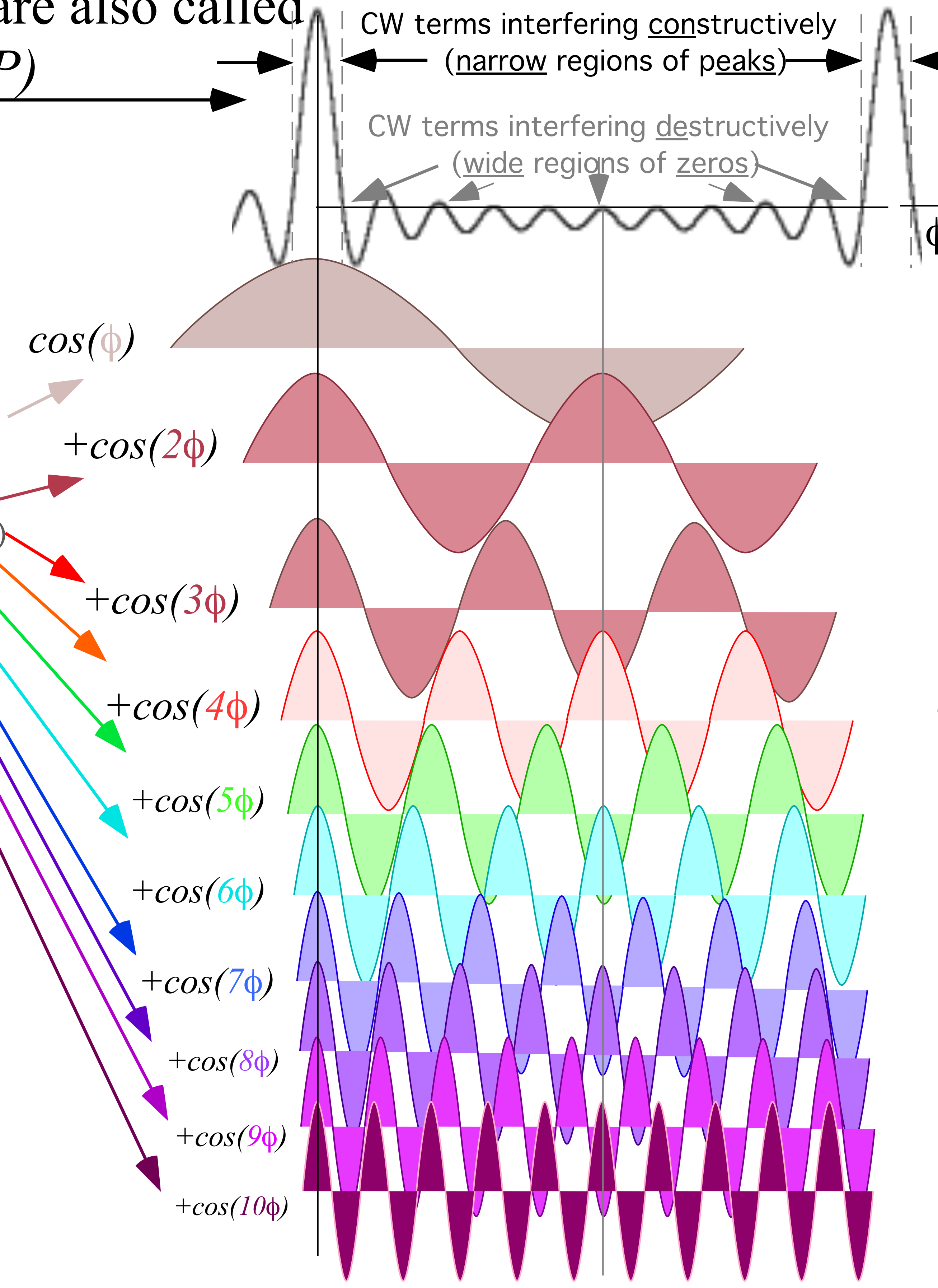
Wavepacket explodes! (Then revives)

Quantum "blasts" of strongly localized ∞-well or rotor waves

A lesson in quantum interference

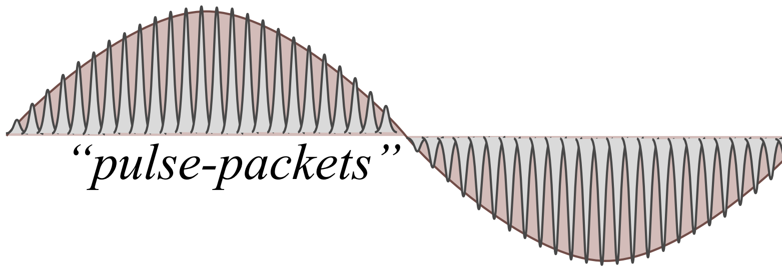
PulseWave forms are also called *Wave Packets (WP)* since they are interfering sums of many *CW* terms

(10-Cosine Waves make up this pulse)



CW terms are also called *Color Waves* or *Fourier Spectral Components*

... and *vice-versa* ... *CW* forms can be made *artificially* from *PW* sums ...



(this is digital *sampling* or digital-to-analog *synthesis*.)

Quantum "blasts" of strongly localized ∞-well or rotor waves

A lesson in quantum interference

PW widths reduce proportionally with more *CW* terms (greater *Spectral* width)

Space-time width (pulse width)

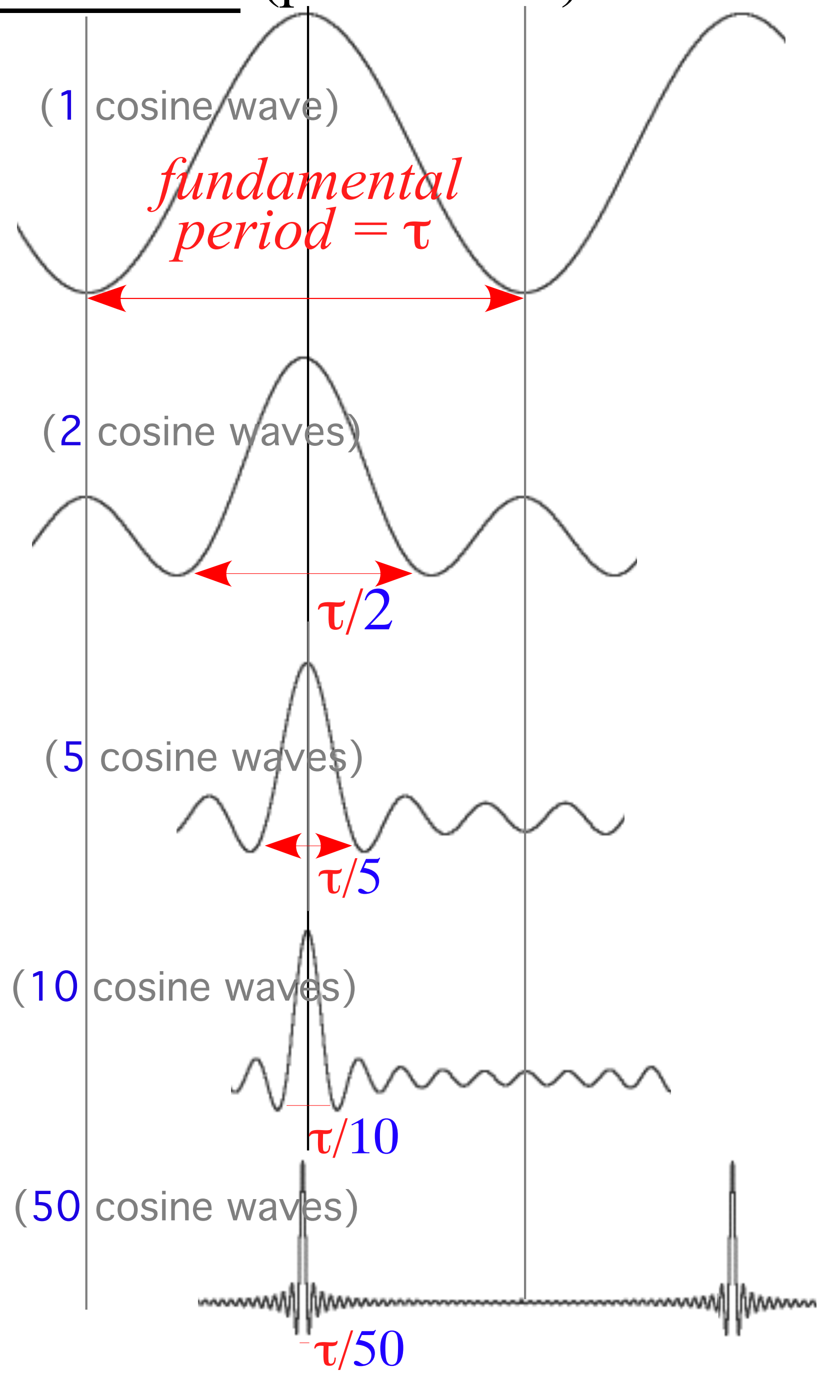
$\Delta t = \tau$

$\Delta t = \tau/2$

$\Delta t = \tau/5$

$\Delta t = \tau/10$

$\Delta t = \tau/50$



this dimension is <u>time</u>

Spectral width (harmonic frequency range)

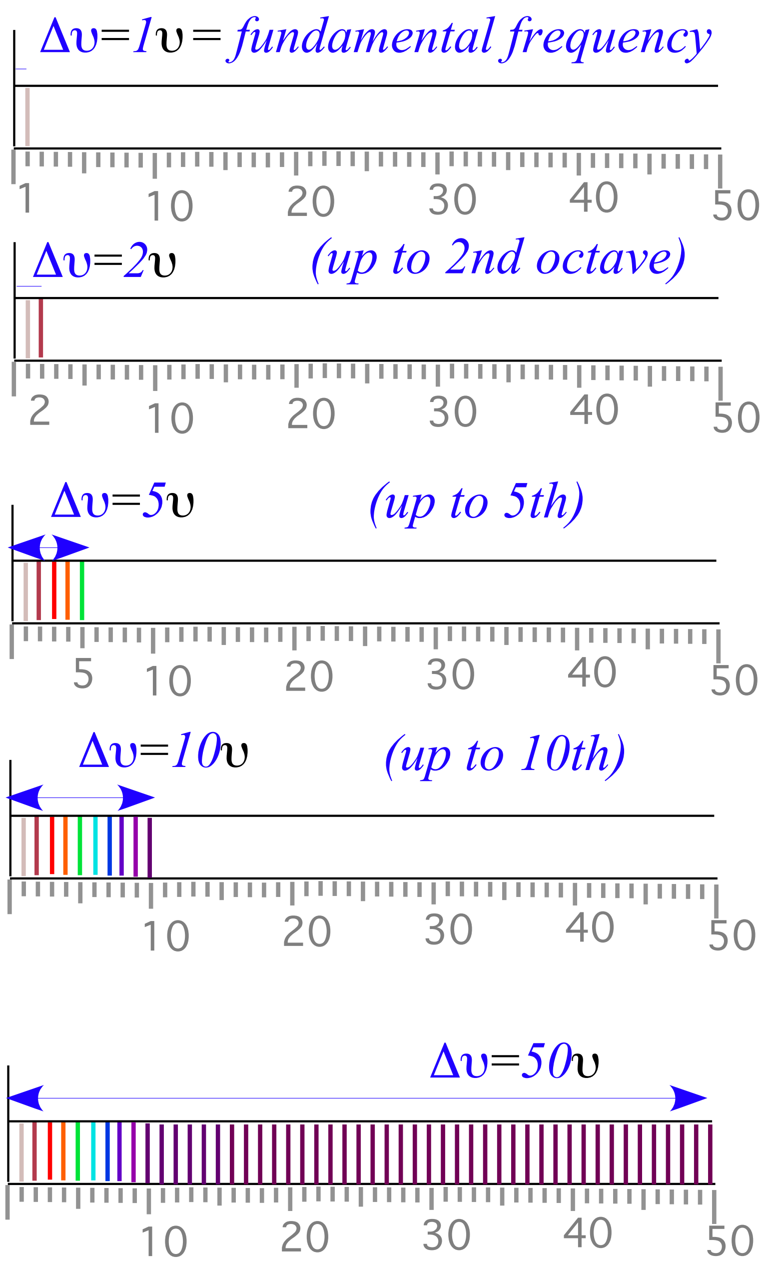
1 *CW* term
$\Delta\upsilon = \upsilon = 1/\tau$

2 *CW* terms
$\Delta\upsilon = 2\upsilon$

5 *CW* terms
$\Delta\upsilon = 5\upsilon$

10 *CW* terms
$\Delta\upsilon = 10\upsilon$

50 *CW* terms
$\Delta\upsilon = 50\upsilon$



this dimension is <u>frequency</u> or <u>per</u>-time

Quantum "blasts" of strongly localized ∞-well or rotor waves

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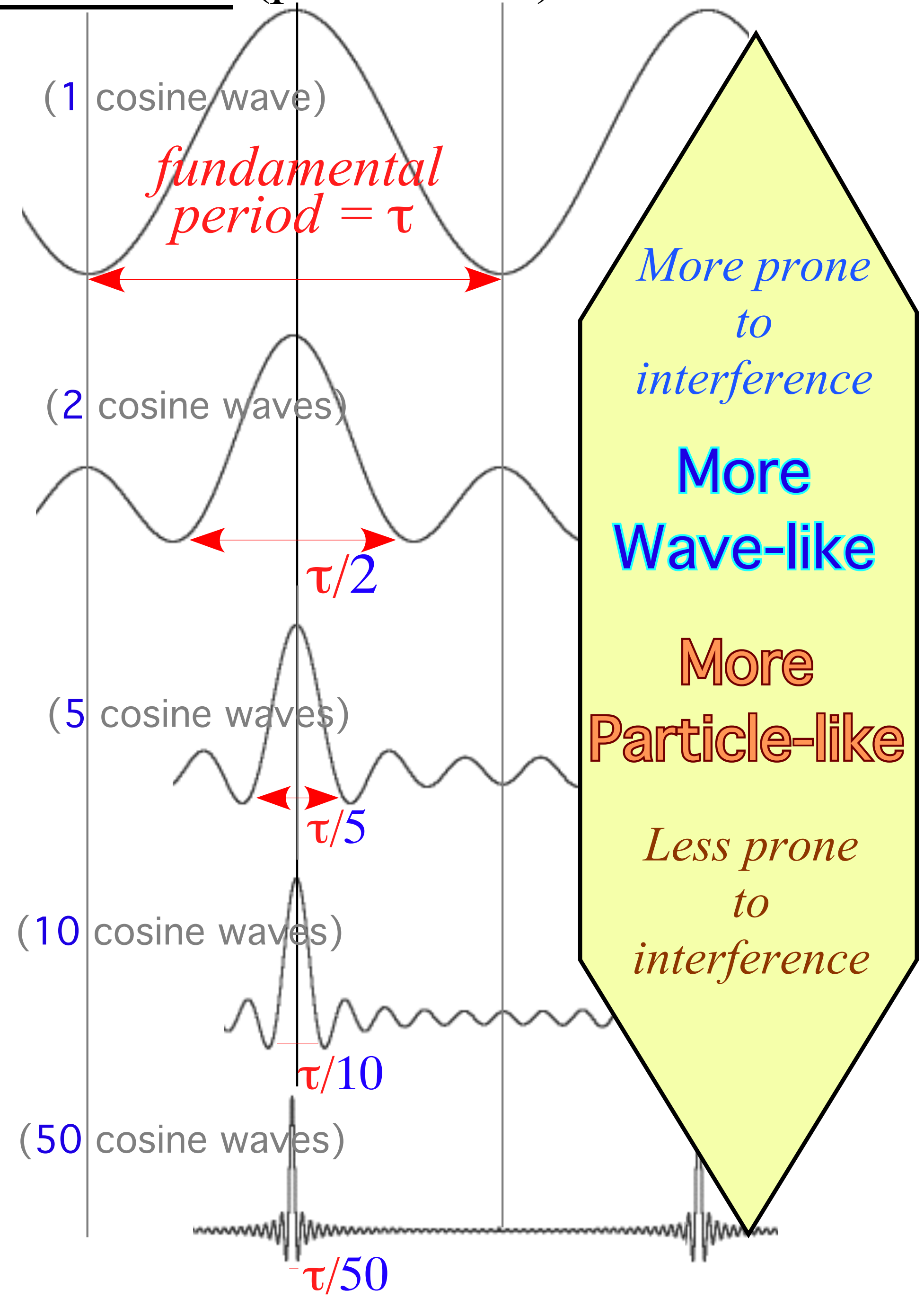

this dimension is time

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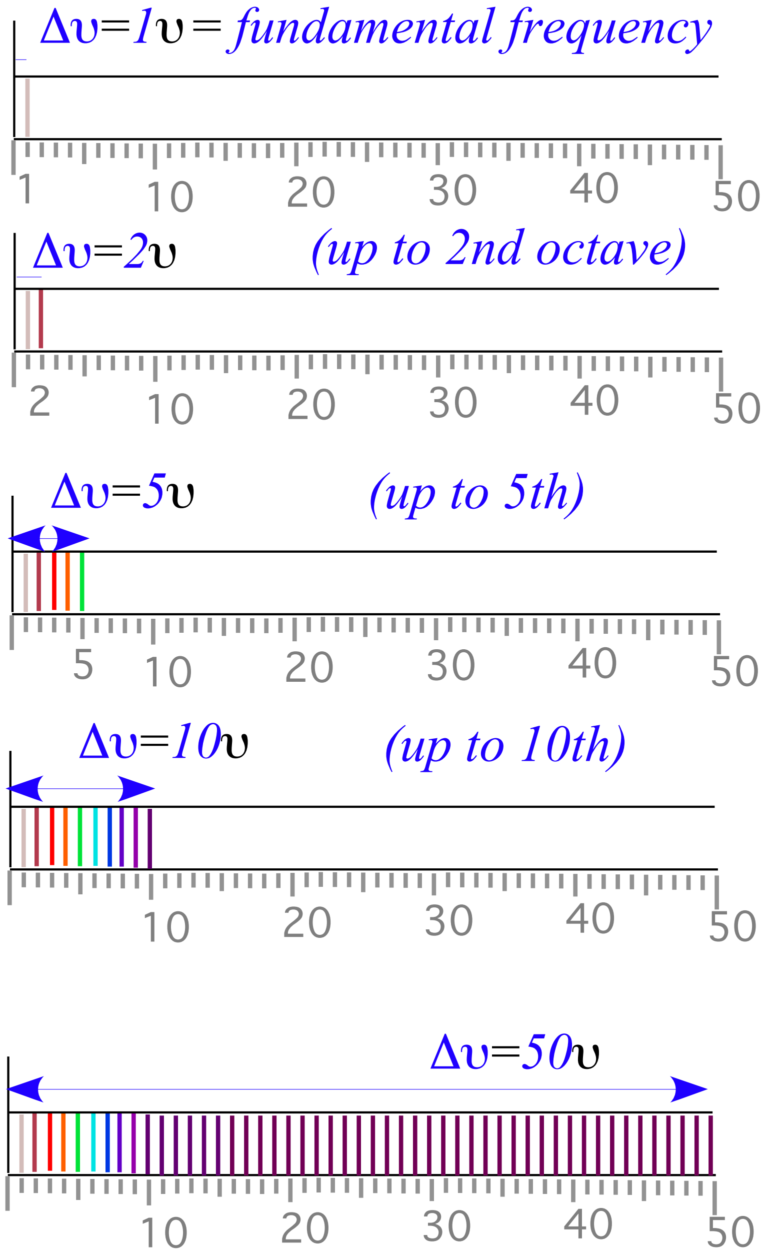

this dimension is frequency or per-time

Fourier-Heisenberg product: $\Delta t \cdot \Delta\upsilon = 1$ (time-frequency uncertainty relation)

Quantum "blasts" of strongly localized ∞-well or rotor waves

A lesson in quantum interference

$$\delta\left(x-a\right)=\left\langle x\middle|a\right\rangle=\sum_{n=1}^{\infty}\left\langle x\middle|\varepsilon_n\right\rangle\left\langle\varepsilon_n\middle|a\right\rangle=\sum_{n=1}^{\infty}a_n\sin k_n x$$

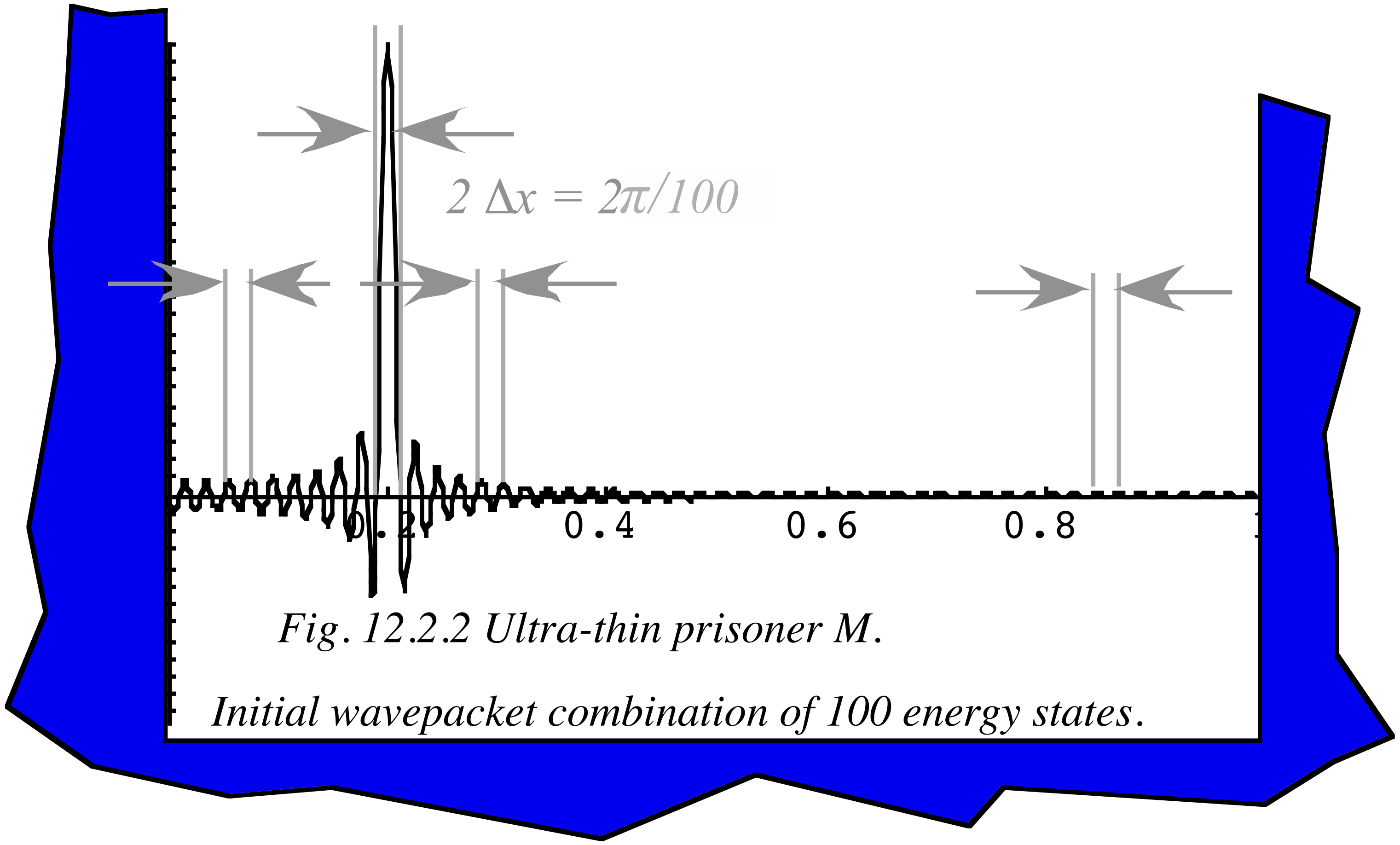

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

Quantum "blasts" of strongly localized ∞-well or rotor waves

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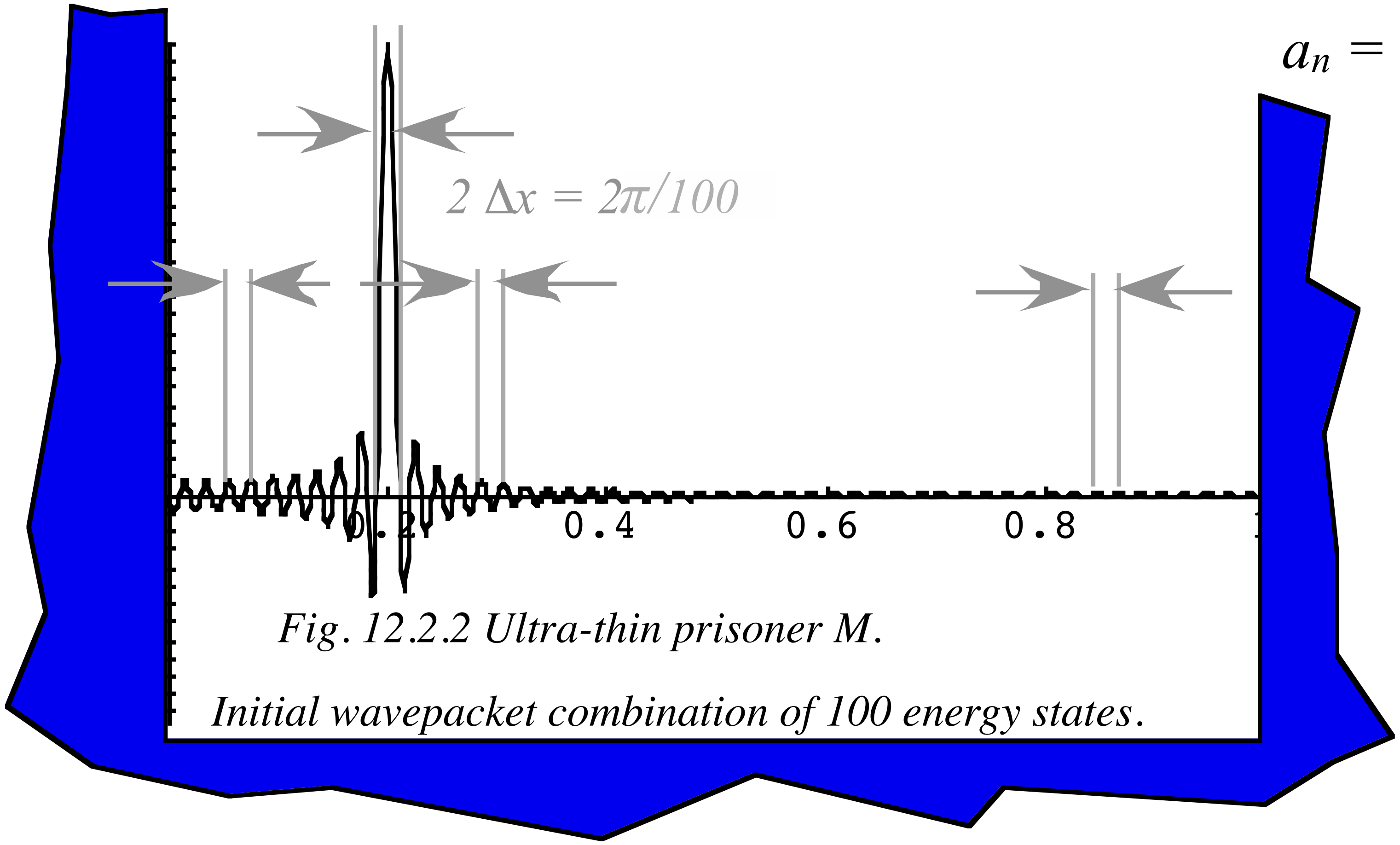
$a_n = \langle\varepsilon_n|a\rangle = (2/W)\sin k_n a \qquad (k_n = n\pi/W)$



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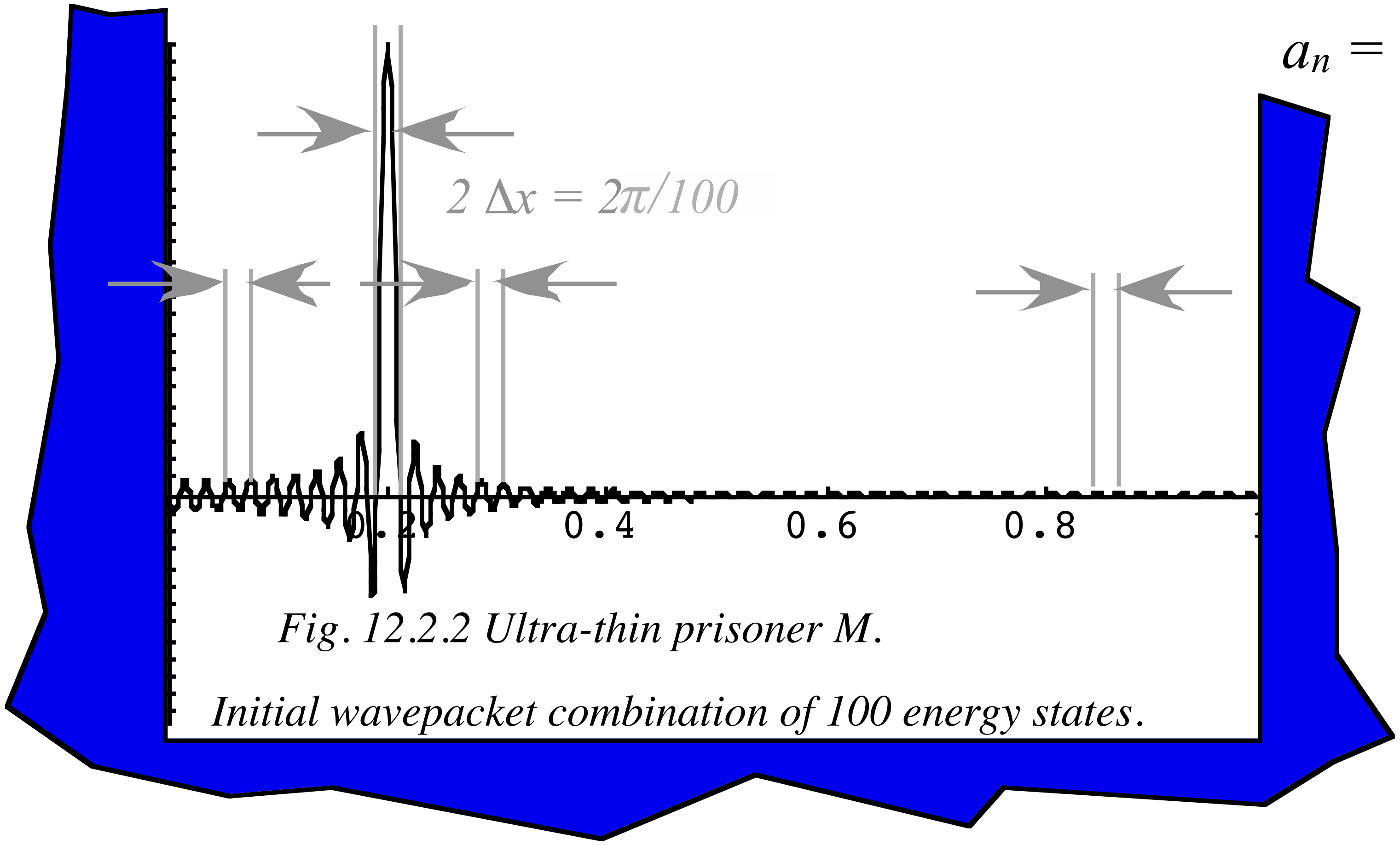

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$$\Psi(x)=\frac{2}{W}\sum_{n}^{N_{\max}}\sin k_n a\,\sin k_n x$$

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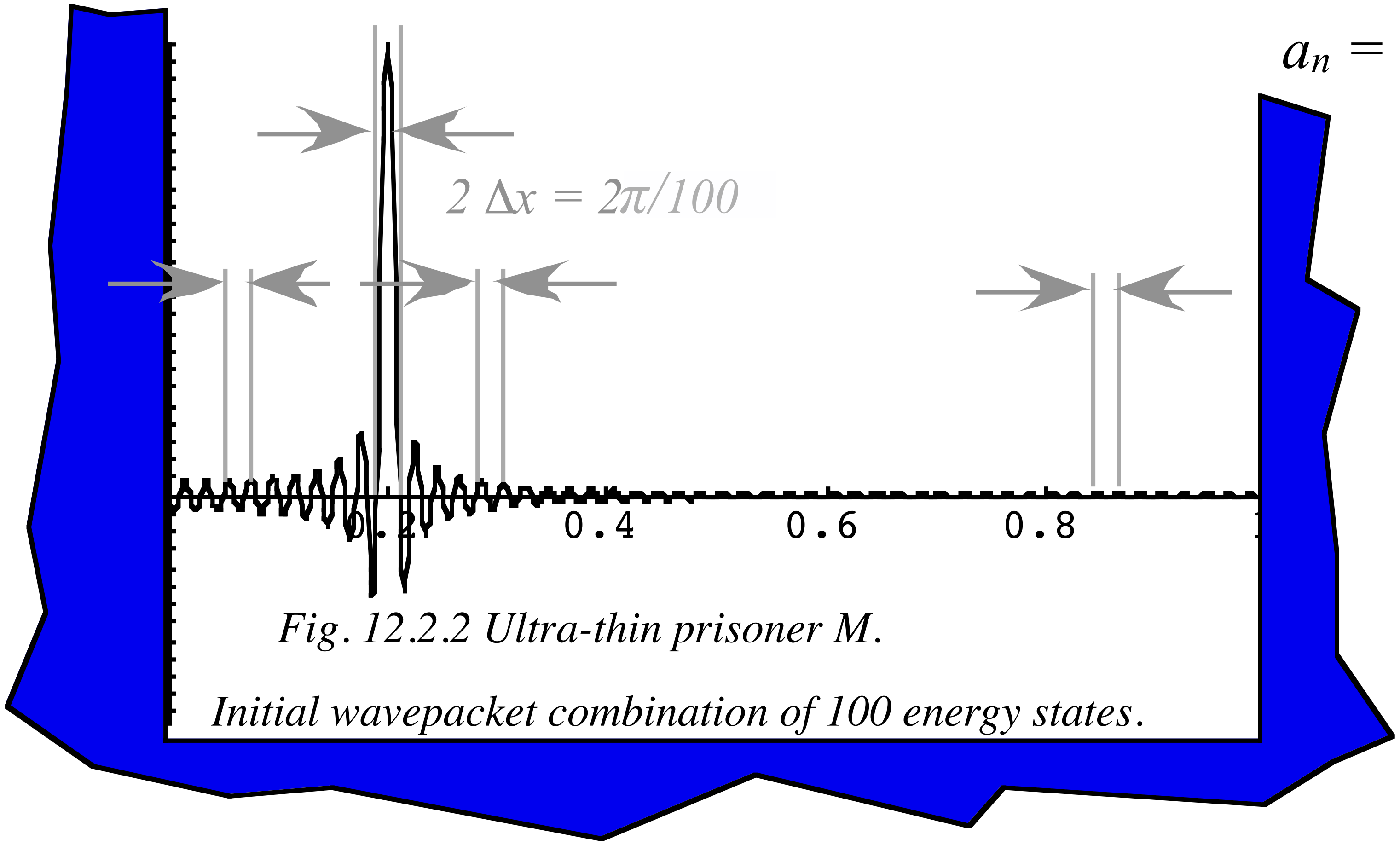
$$\delta(x-a) = \langle x|a\rangle = \sum_{n=1}^{\infty}\langle x|\varepsilon_n\rangle\langle\varepsilon_n|a\rangle = \sum_{n=1}^{\infty} a_n \sin k_n x$$



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$$\Psi(x) = \frac{2}{W}\sum_{n}^{N_{\max}} \sin k_n a \sin k_n x$$

$$\rightarrow \frac{2}{W}\int_0^{K_{\max}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

QTCA Unit 4 Ch.12.2

Quantum "blasts" of strongly localized ∞-well or rotor waves

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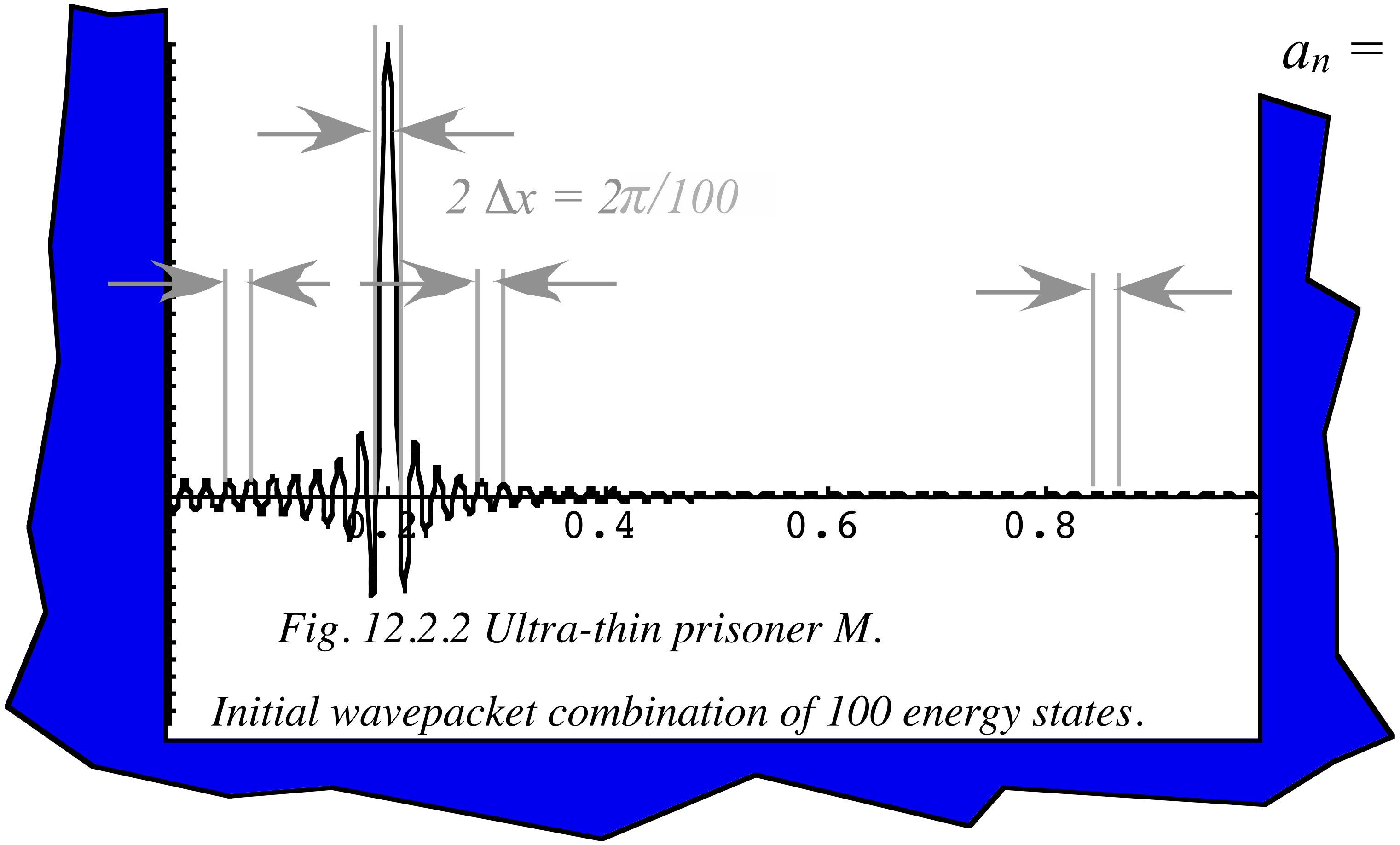

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$$= \frac{2}{W}\frac{W}{\pi}\int_{0}^{K_{\max}} dk \sin ka \sin kx$$

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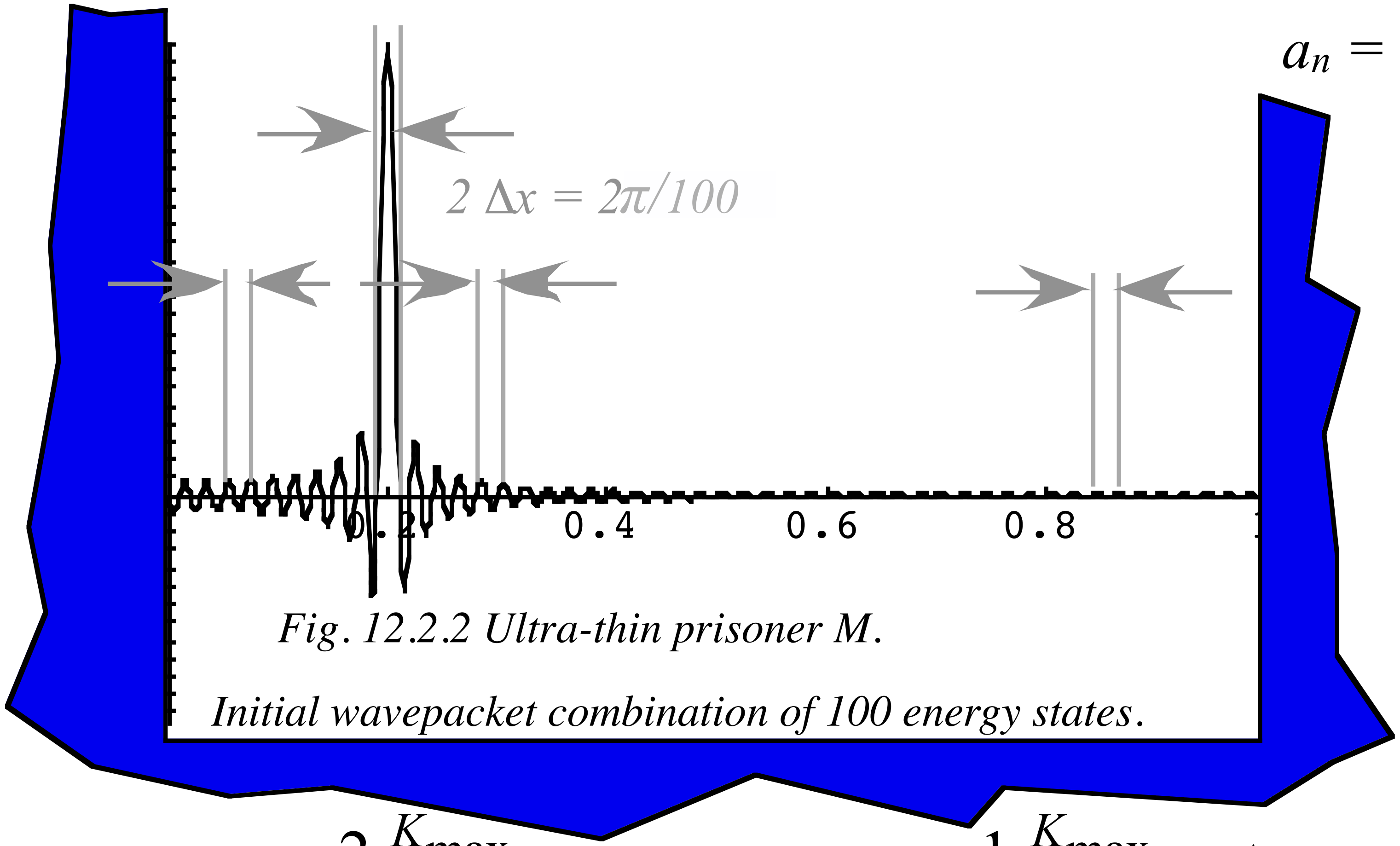

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$$\rightarrow \frac{2}{W}\int_0^{K_{\max}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

$$= \frac{2}{W}\frac{W}{\pi}\int_0^{K_{\max}} dk \sin ka \sin kx$$

$$\Psi(x) \cong \frac{2}{\pi}\int_0^{K_{\max}} dk \sin ka \sin kx = \frac{1}{\pi}\int_0^{K_{\max}} dk\left(\cos k(x-a) - \cos k(x+a)\right)$$

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A lesson in quantum interference

$$\delta\left(x-a\right)=\left\langle x\middle|a\right\rangle=\sum_{n=1}^{\infty}\left\langle x\middle|\varepsilon_n\right\rangle\left\langle\varepsilon_n\middle|a\right\rangle=\sum_{n=1}^{\infty}a_n\sin k_n x$$

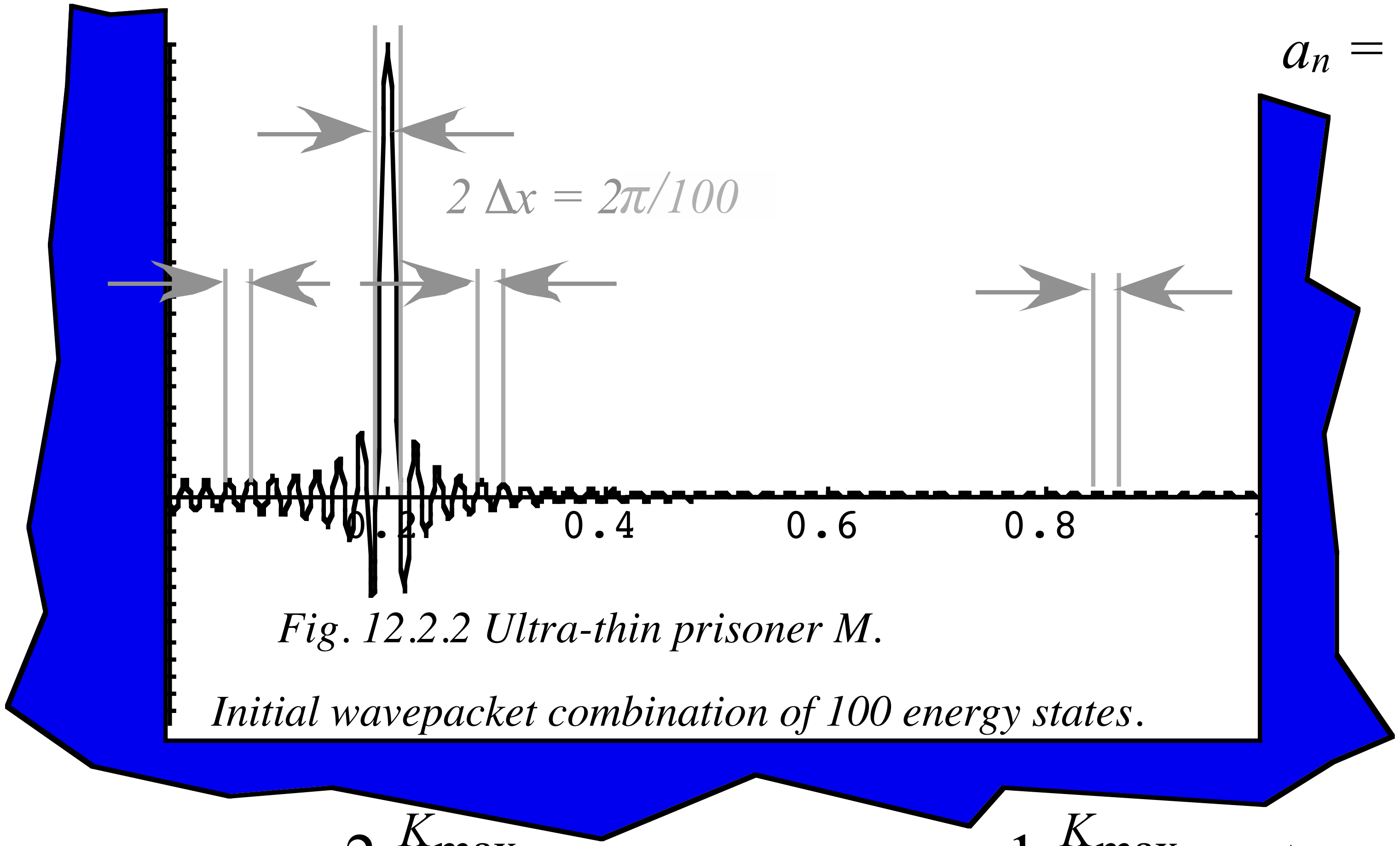

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

$a_n = \langle\varepsilon_n|a\rangle = (2/W)\sin k_n a \qquad (k_n = n\pi/W)$

$$\Psi\left(x\right)=\frac{2}{W}\sum_{n}^{N_{\max}}\sin k_n a\,\sin k_n x$$

$$\rightarrow\frac{2}{W}\int_0^{K_{\max}}dk\,\frac{\Delta n}{\Delta k}\sin ka\,\sin kx$$

$$=\frac{2}{W}\frac{W}{\pi}\int_0^{K_{\max}}dk\,\sin ka\,\sin kx$$

$$\Psi\left(x\right)\cong\frac{2}{\pi}\int_0^{K_{\max}}dk\,\sin ka\,\sin kx=\frac{1}{\pi}\int_0^{K_{\max}}dk\left(\cos k\left(x-a\right)-\cos k\left(x+a\right)\right)$$

$$\cong\frac{\sin K_{\max}(x\text{-}a)}{\pi(x\text{-}a)}-\frac{\sin K_{\max}(x+a)}{\pi(x+a)}\cong\frac{\sin K_{\max}(x\text{-}a)}{\pi(x\text{-}a)}\quad\text{for: } x\approx a$$

Quantum "blasts" of strongly localized ∞-well or rotor waves

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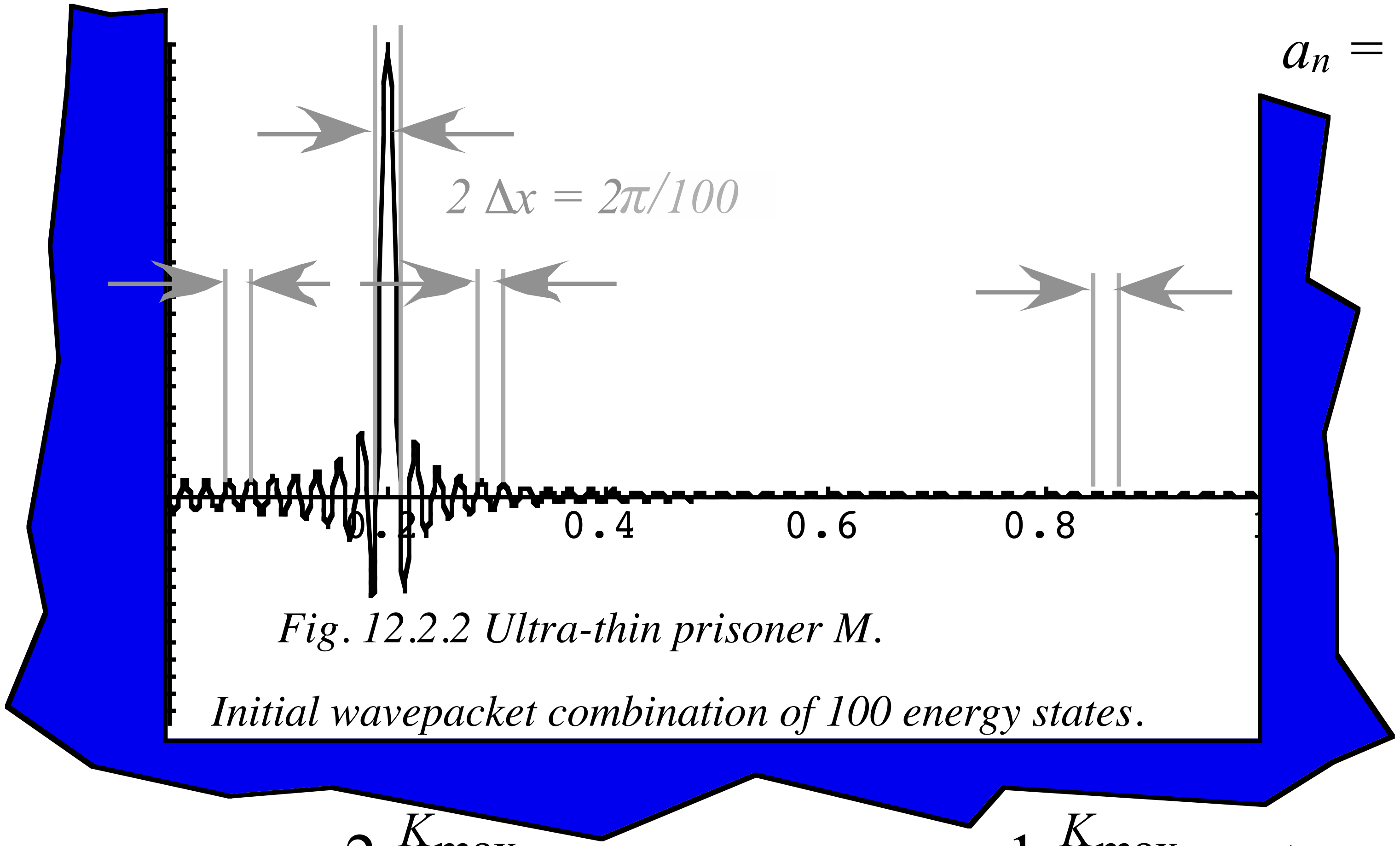

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$$\cong\frac{\sin K_{\max}(x-a)}{\pi(x-a)}-\frac{\sin K_{\max}(x+a)}{\pi(x+a)}\cong\frac{\sin K_{\max}(x-a)}{\pi(x-a)}\quad\text{for: } x\approx a$$

"Last-in-first-out" effect. Last $K_{\max}$-value dominates and "inside" K get "smothered" by interference with neighbors.

Spectral hierarchy of Born-Oppenheimer approximations to *AMOP*

Sketch of modern molecular spectroscopy

Example of16µm spectra of CF_4 *1996 AMOP Handbook*
2005 AMOP Handbook
Example of16µm spectra of SF_6 *2018?AMOP Handbook*

Example of ??µm spectra of C_{60} *?*

Units of frequency (Hz), wavelength (m), and energy (eV)
Spectral windows in atmosphere due to molecules

Simple molecular-spectra models
- *2-well tunneling, Bohr mass-on-ring, 1D harmonic oscillator, Coulomb PE models*

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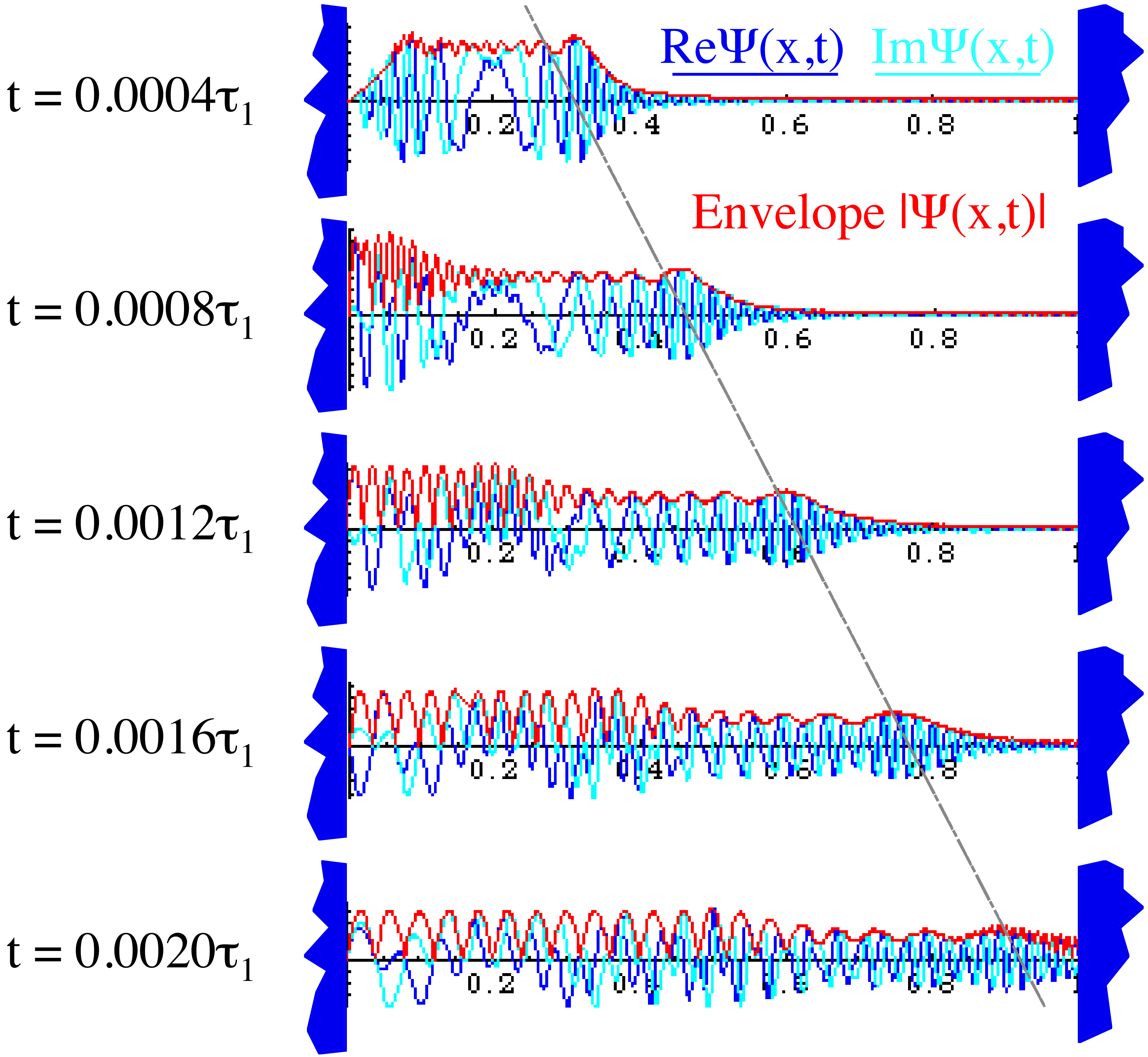
➡ *Quantum "blasts" of strongly localized ∞-well or rotor waves: A lesson in quantum interference*

➡ **Wavepacket explodes! (Then revives)**

Wavepacket explodes!

Time given in units of period τ_1 (slowest phasor of ground level).

fundamental zero-point period $\tau_1 = 1/\nu_1$



Wavepacket explodes!

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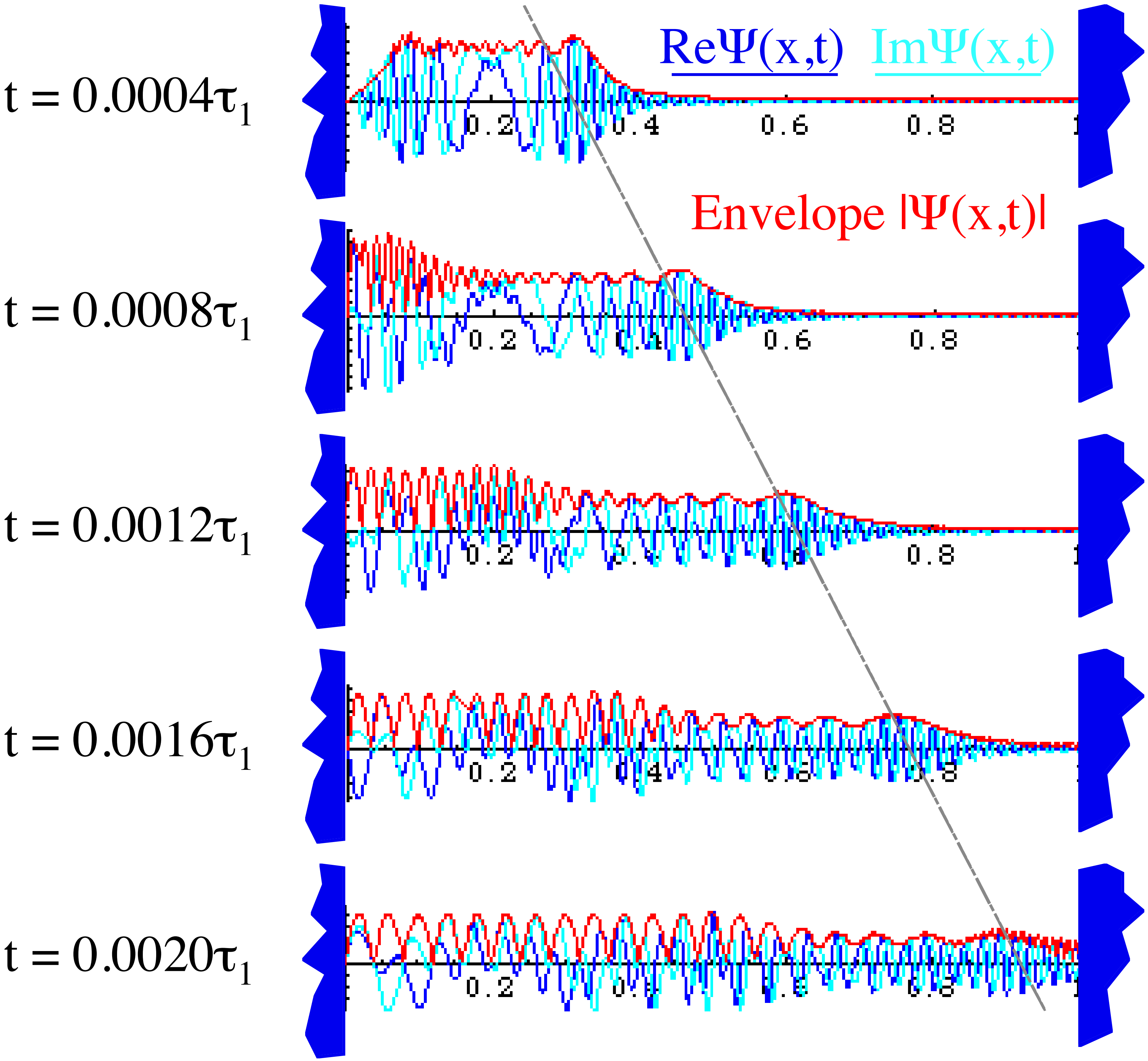
fundamental zero-point period $\tau_1 = 1/\nu_1$ is

$$\tau_1 = \frac{2\pi}{\omega_1} = \frac{2\pi\hbar}{\varepsilon_1}$$

$$= \frac{h}{h^2/8MW^2} = \frac{8MW^2}{h}$$



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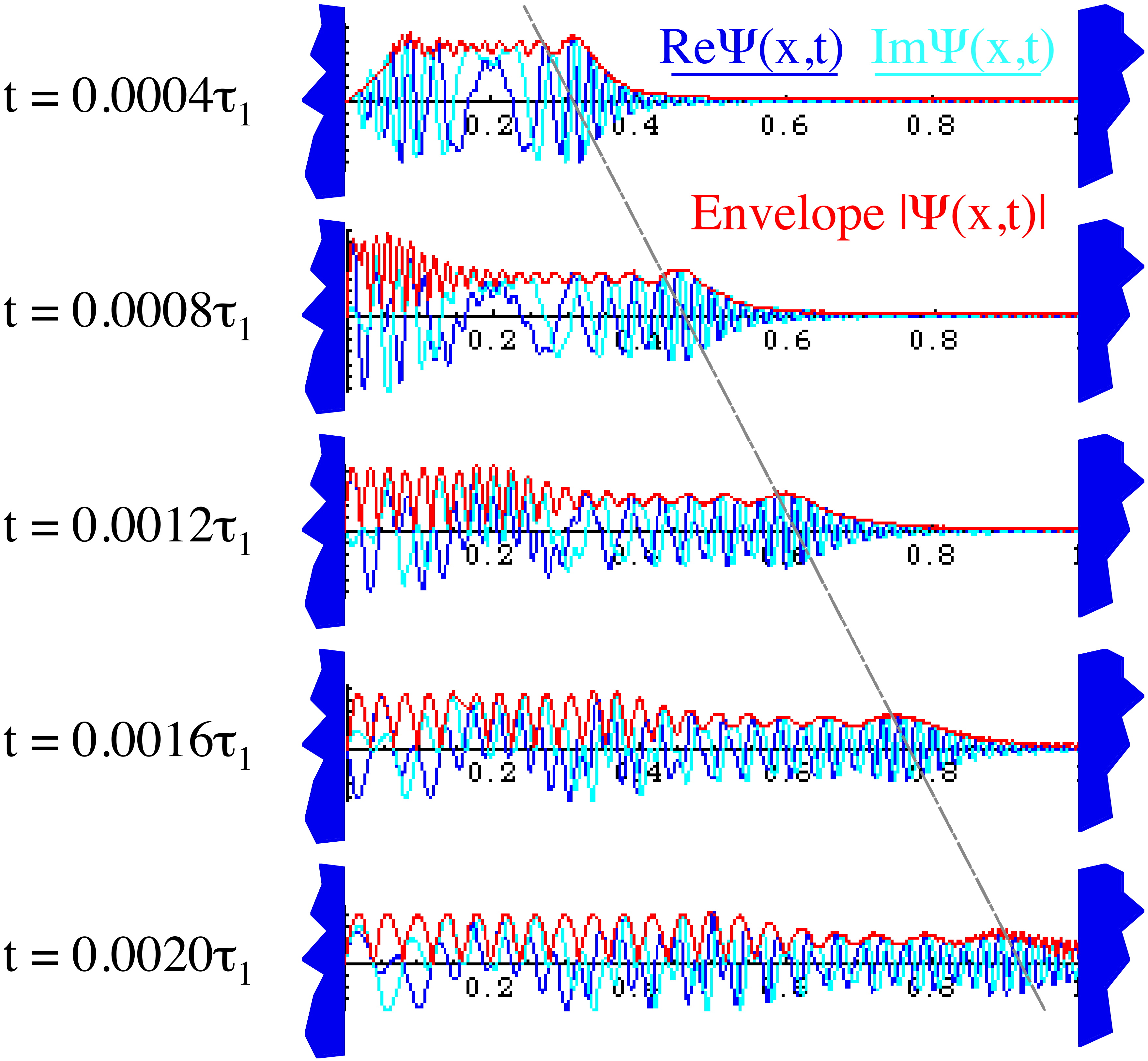

ε_n-level classical velocity:

$$V_n = \frac{d\omega_n}{dk} = \frac{1}{\hbar}\frac{d\varepsilon_n}{dk}$$

$$= \frac{1}{\hbar}\frac{\hbar^2}{2M}\frac{dk^2}{dk}$$

$$= \frac{\hbar 2k_n}{2M} = \frac{\hbar n\pi}{MW} = \frac{hn}{2MW}$$

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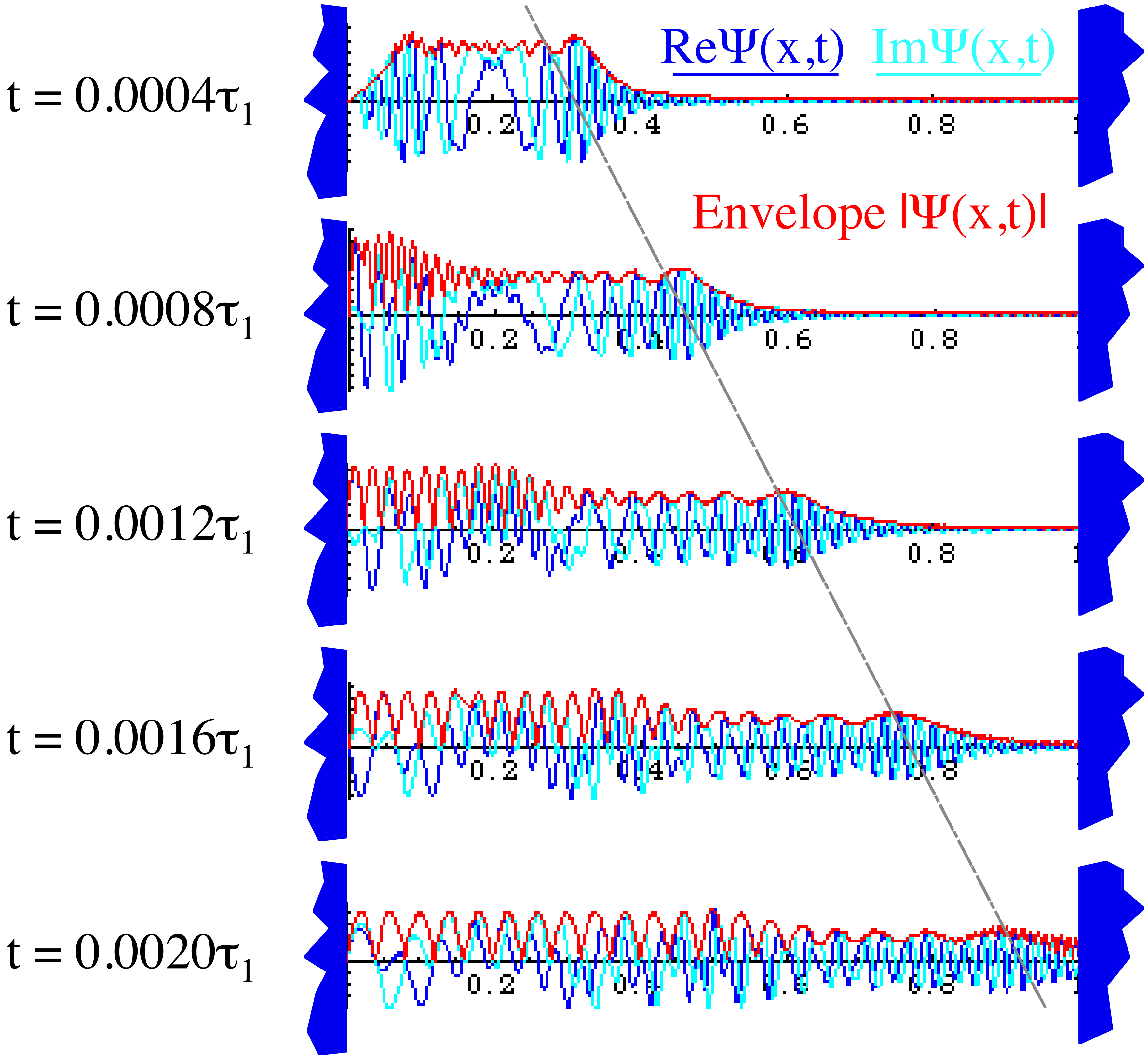

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εn-level classical round trip time Tn(2W)

$$T_n(2W) = \frac{2W}{V_n} = 2W\frac{2MW}{hn} = \frac{4MW^2}{hn}$$

$$= \frac{1}{2n}\frac{8MW^2}{h} = \frac{\tau_1}{2n}$$

QTCA Unit 4 Ch.12.2

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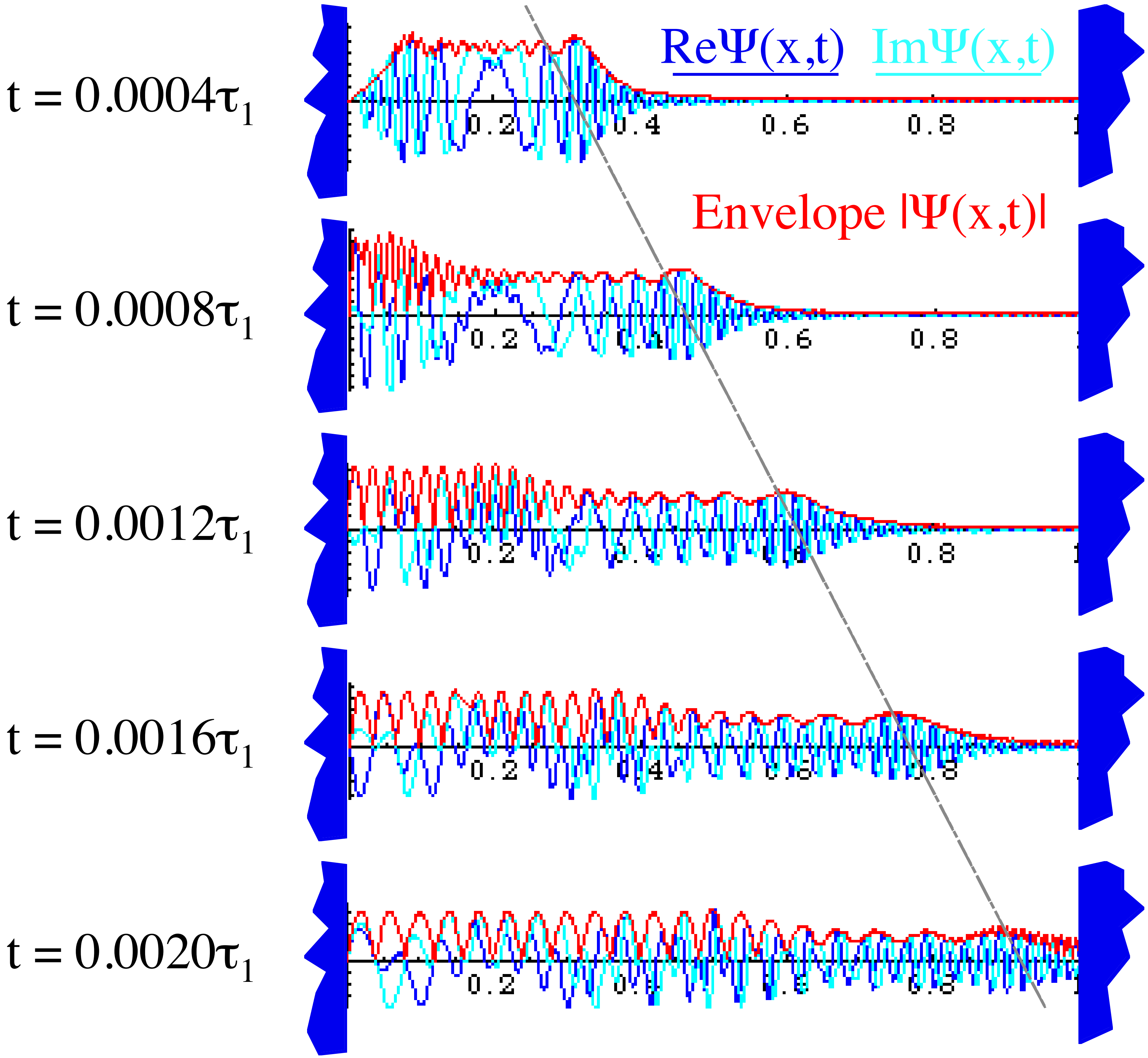

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εn-level 1-way time Tn(W)

$$T_n(W) = T_n(2W)/2 = \frac{\tau_1}{4n}$$

$$\left(= 0.0025\,\tau_1 \quad \text{for: } n{=}100\right)$$

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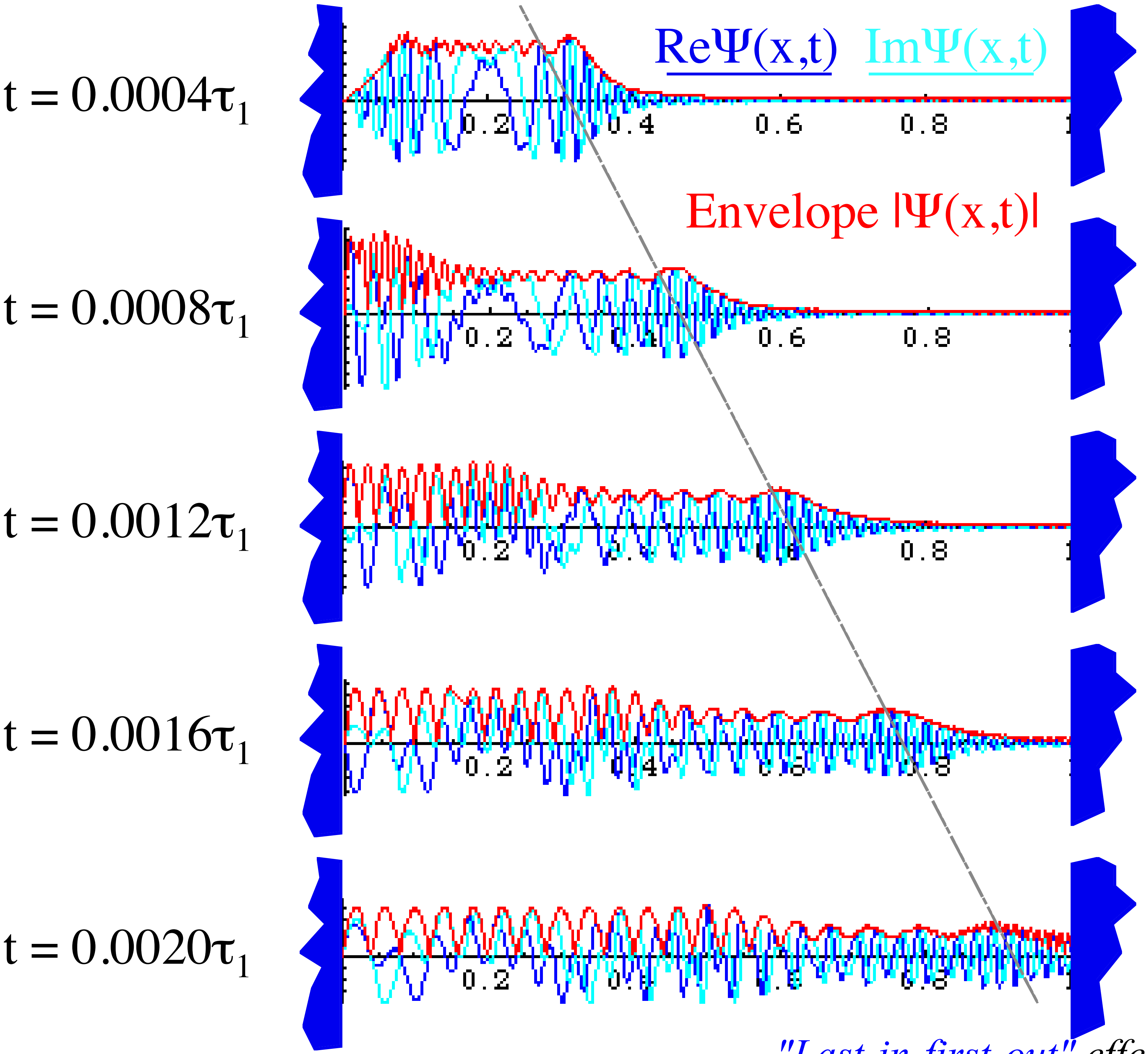

"Last-in-first-out" effect

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Wavepacket explodes! (Then revives)

Wavepacket explodes! (Then revives)

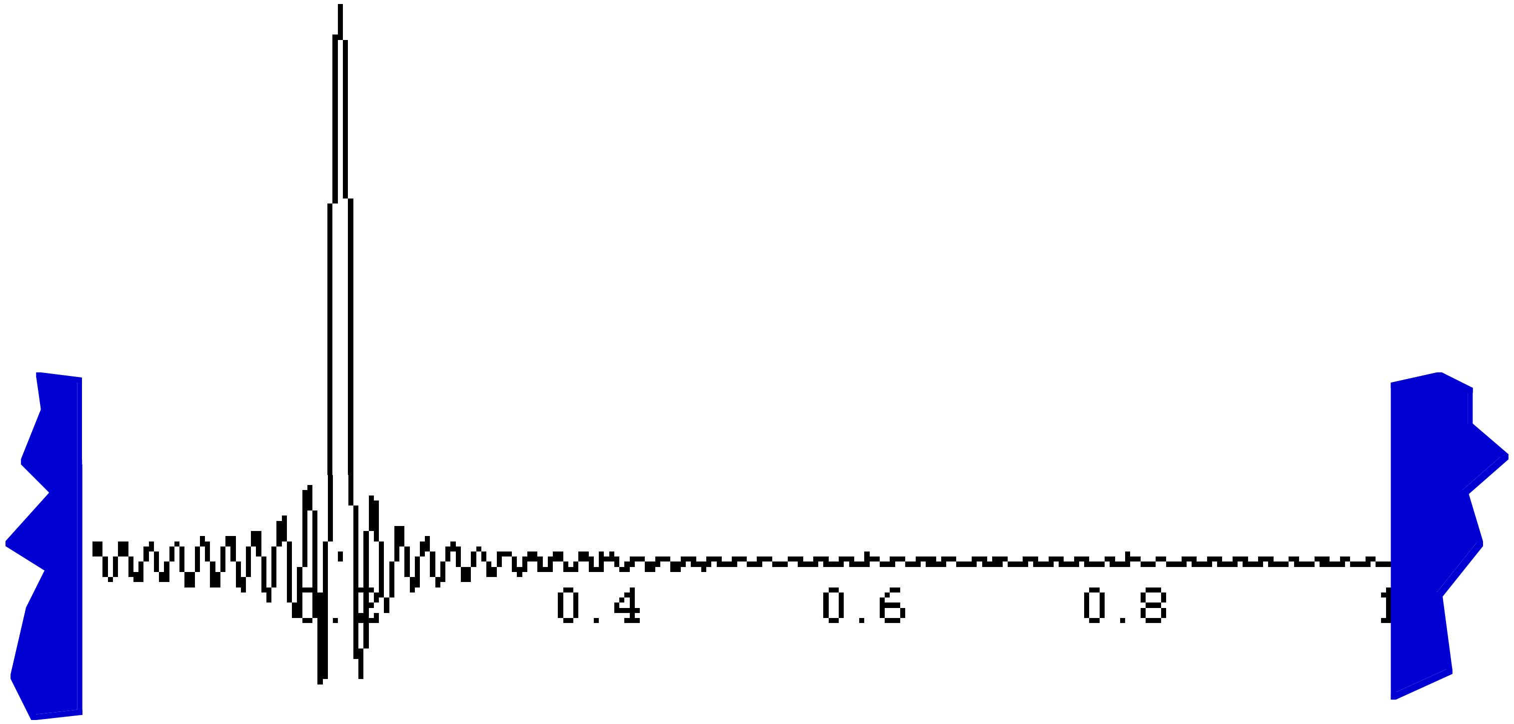
Zero-point period τ_1 is just enough time for "particle" in ε_n-level to make *2n* round trips.

$$\tau_1 = 2n\,T_n(2W) = \frac{8ML^2}{h}$$

In time τ_1 ground ε_1-level particle does 2 round trips,
ε_2-level particle makes 4 round trips,
ε_3-level particle makes 6 round trips,..,

At time τ_1, *M* undergoes a *full revival* and "unexplodes" into his original spike at $x=0.2W$,

$t = 1.0000\tau_1$
$= 3.0\tau_{\text{beat}}$



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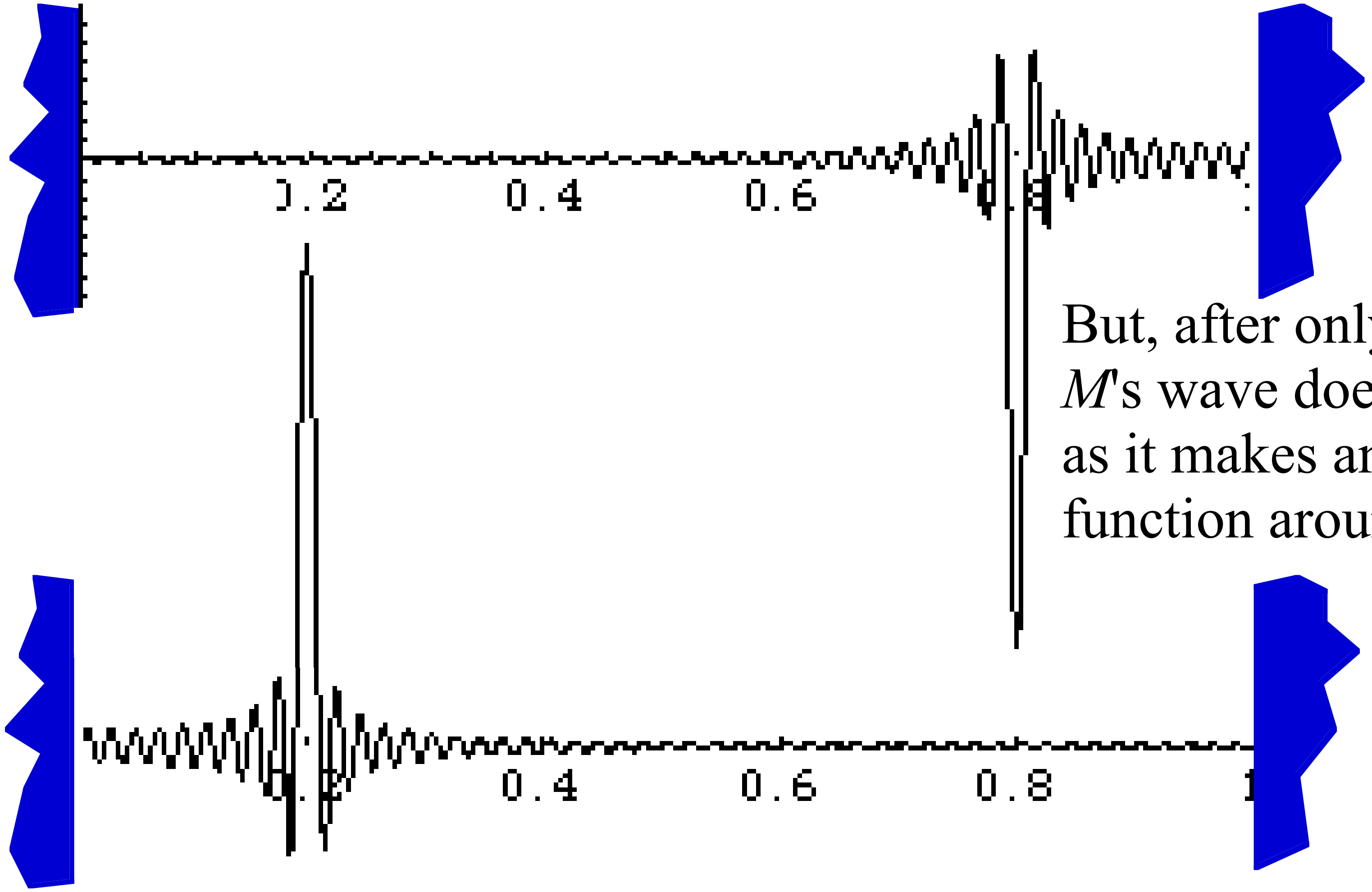
$$t = 0.5000\tau_1$$
$$= 1.5\tau_{beat}$$



$$t = 1.0000\tau_1$$
$$= 3.0\tau_{beat}$$

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

At fractional times τ_1/n *M* undergoes a number of *fractional revivals*

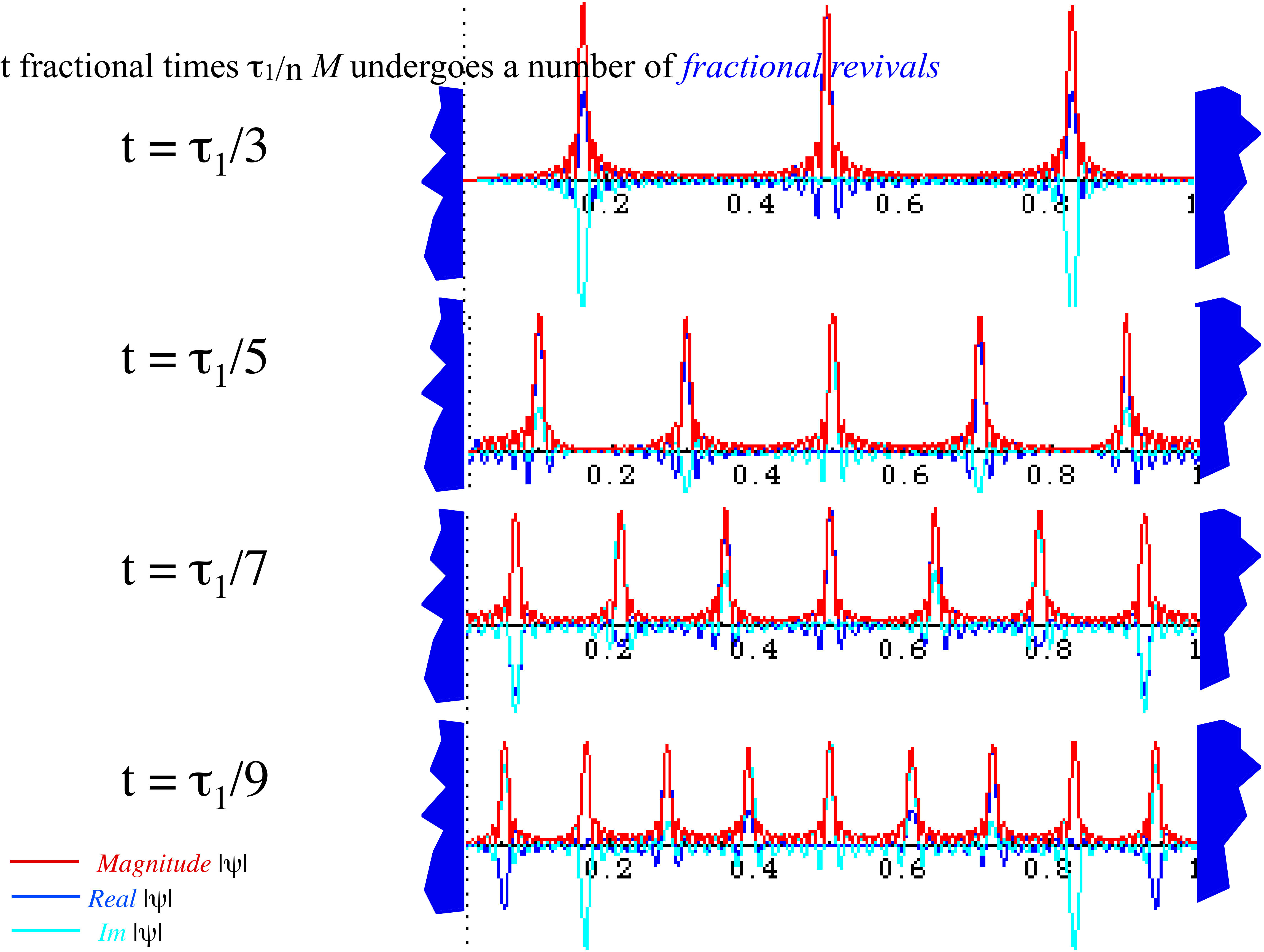


Fig. 12.2.5 The "Dance of the deltas." Mini-Revivals for prisoner M's wavepacket envelope function.

A sketch of modern molecular spectroscopy

The frequency hierarchy   *Example of16μm spectra of CF_4*

Units of frequency (Hz), wavelength (m), and energy (eV)

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Wavepacket explodes! (Then revives)

Quantum "revivals" of gently localized rotor waves: A lesson in quantum number theory

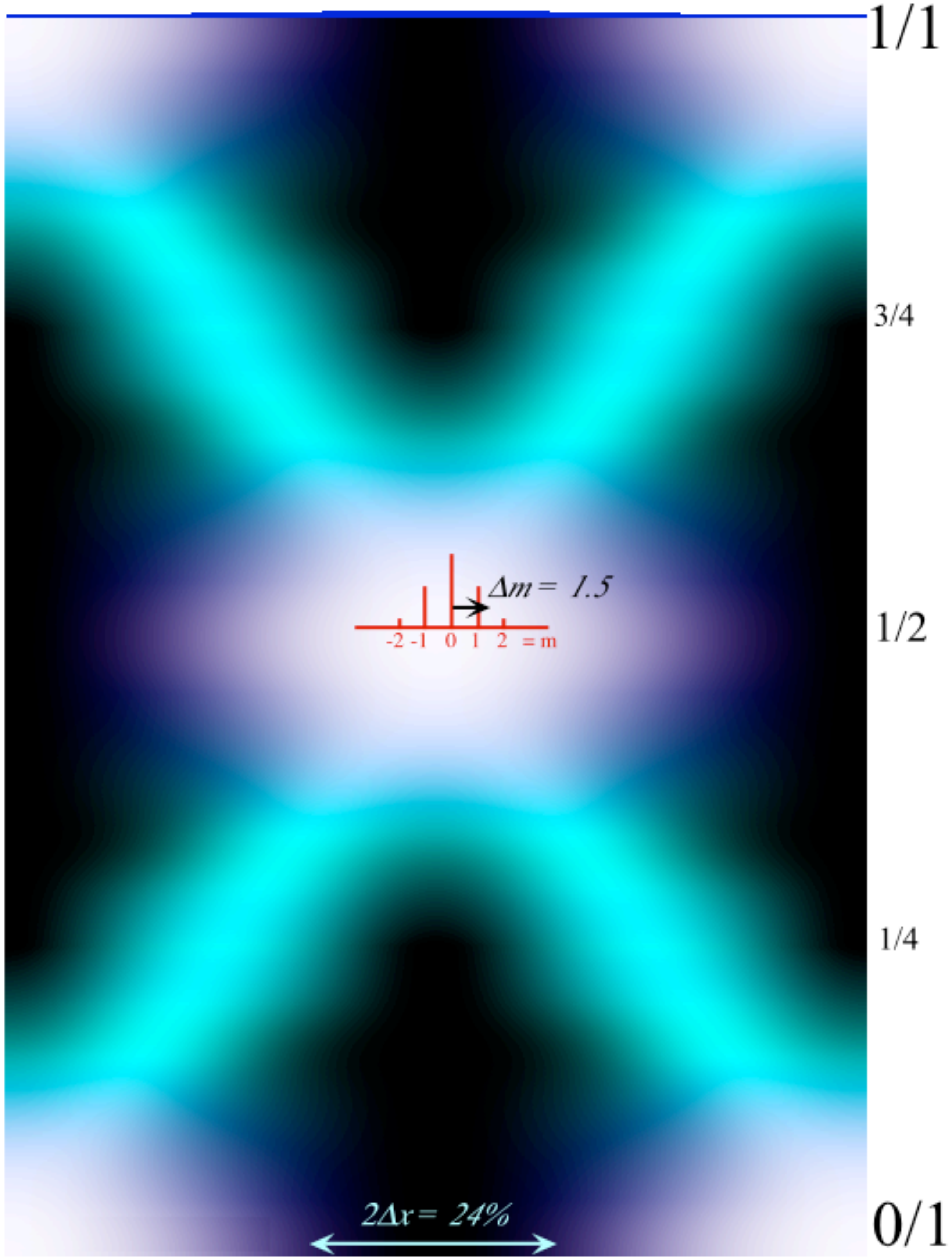
Farey-Sums and Ford-products

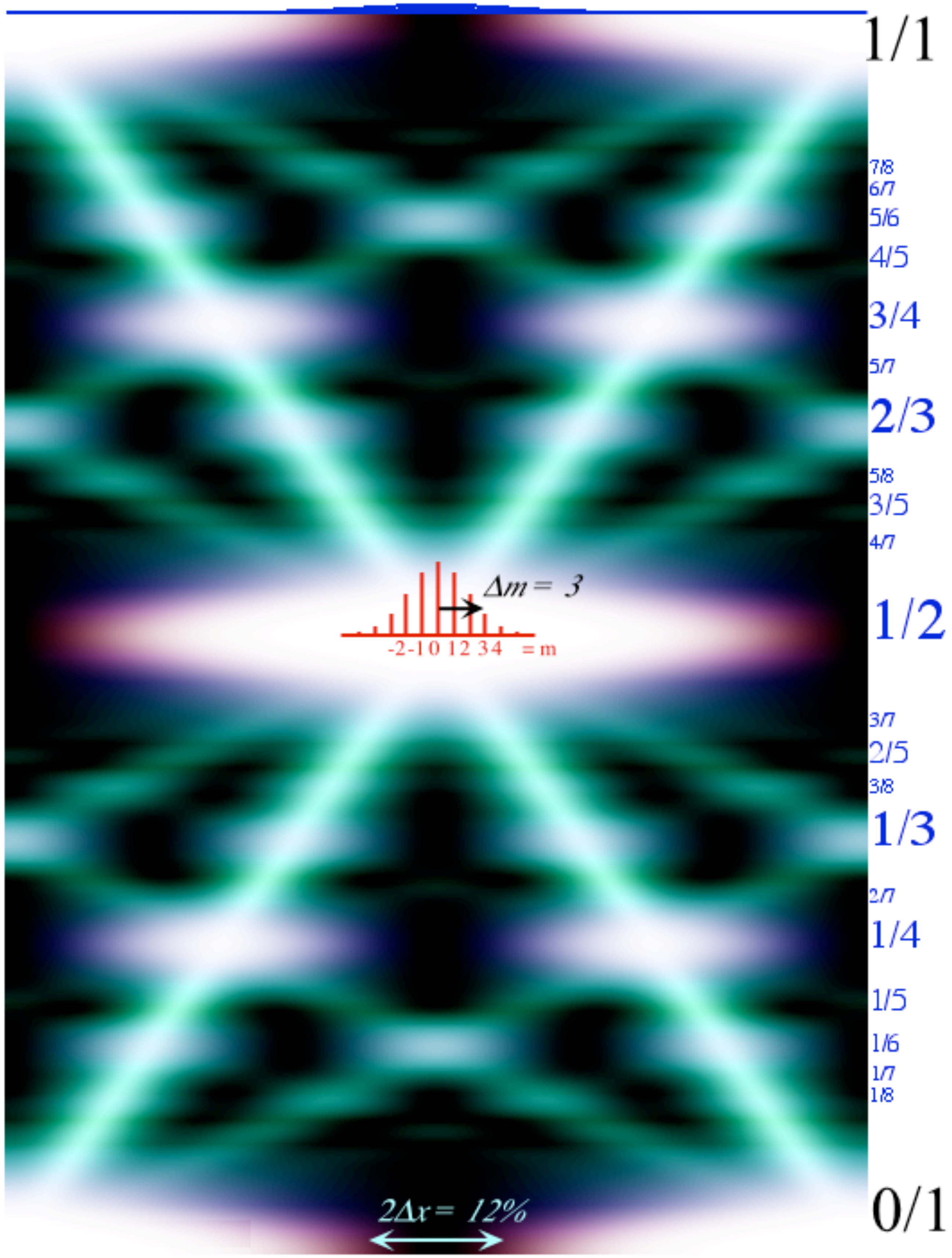
Ford Circles and Farey-Trees

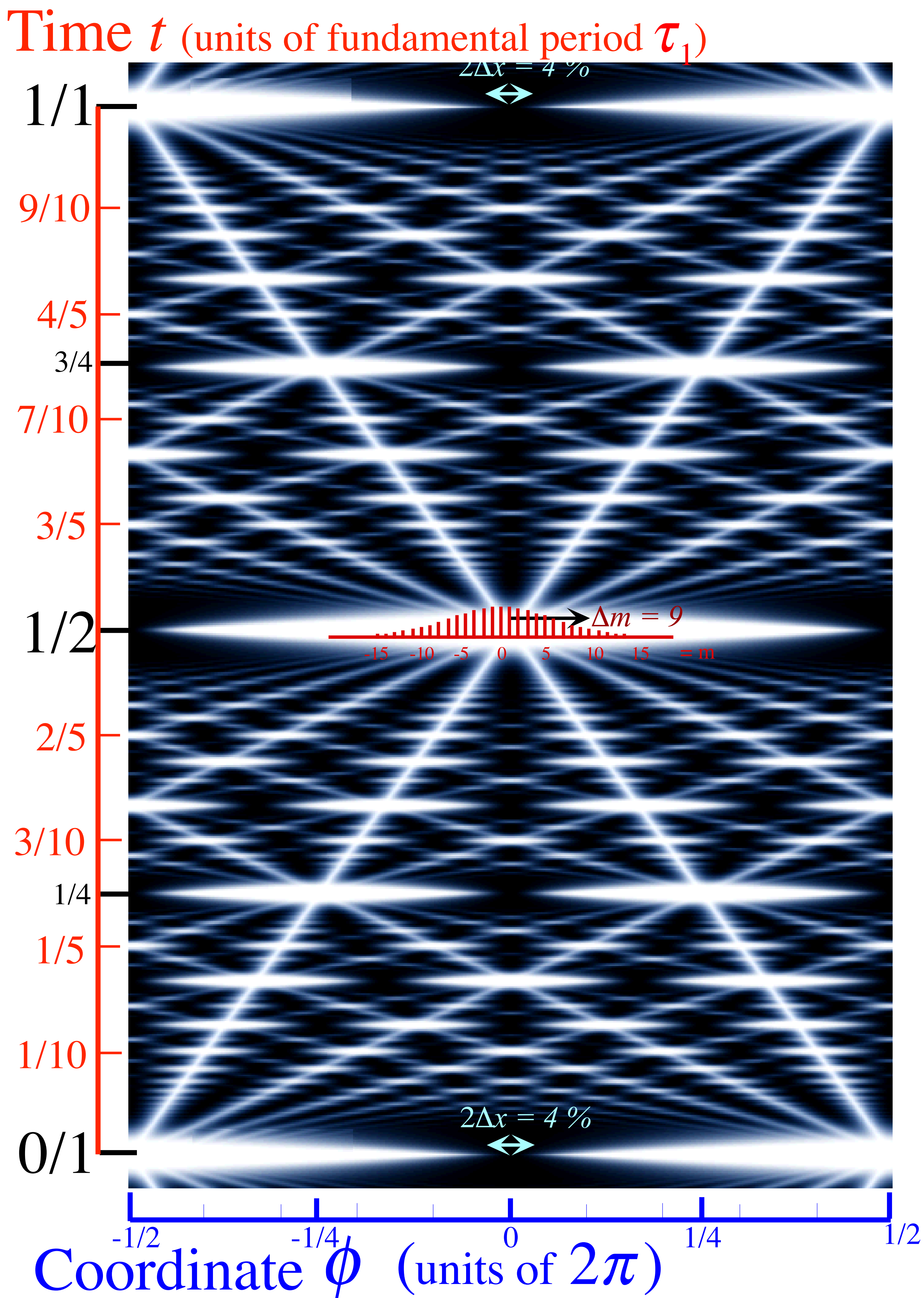
*Quantum "revivals" of gently*localized rotor waves*

A lesson in quantum number theory

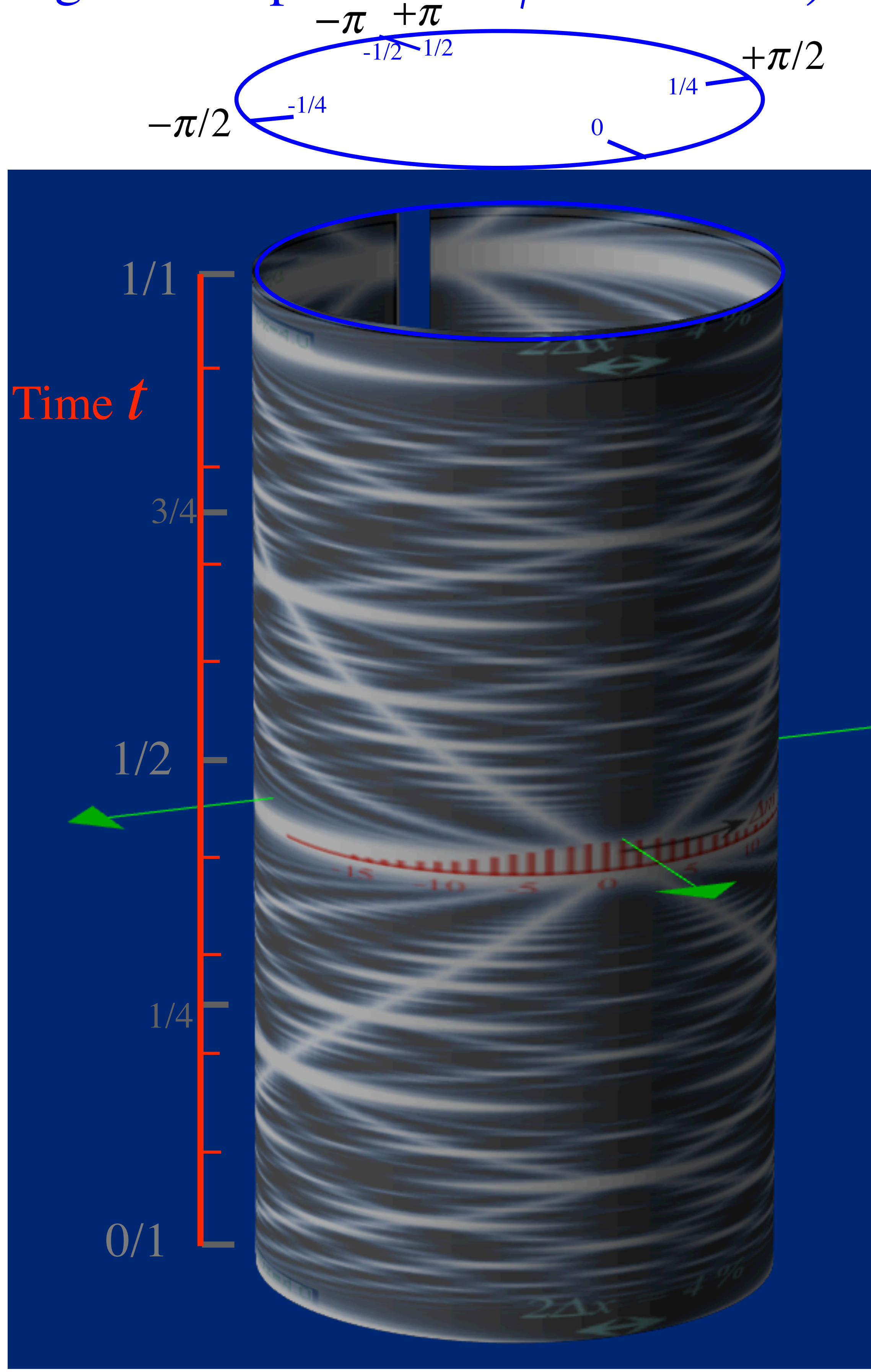
**gently means gently-truncated Gaussian distributions*





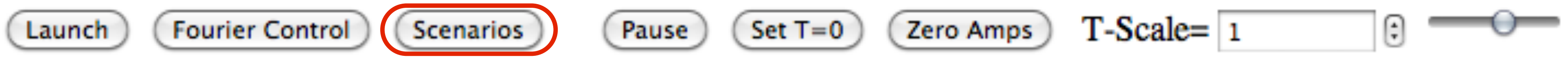


(Imagine "wrap-around" ϕ-coordinate)

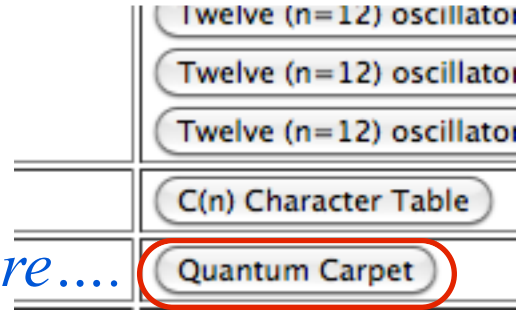


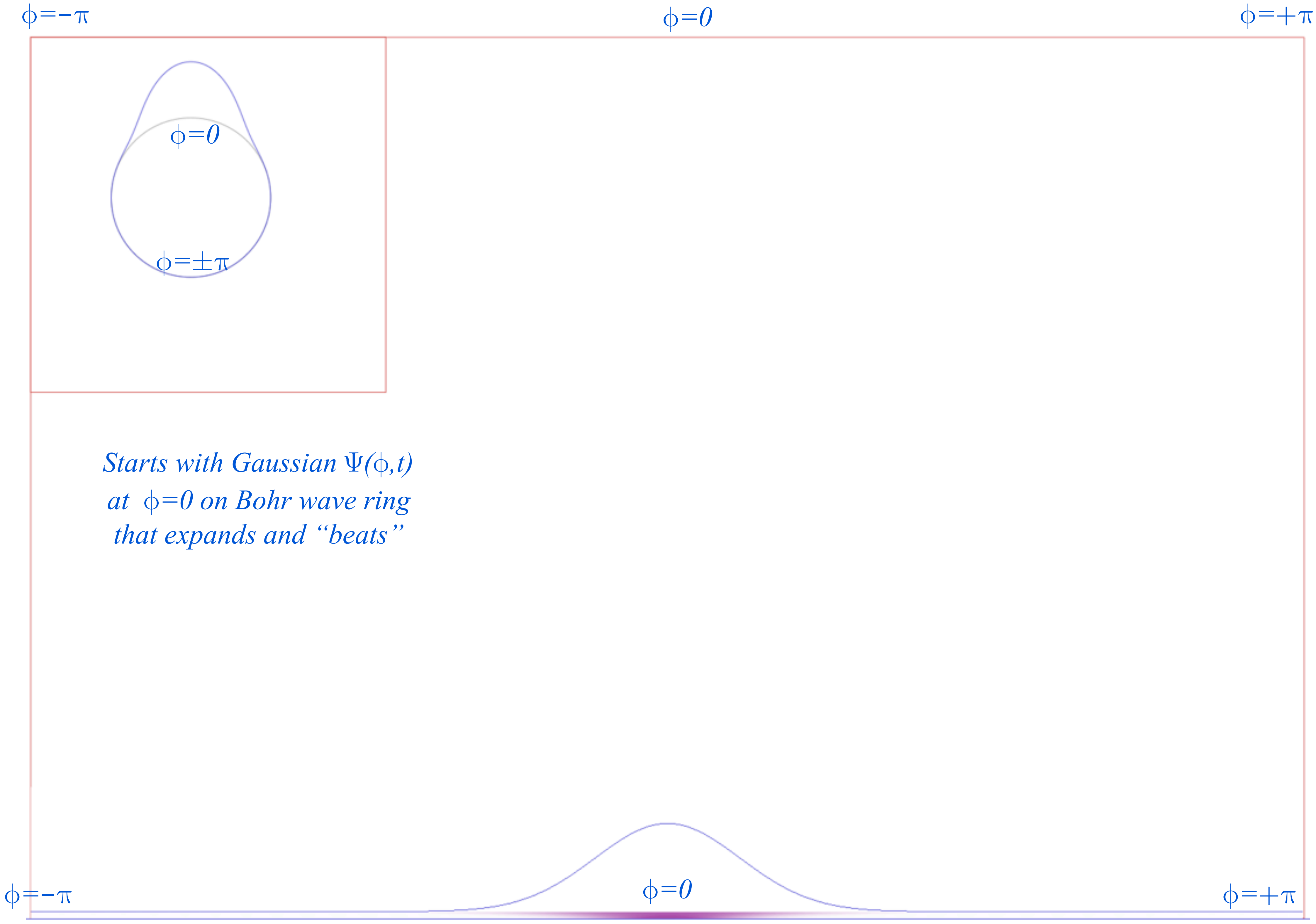
WaveIt Web simulation https://www.uark.edu/ua/modphys/markup/WaveItWeb.html?scenario=Quantum%20Carpet

Click here....



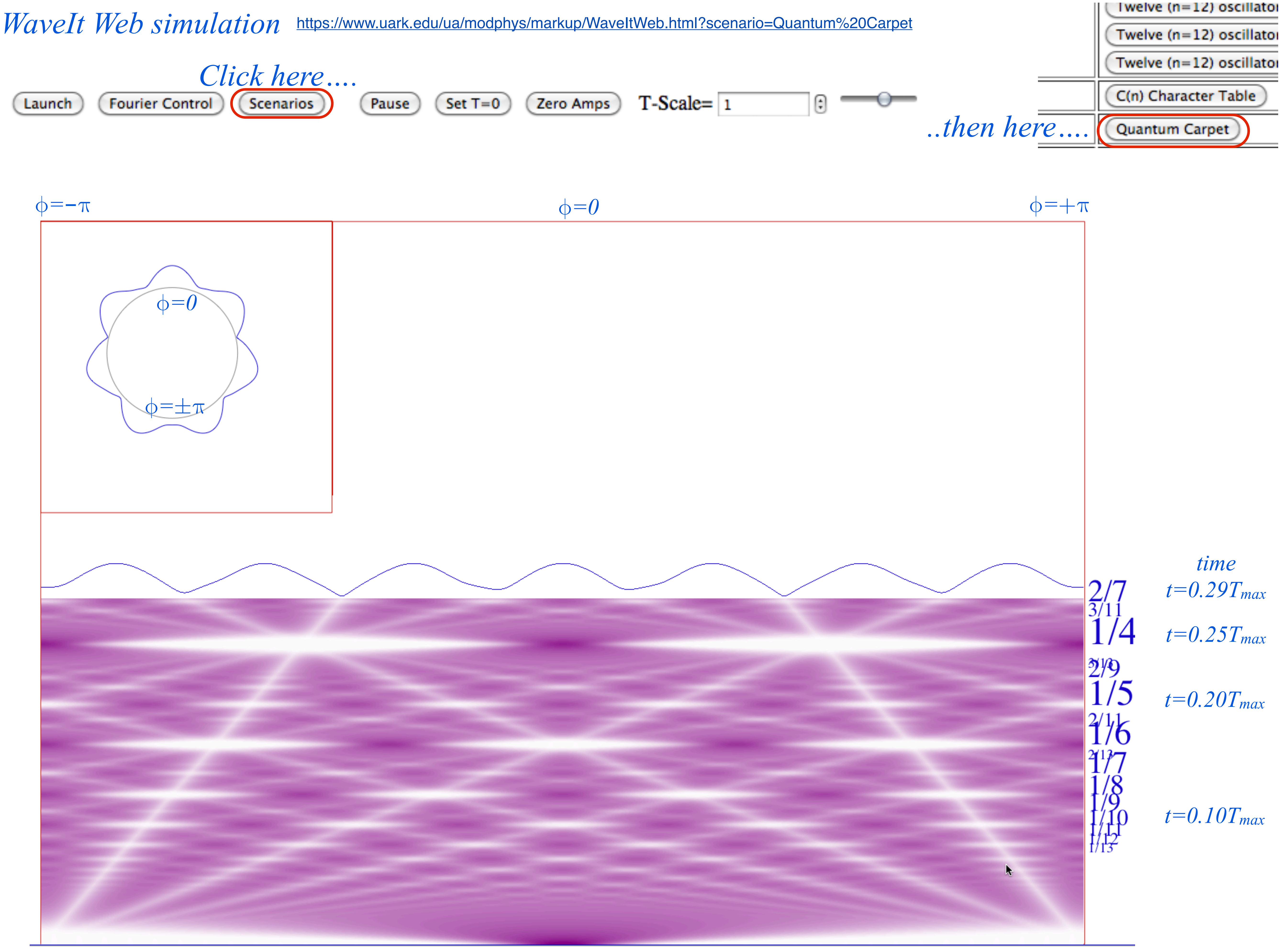
..then here....



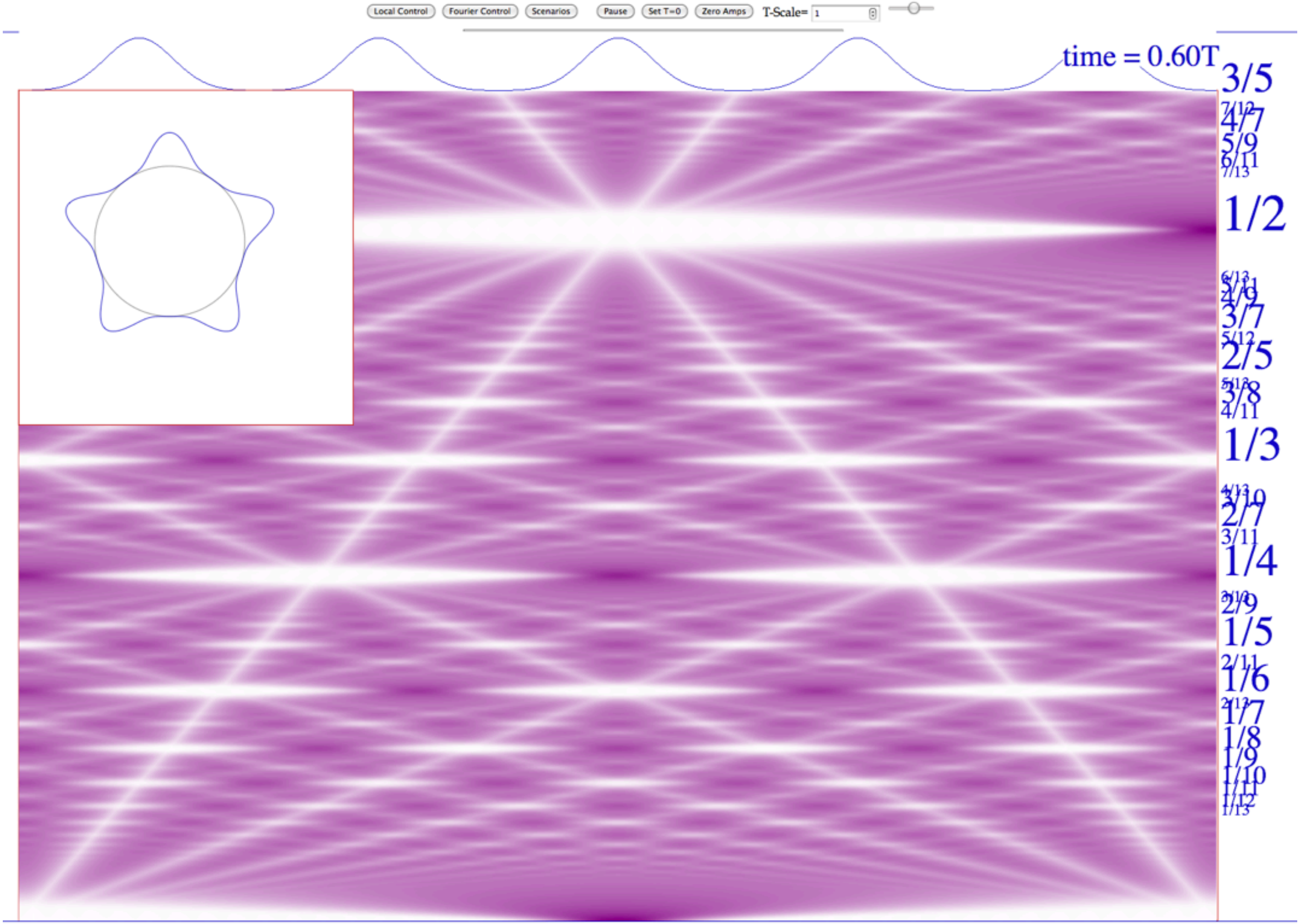


Starts with Gaussian Ψ(φ,t)
at φ=0 on Bohr wave ring
that expands and "beats"

WaveIt Web simulation https://www.uark.edu/ua/modphys/markup/WaveItWeb.html?scenario=Quantum%20Carpet


Click here....

..then here....


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
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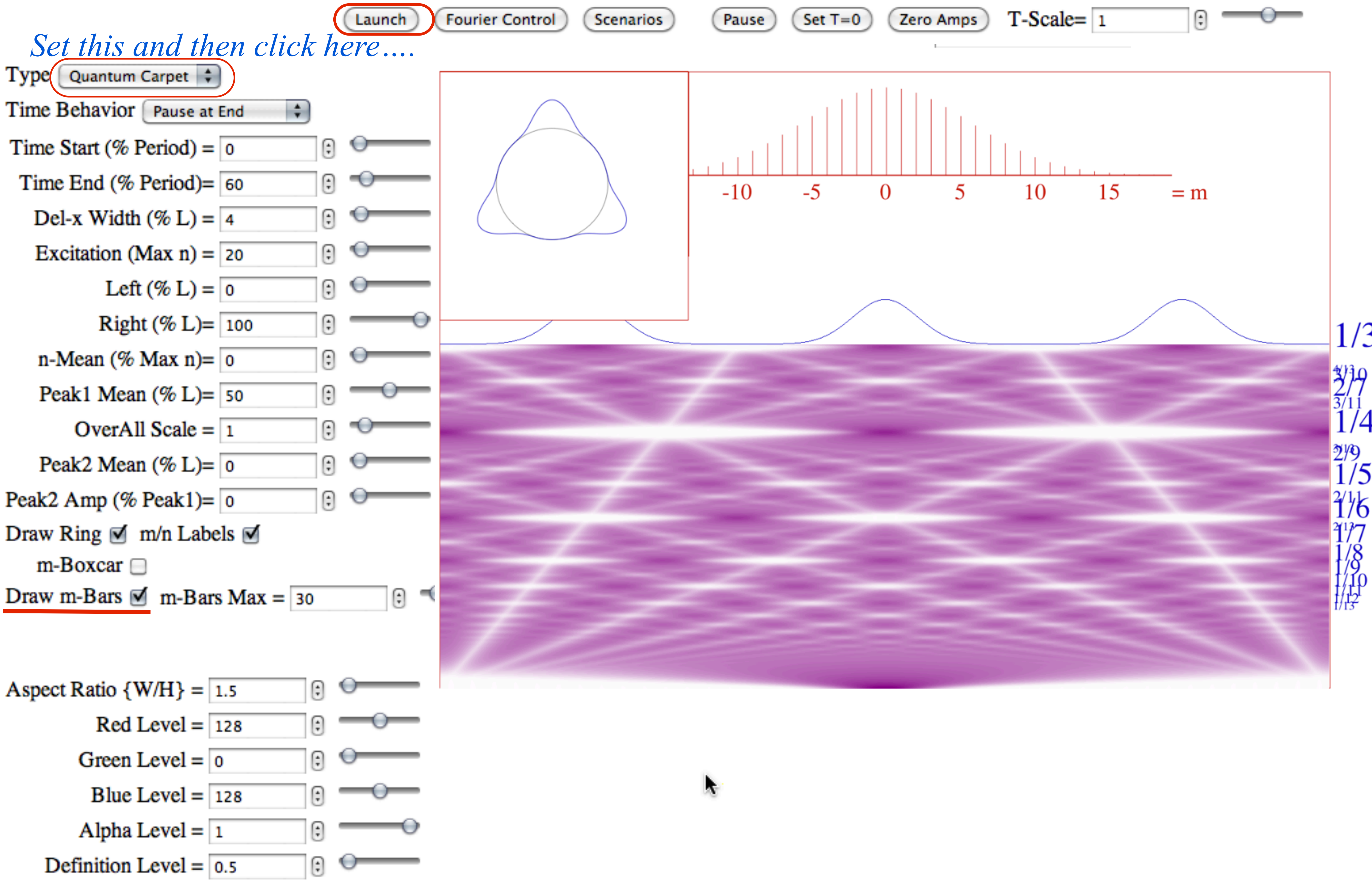
1/12
1/13



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

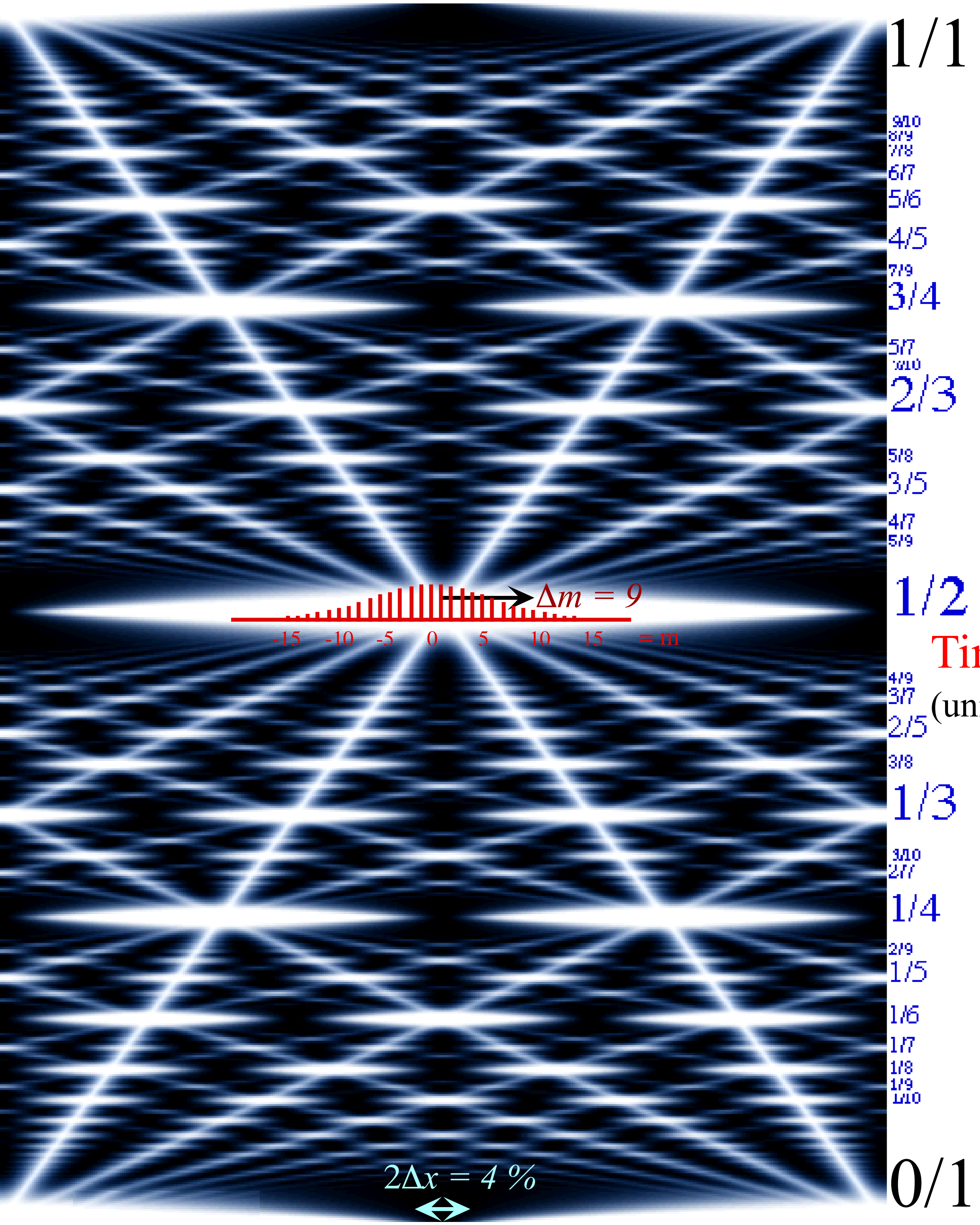
Alpha Level = 1

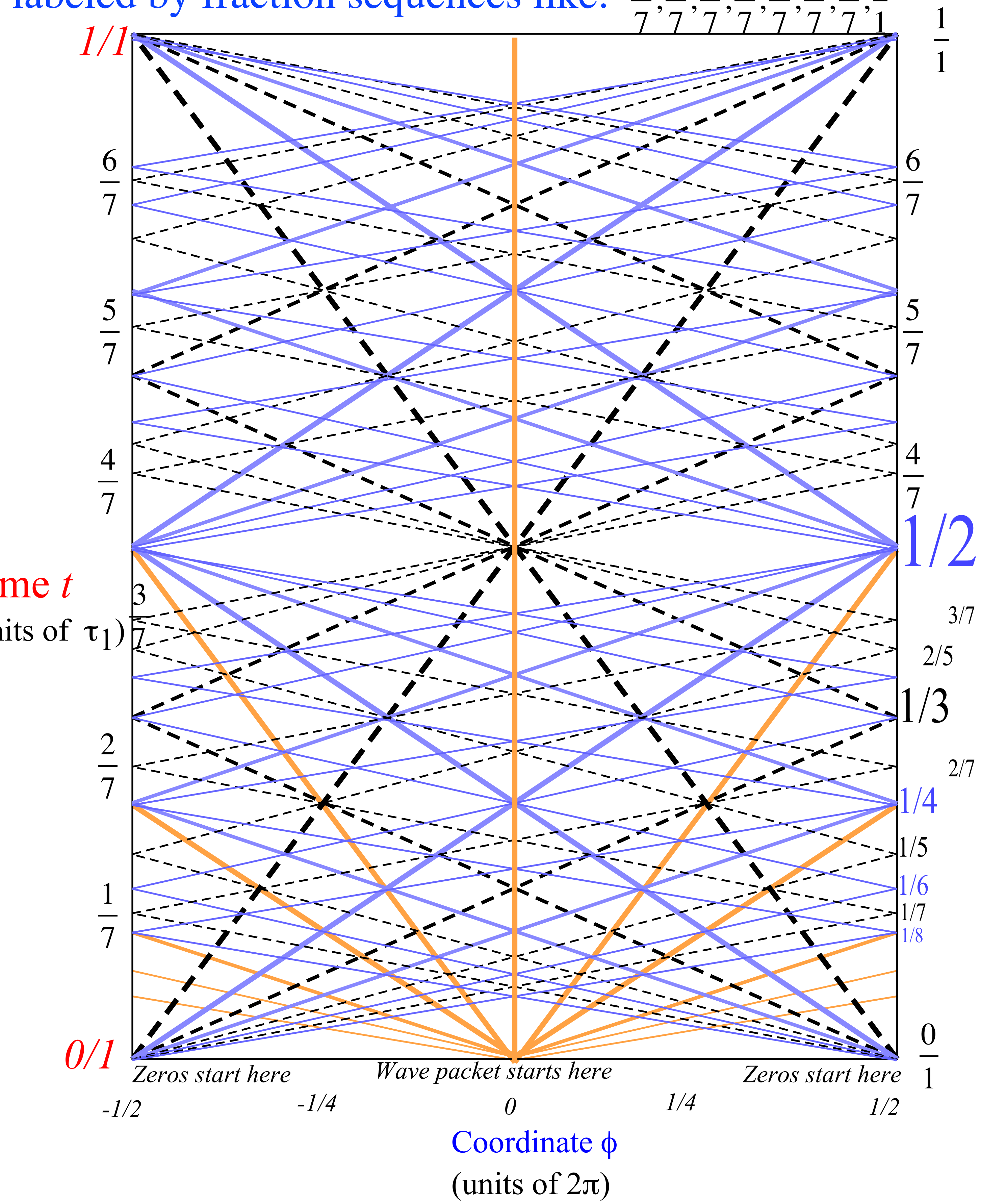
Definition Level = 0.5

N-level-system and revival-beat wave dynamics

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

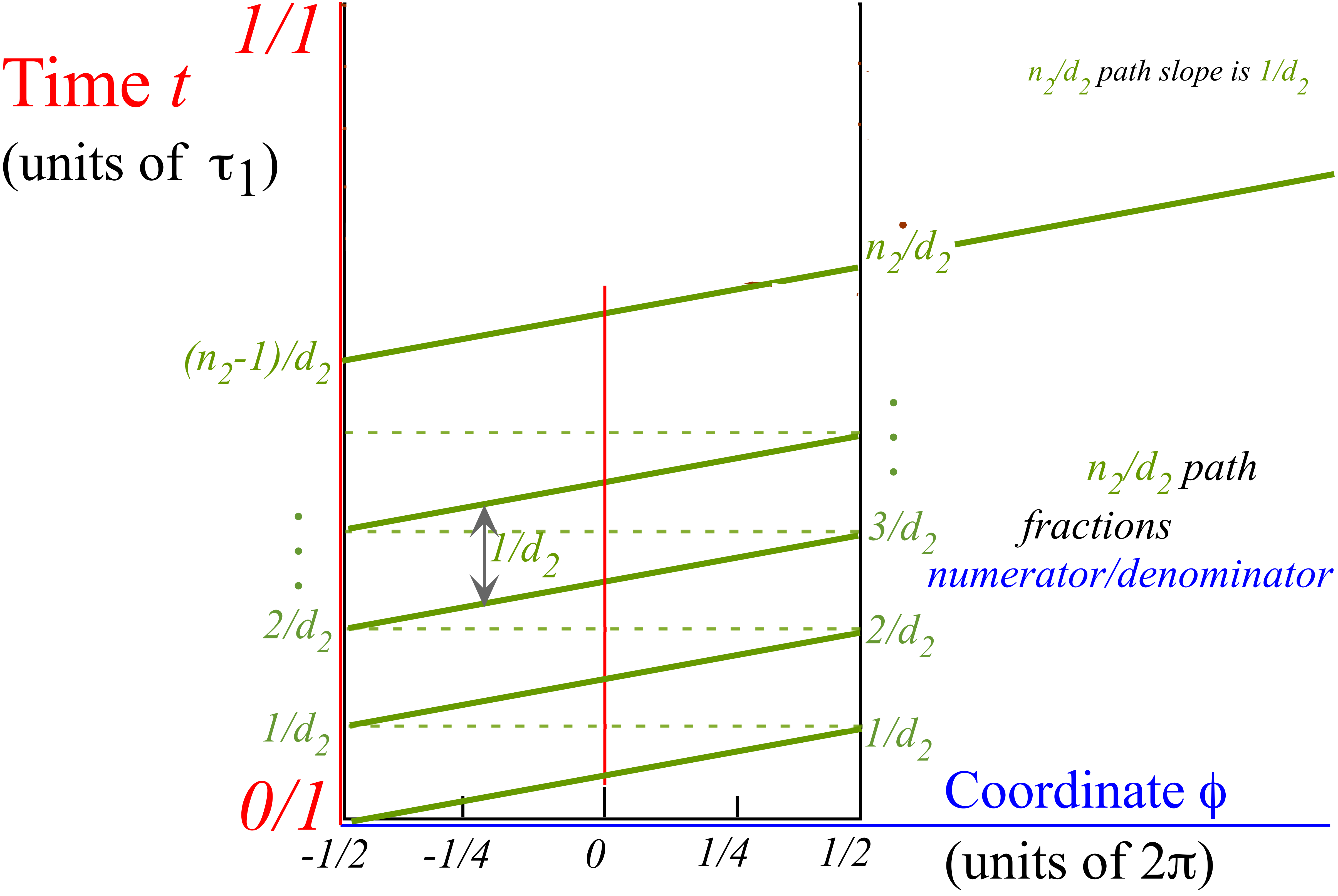
Zeros (clearly) and "particle-packets" (faintly) have paths labeled by fraction sequences like: $\frac{0}{7}, \frac{1}{7}, \frac{2}{7}, \frac{3}{7}, \frac{4}{7}, \frac{5}{7}, \frac{6}{7}, \frac{1}{1}$





Farey Sum algebra of revival-beat wave dynamics

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



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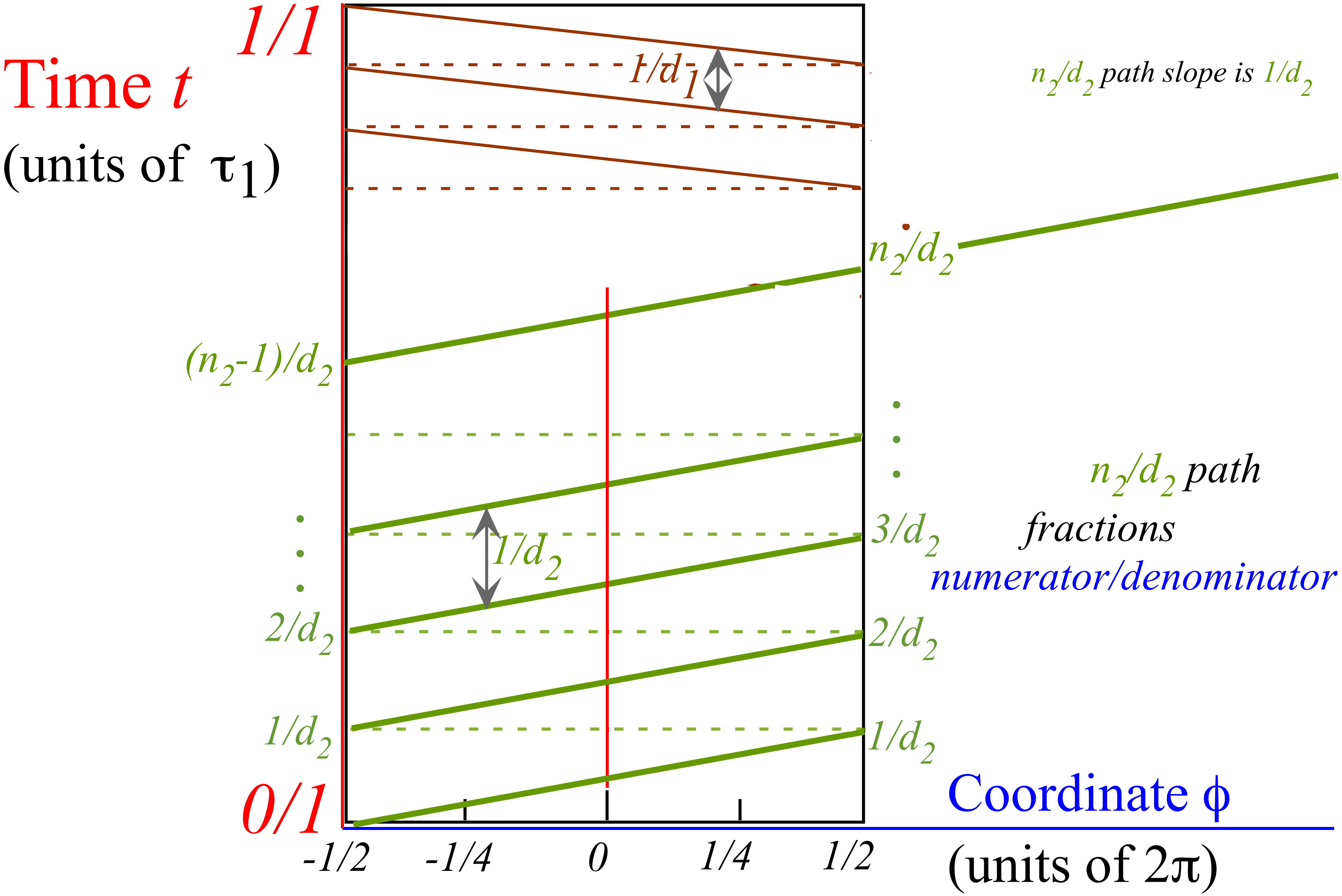

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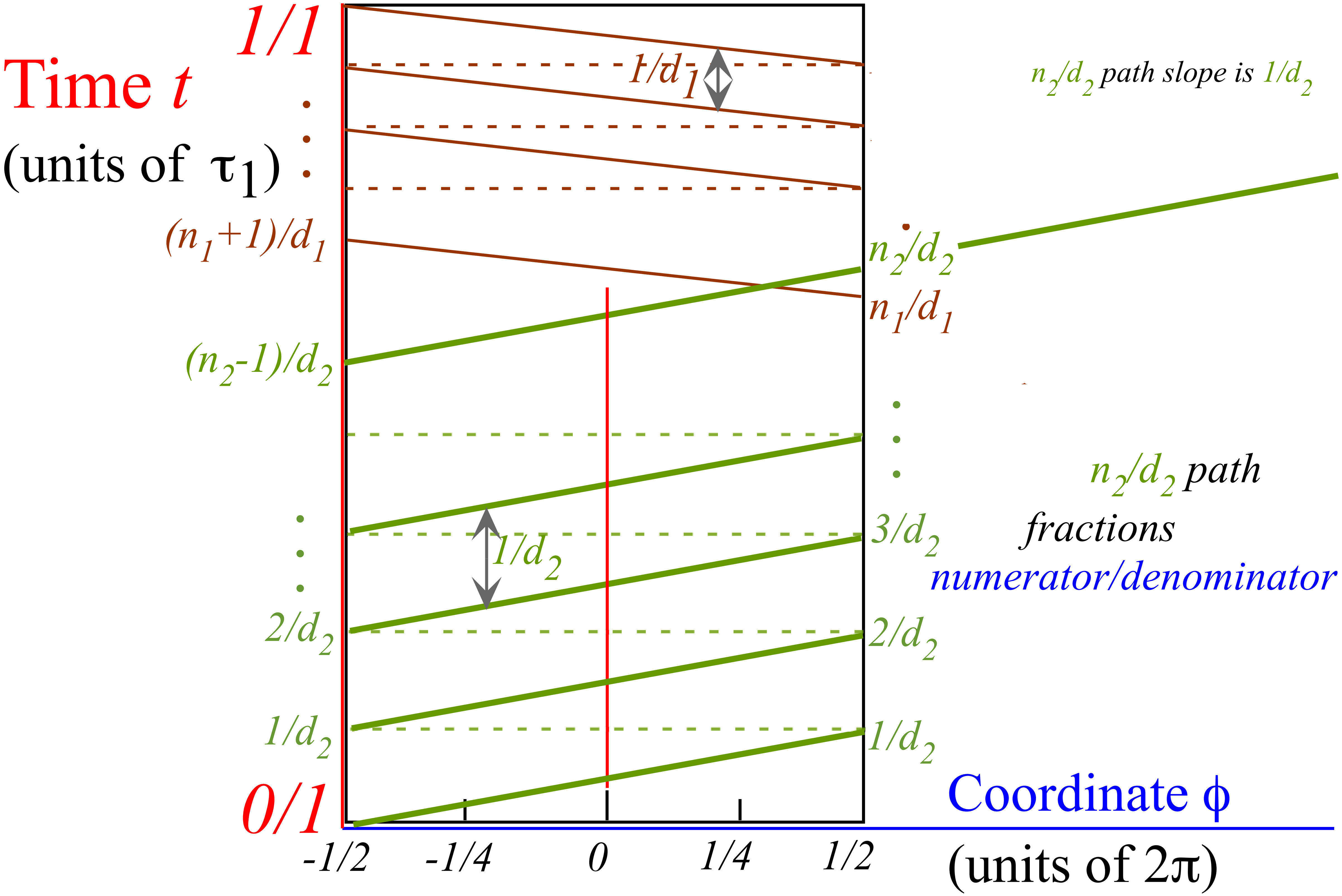

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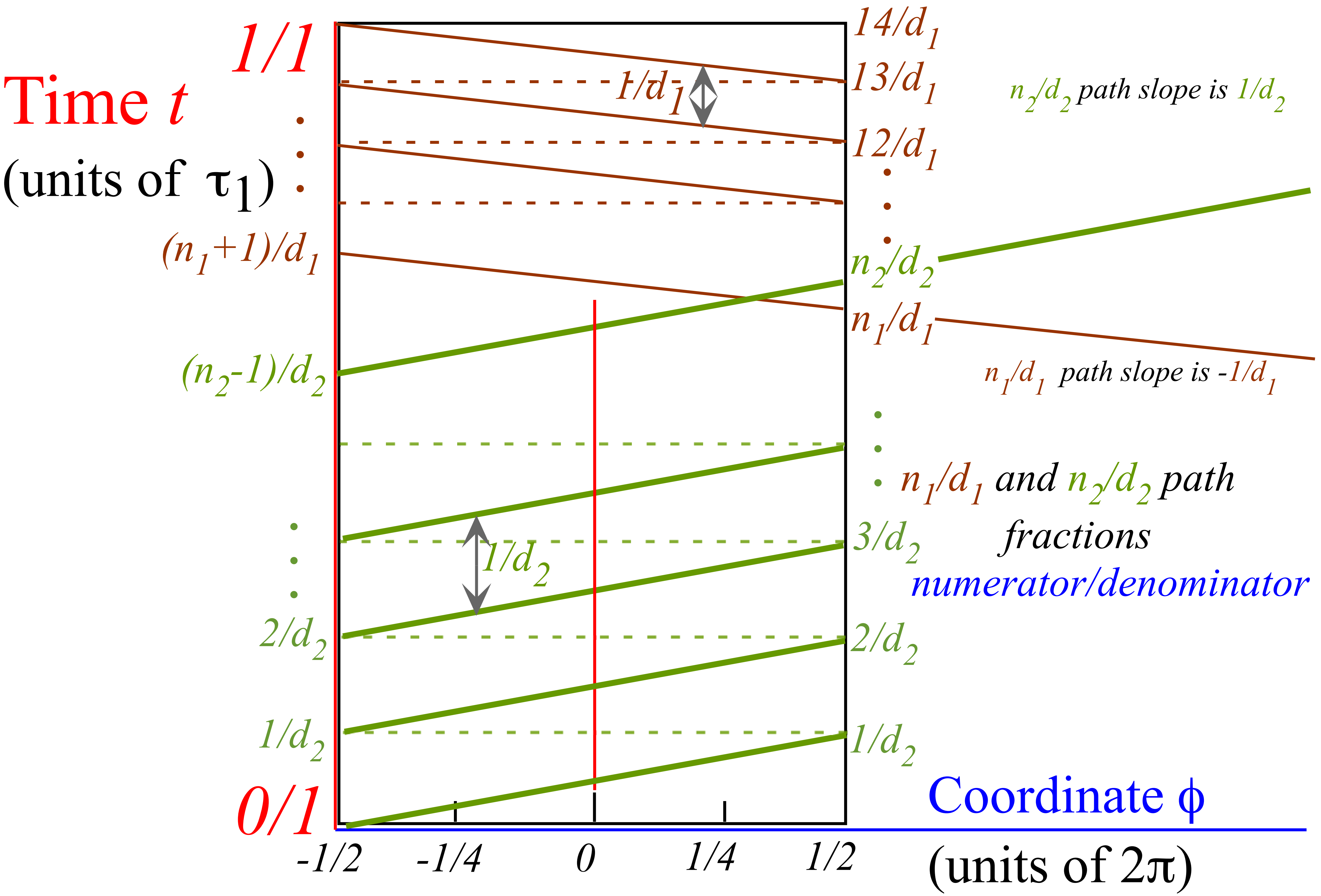

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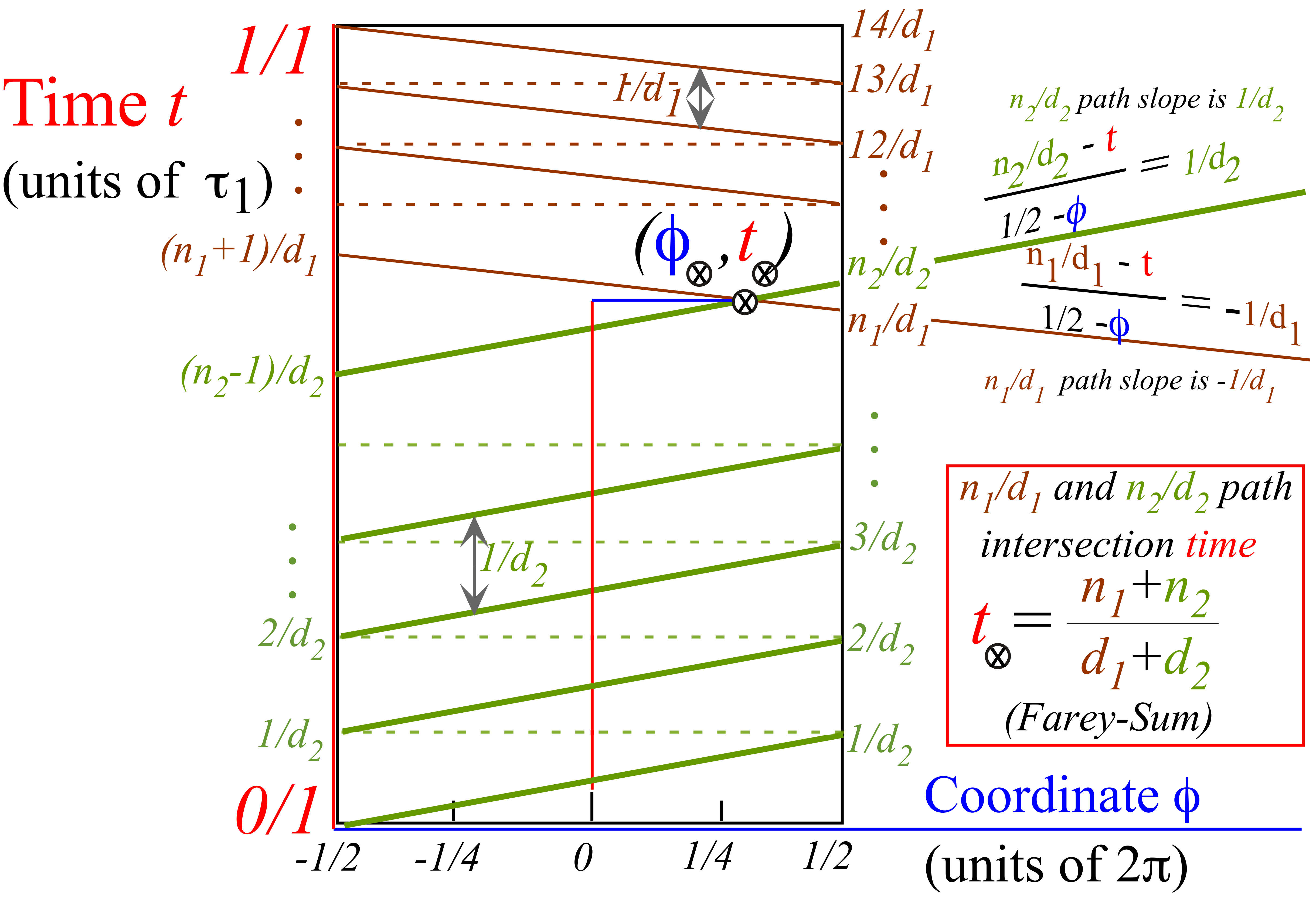


n_1/d_1 and n_2/d_2 path intersection time

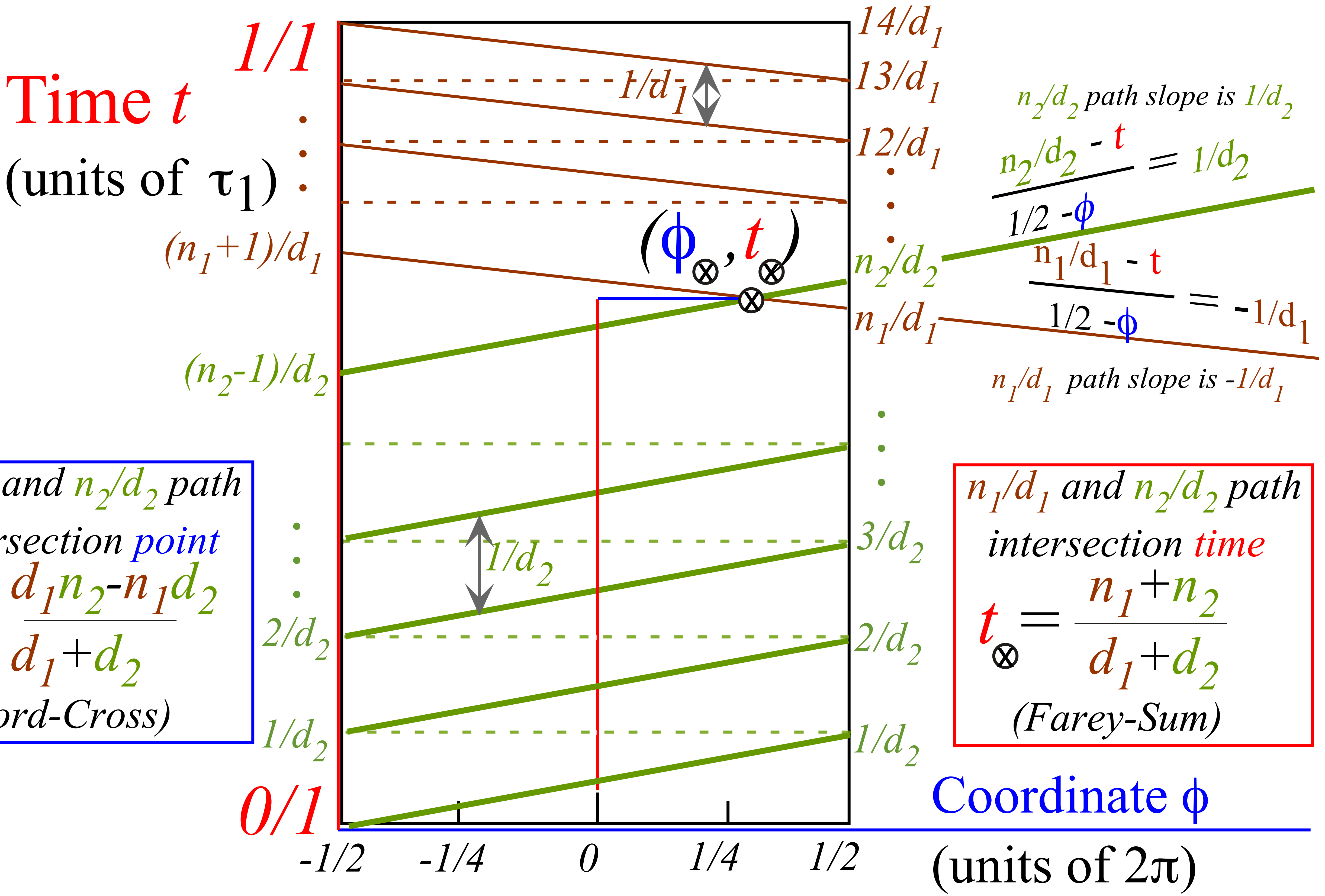
$$t_\otimes = \frac{n_1+n_2}{d_1+d_2}$$

(Farey-Sum)

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

Farey Sum algebra of revival-beat wave dynamics

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



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)]

“Monster Mash” classical segue to Heisenberg action relations

Example of very very large M_1 ball-walls crushing a poor little m_2

How m_2 keeps its action

An interesting wave analogy: The “Tiny-Big-Bang” [*Harter, J. Mol. Spec. 210, 166-182 (2001)*],[*Harter, Li IMSS (2012)**]

A lesson in geometry of fractions and fractals: Ford Circles and Farey Sums

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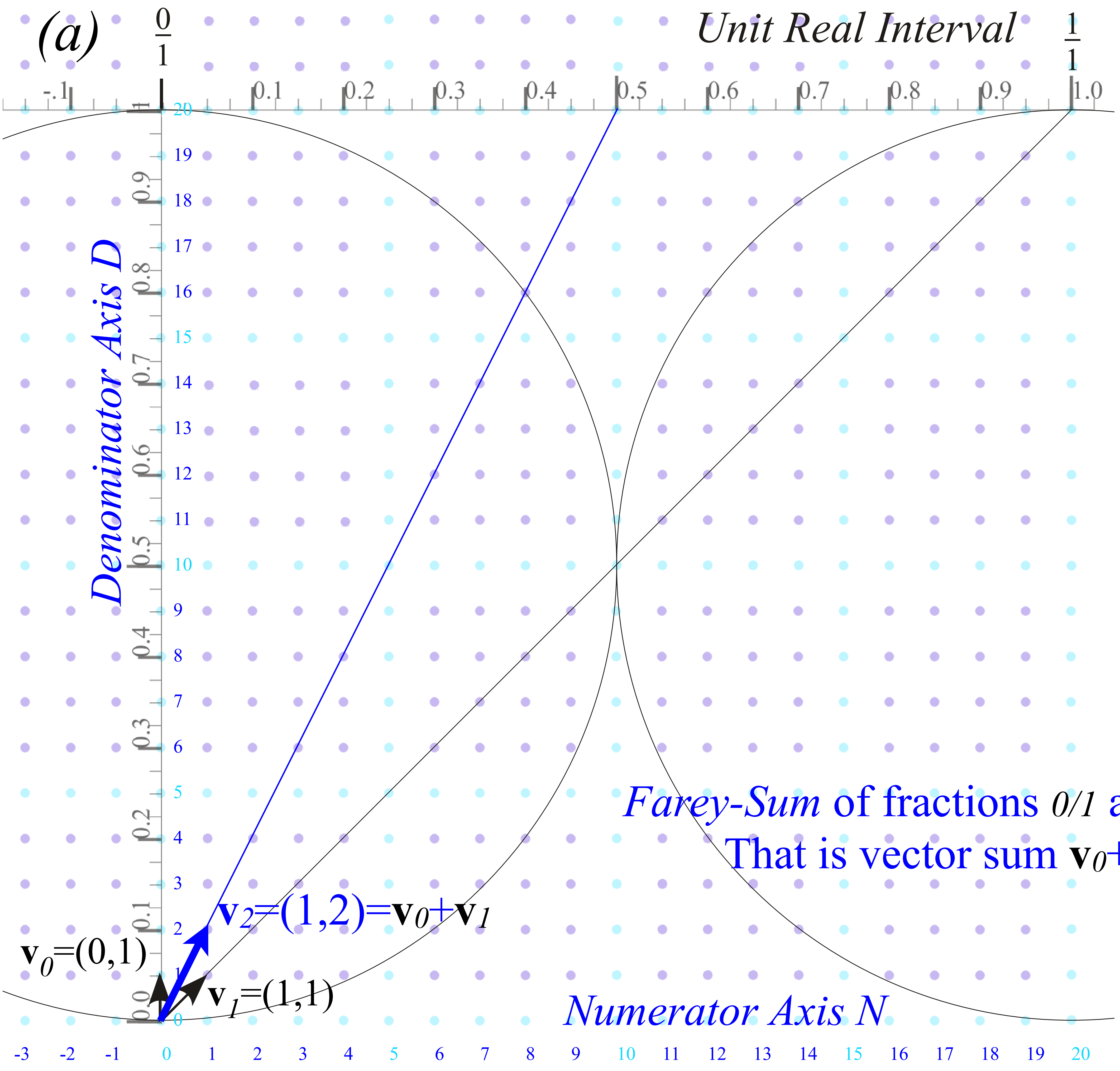
Farey Sum related to vector sum and *Ford Circles*

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 (2015)*]

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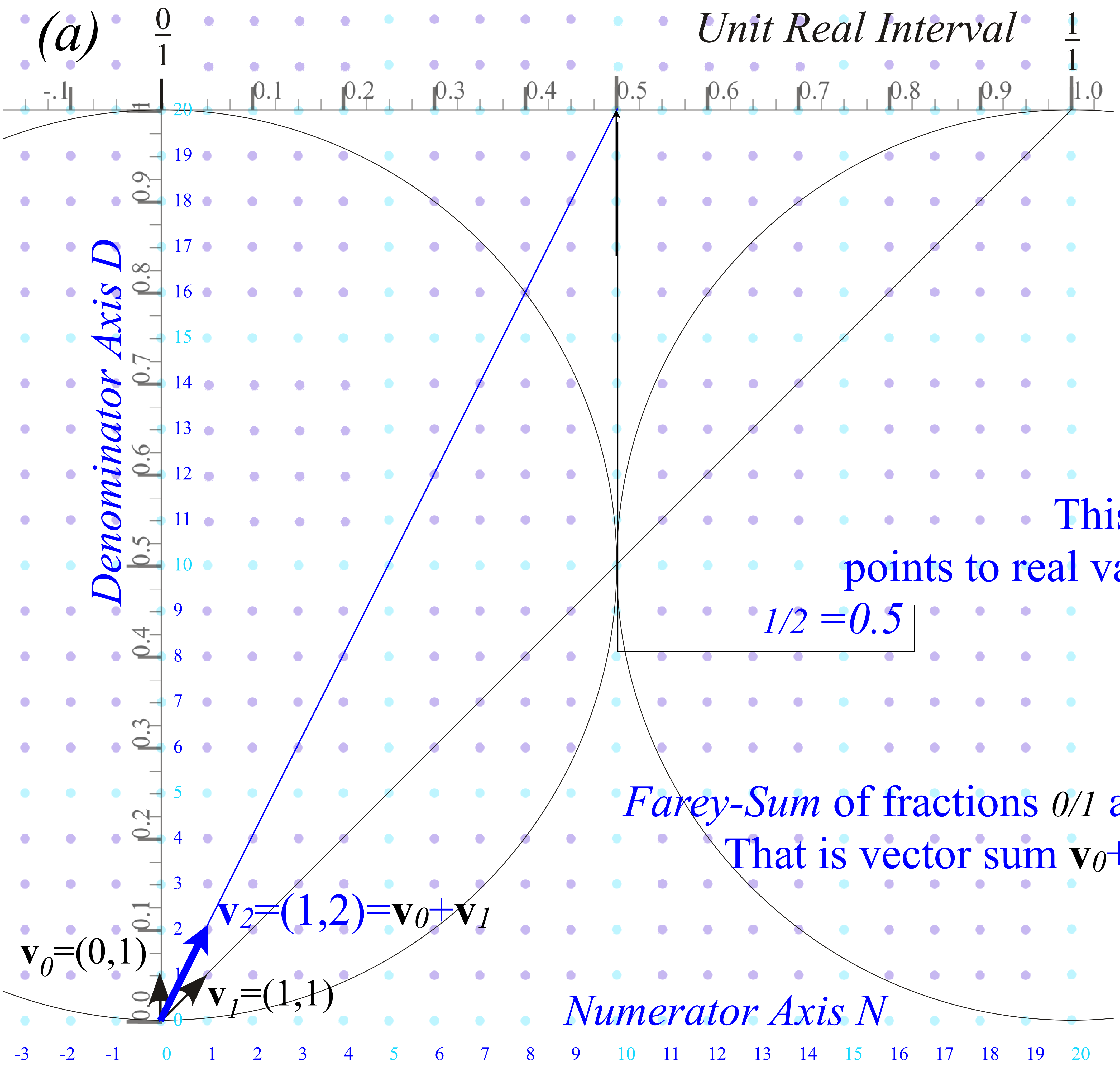

$\mathbf{v}_0$=(0,1)

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

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

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

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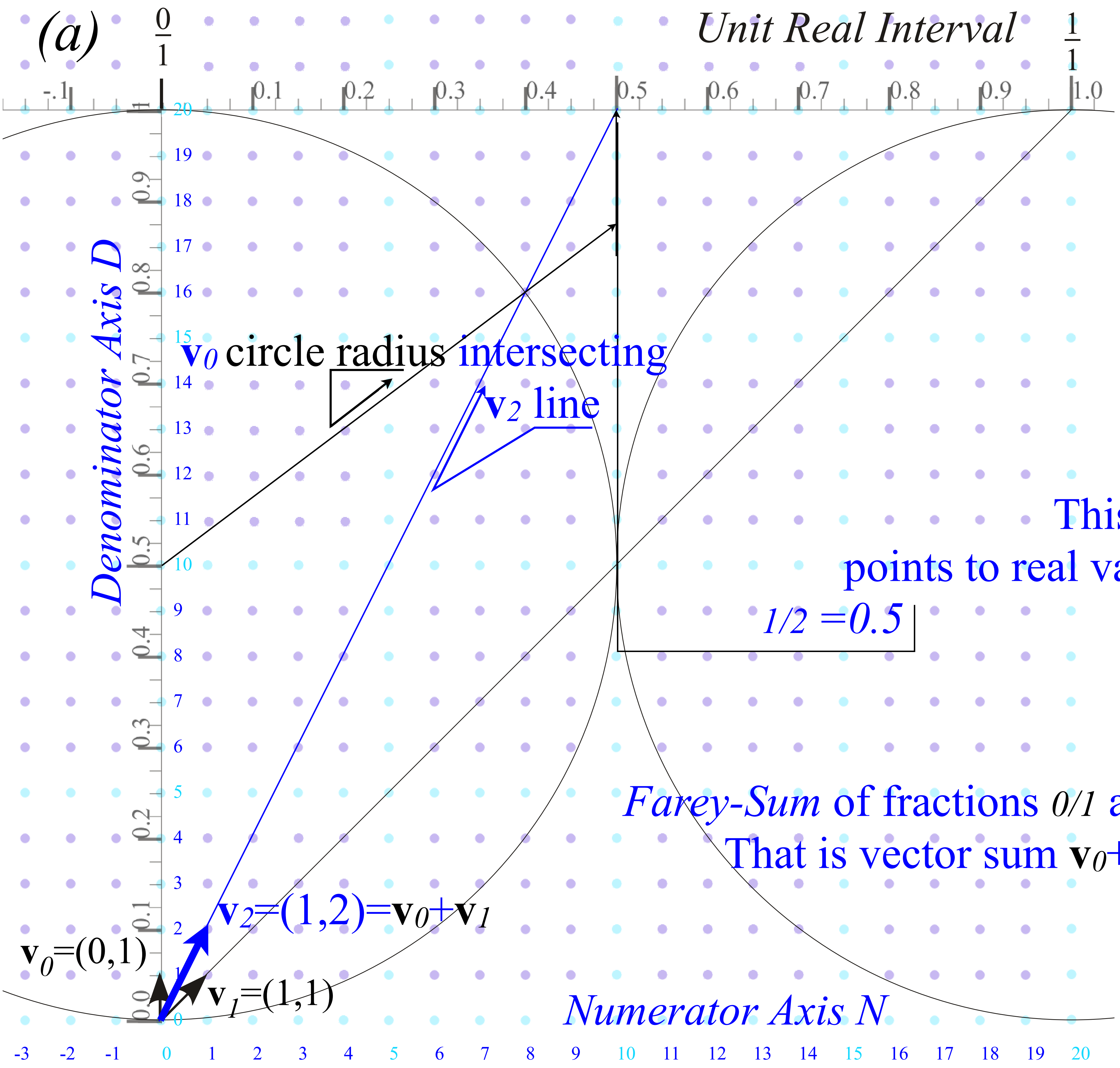

$\mathbf{v}_0$ circle radius intersecting $\mathbf{v}_2$ line

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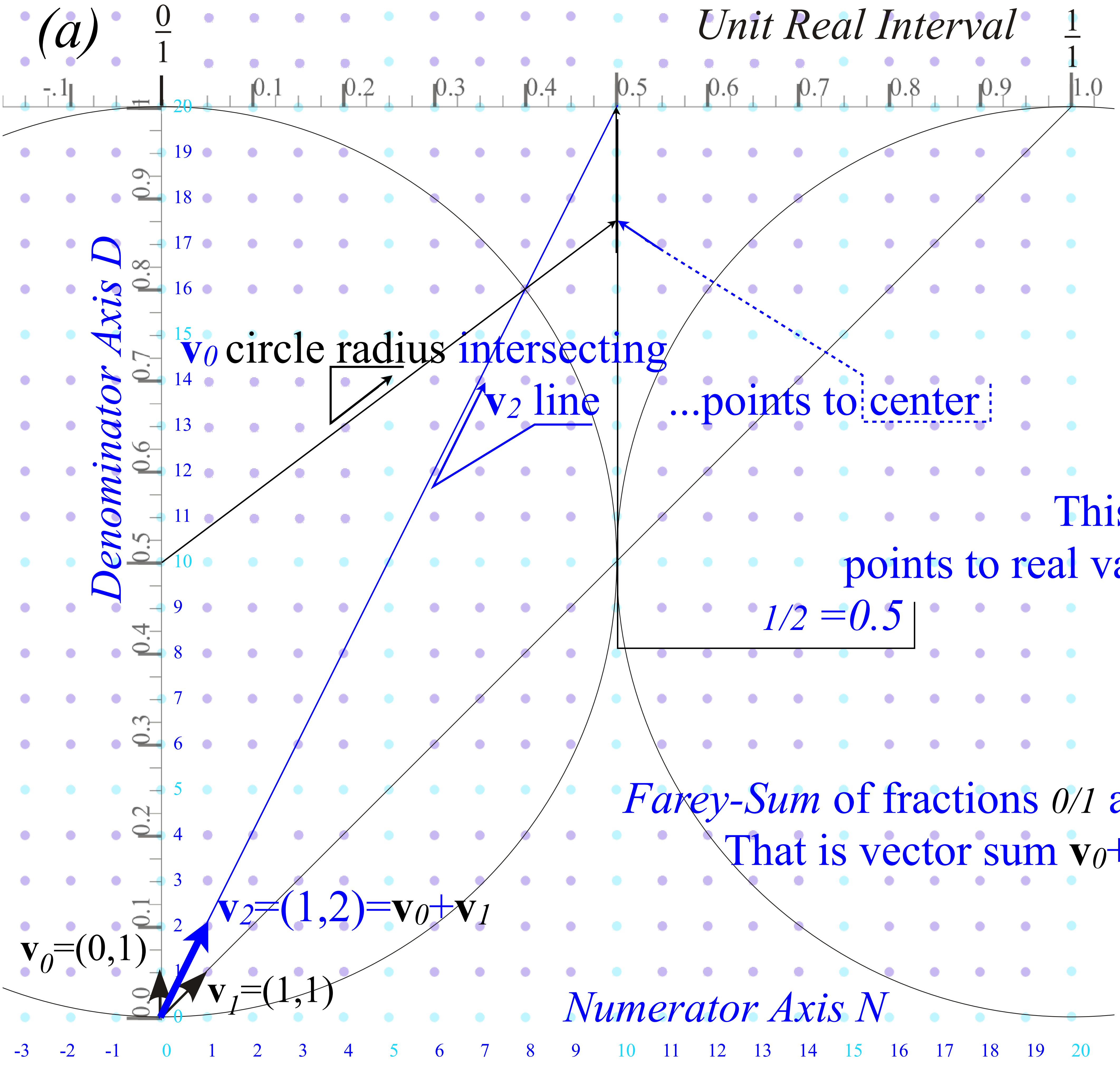

$\mathbf{v}_0$ circle radius intersecting $\mathbf{v}_2$ line

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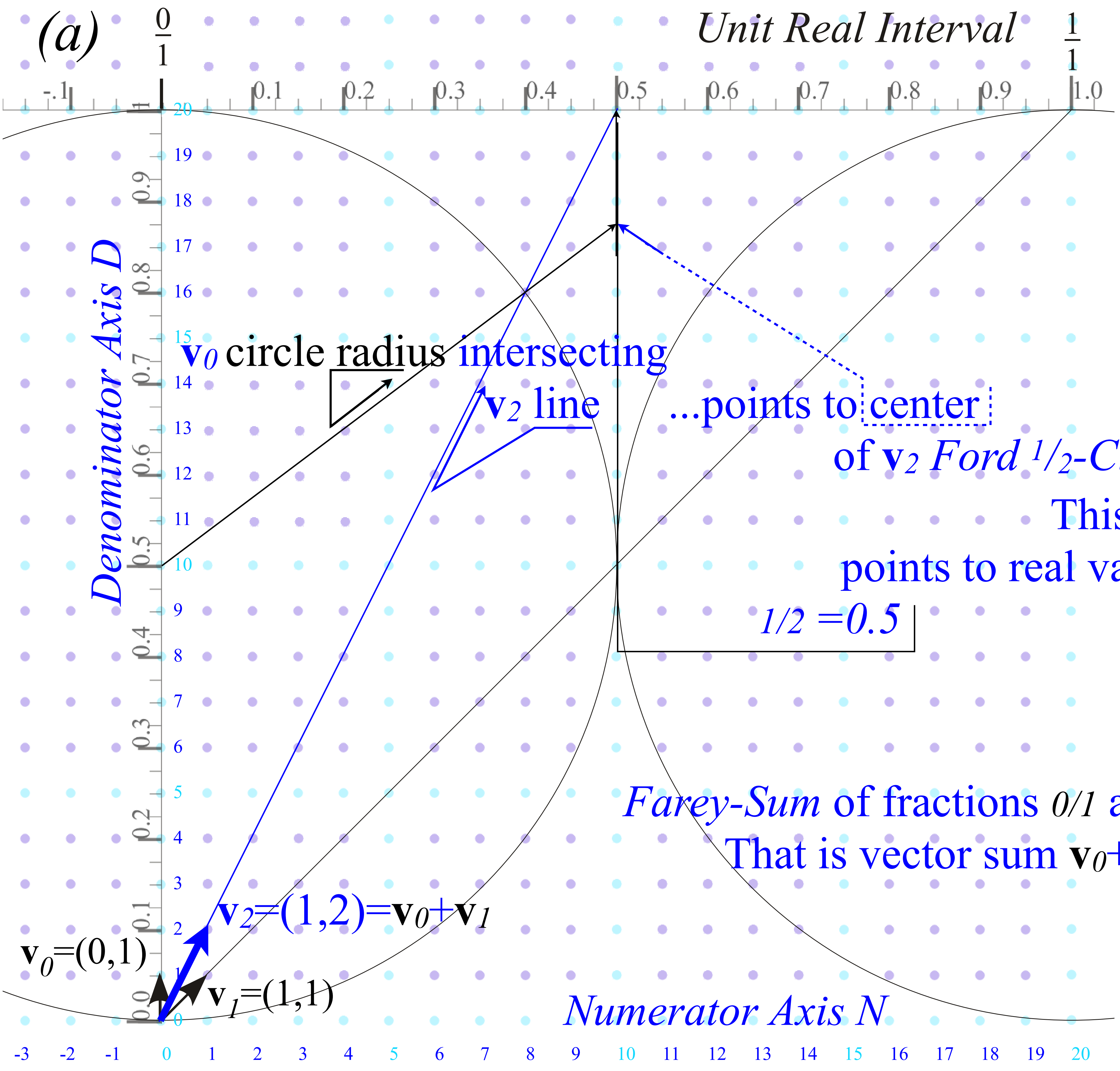

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...points to center of $\mathbf{v}_2$ *Ford* $^1/_2$*-Circle*

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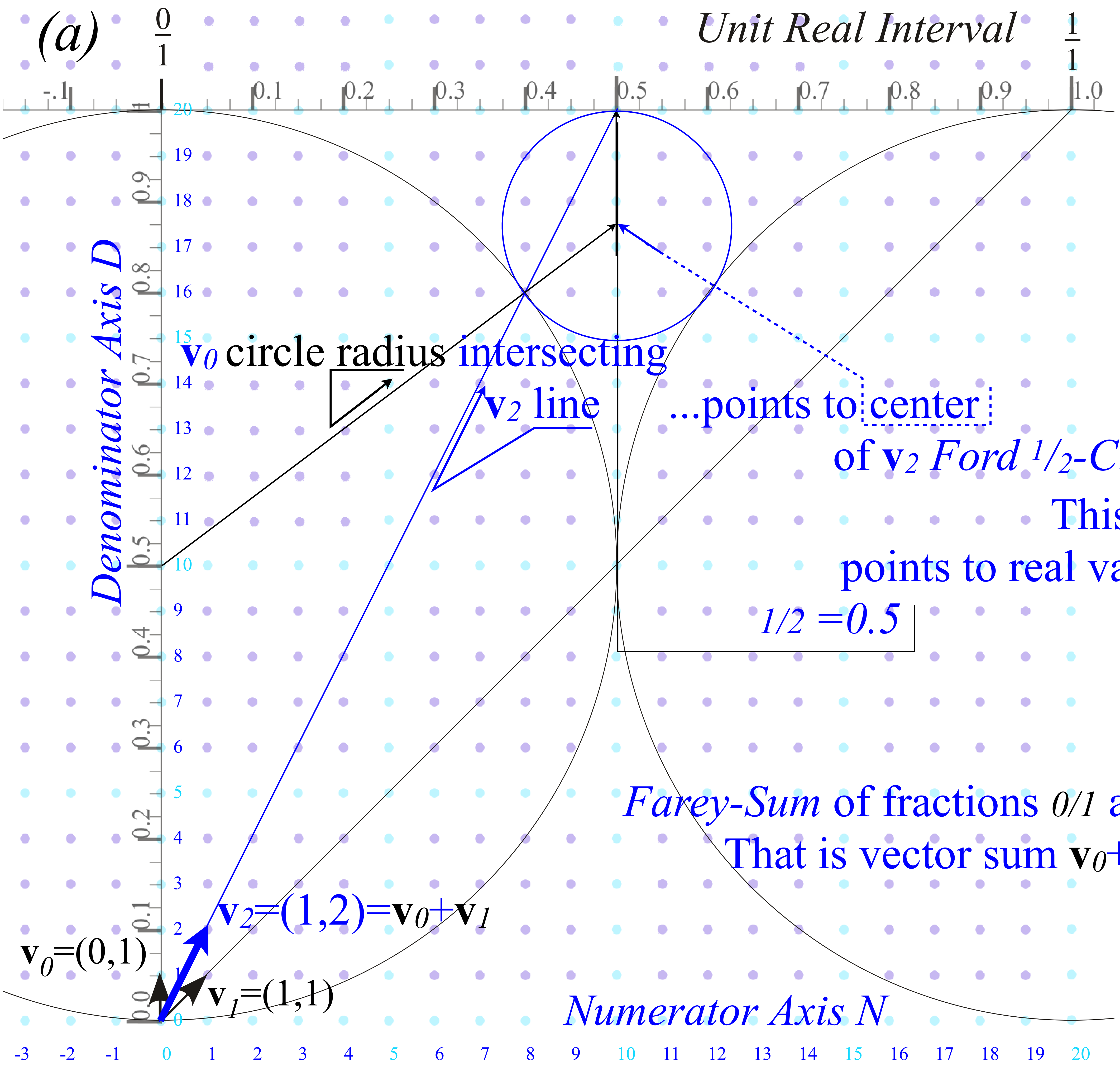

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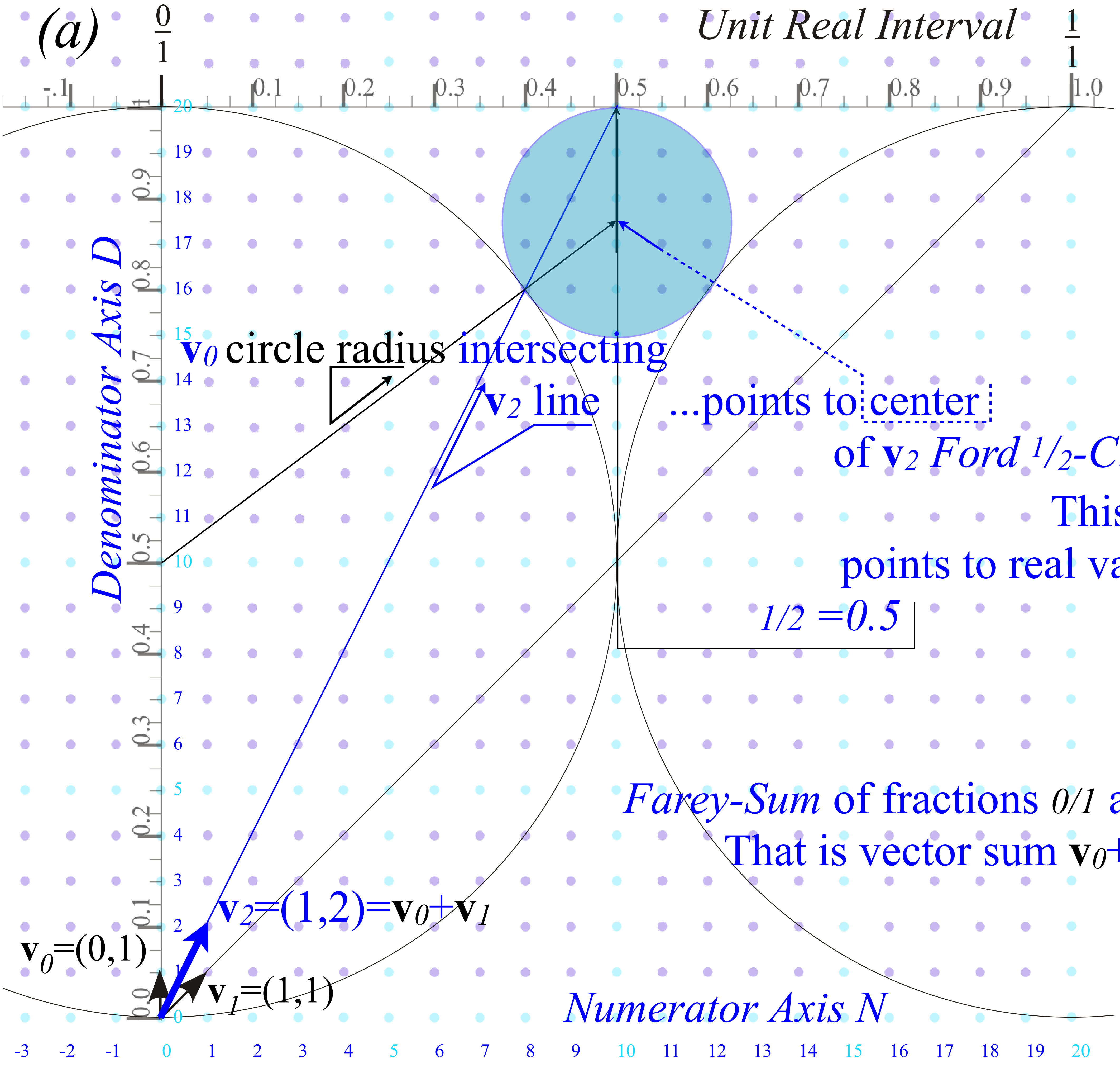

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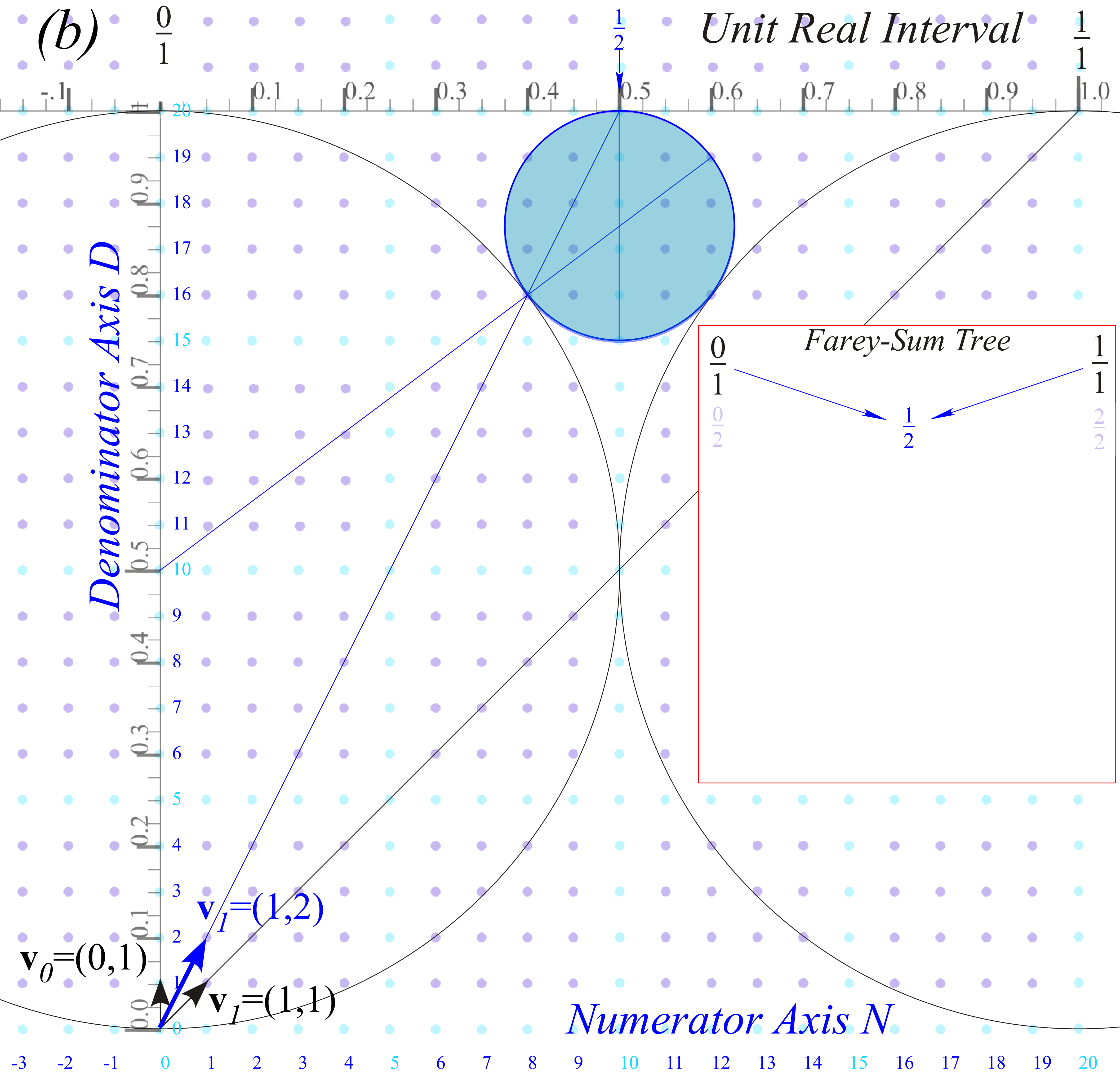
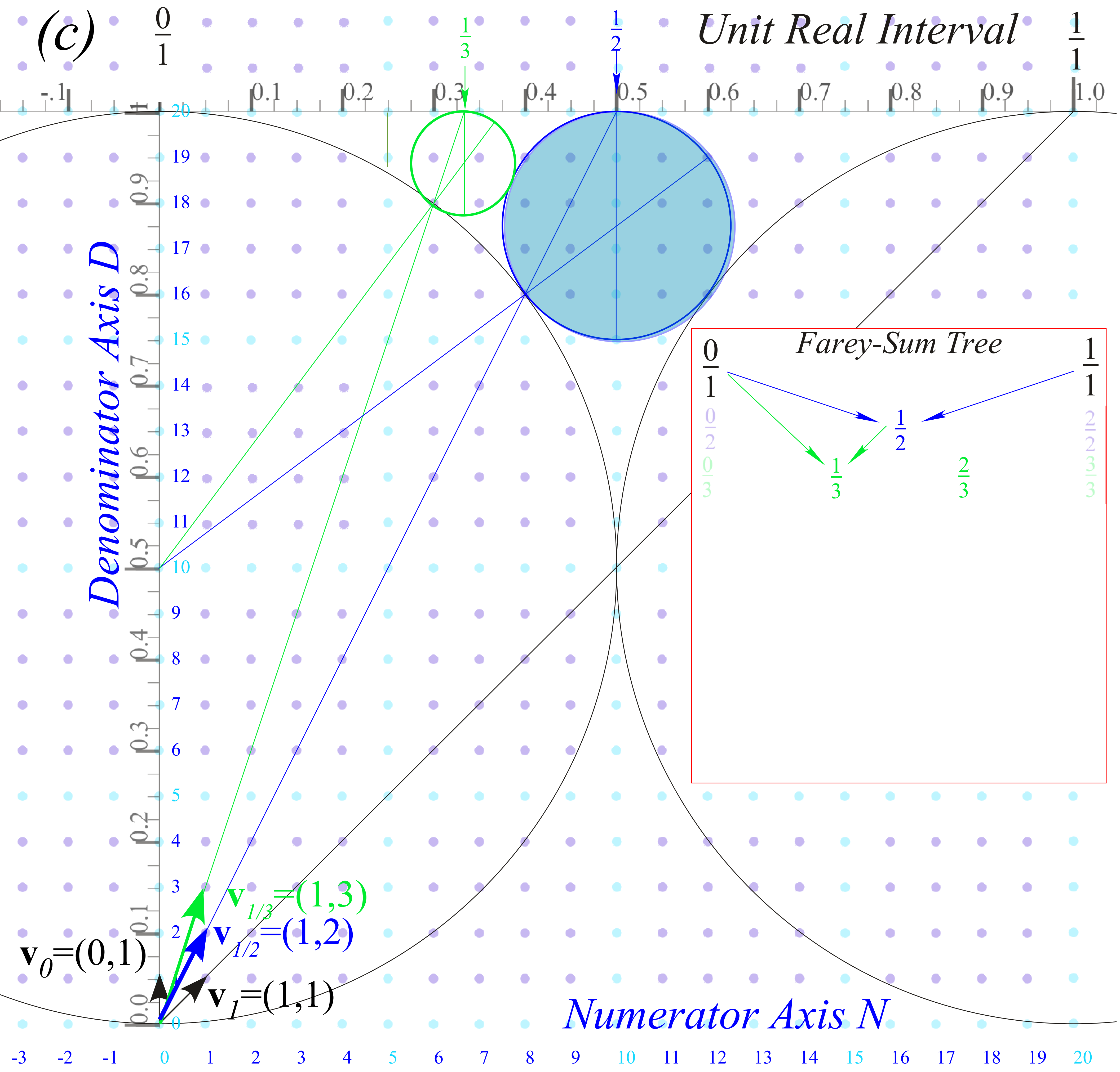


Farey Sum related to vector sum and *Ford Circles*

1/1-circle has diameter *1*

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

[Li, Harter, Chem.Phys.Letters (2015)]



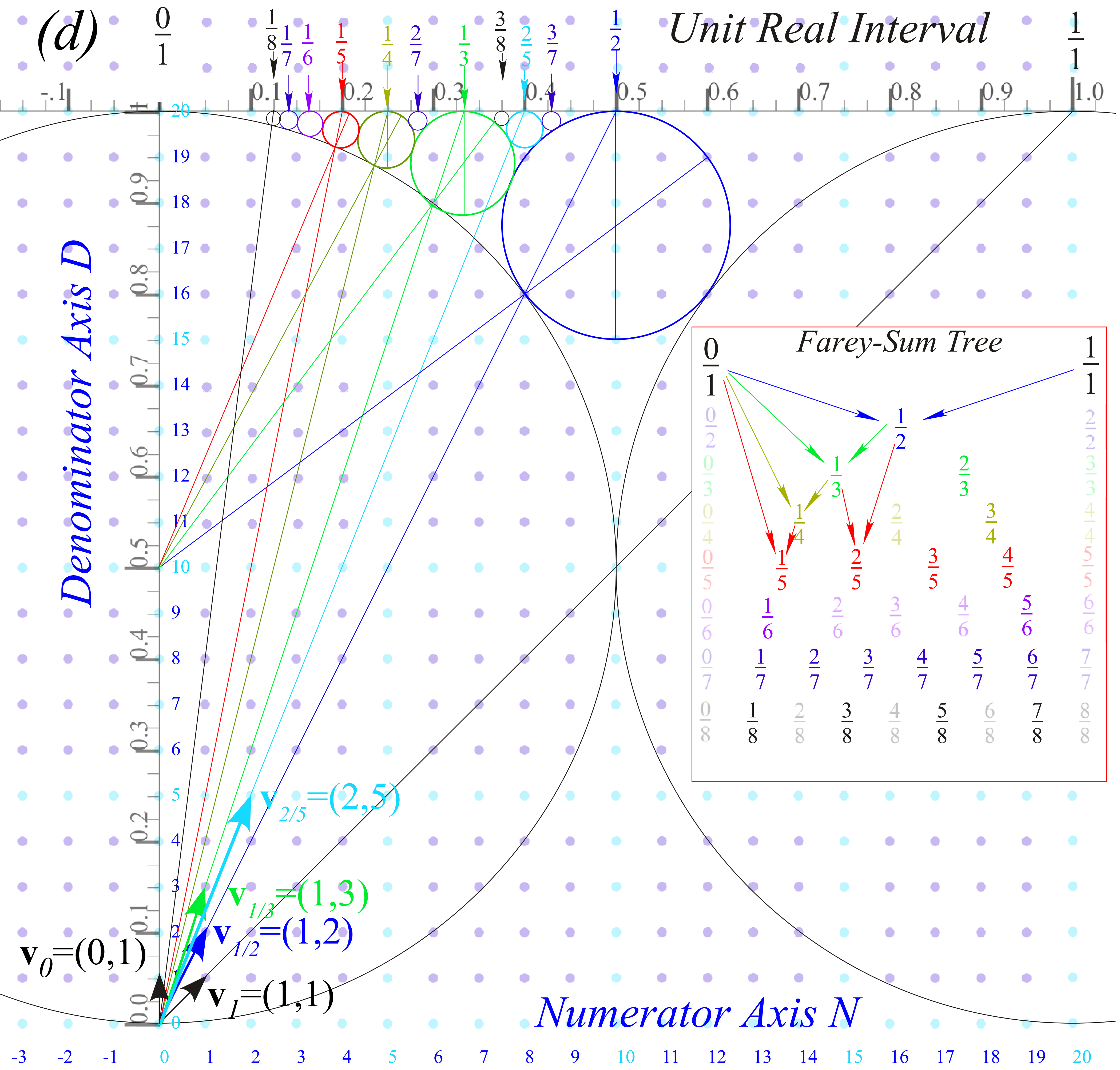
Farey Sum related to vector sum and *Ford Circles*

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 (2015)*]

Farey Sum related to vector sum and *Ford Circles*



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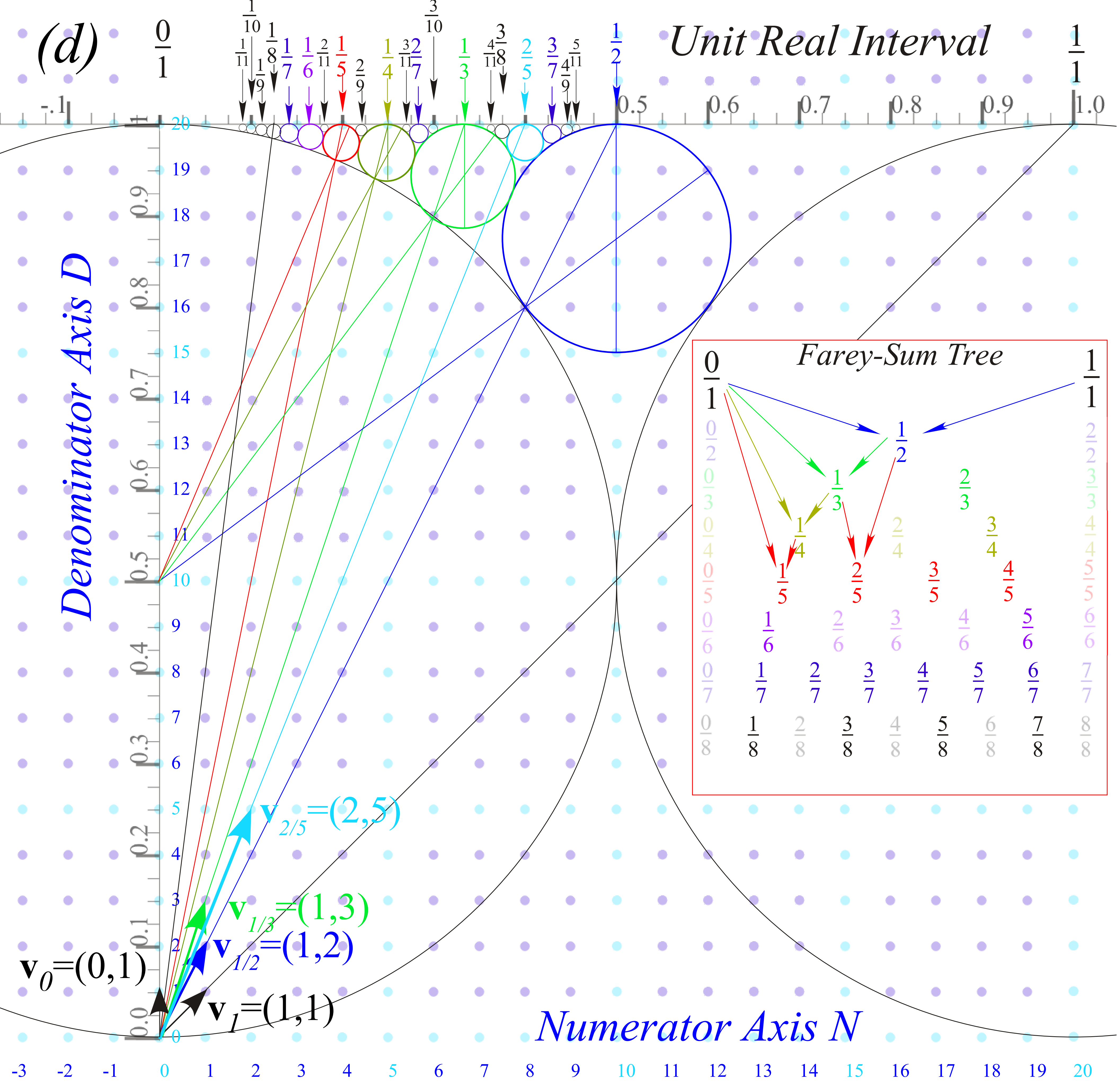
1/3-circles have diameter $1/3^2=1/9$

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

[Li, Harter, Chem.Phys.Letters (2015)]



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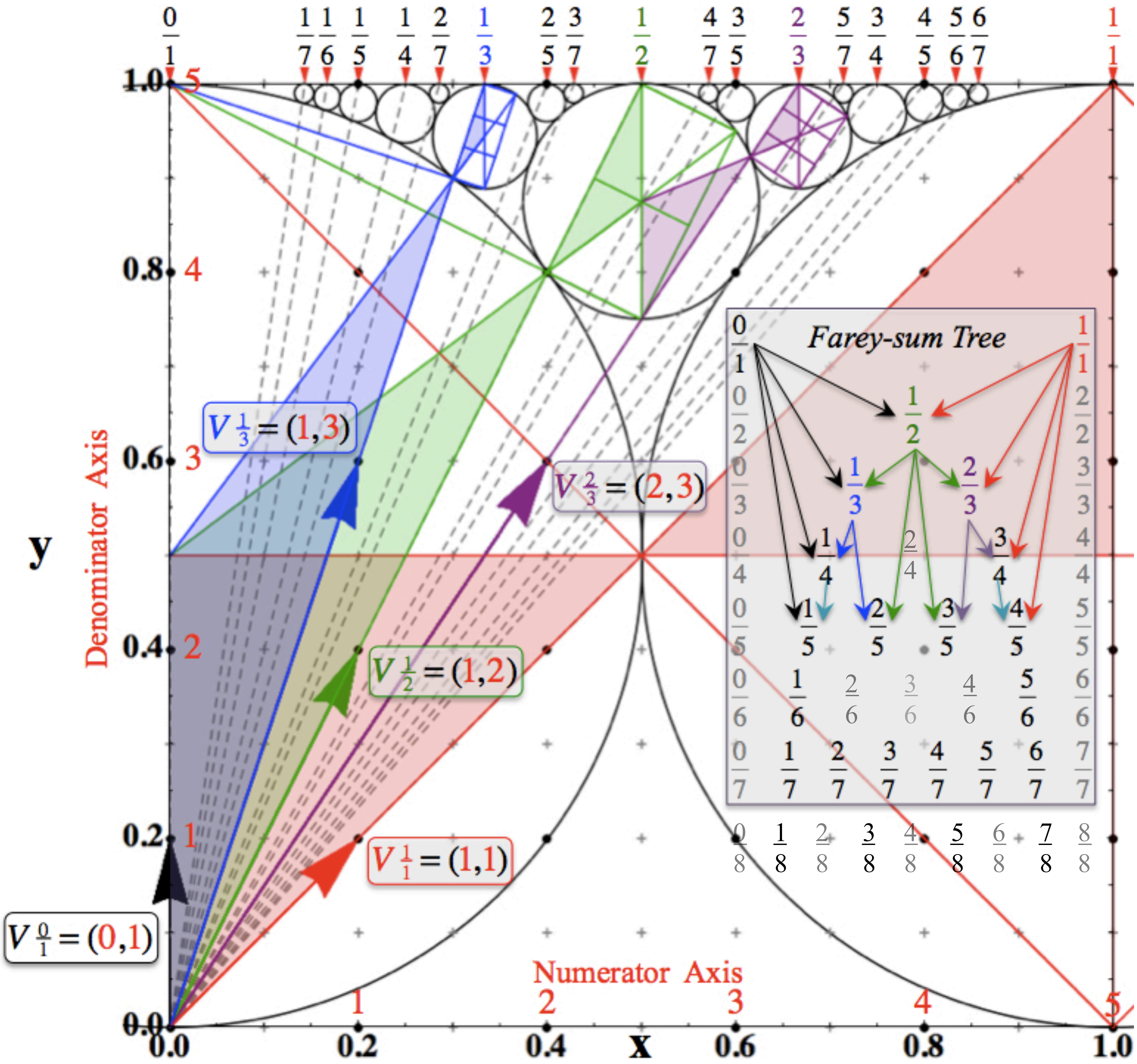
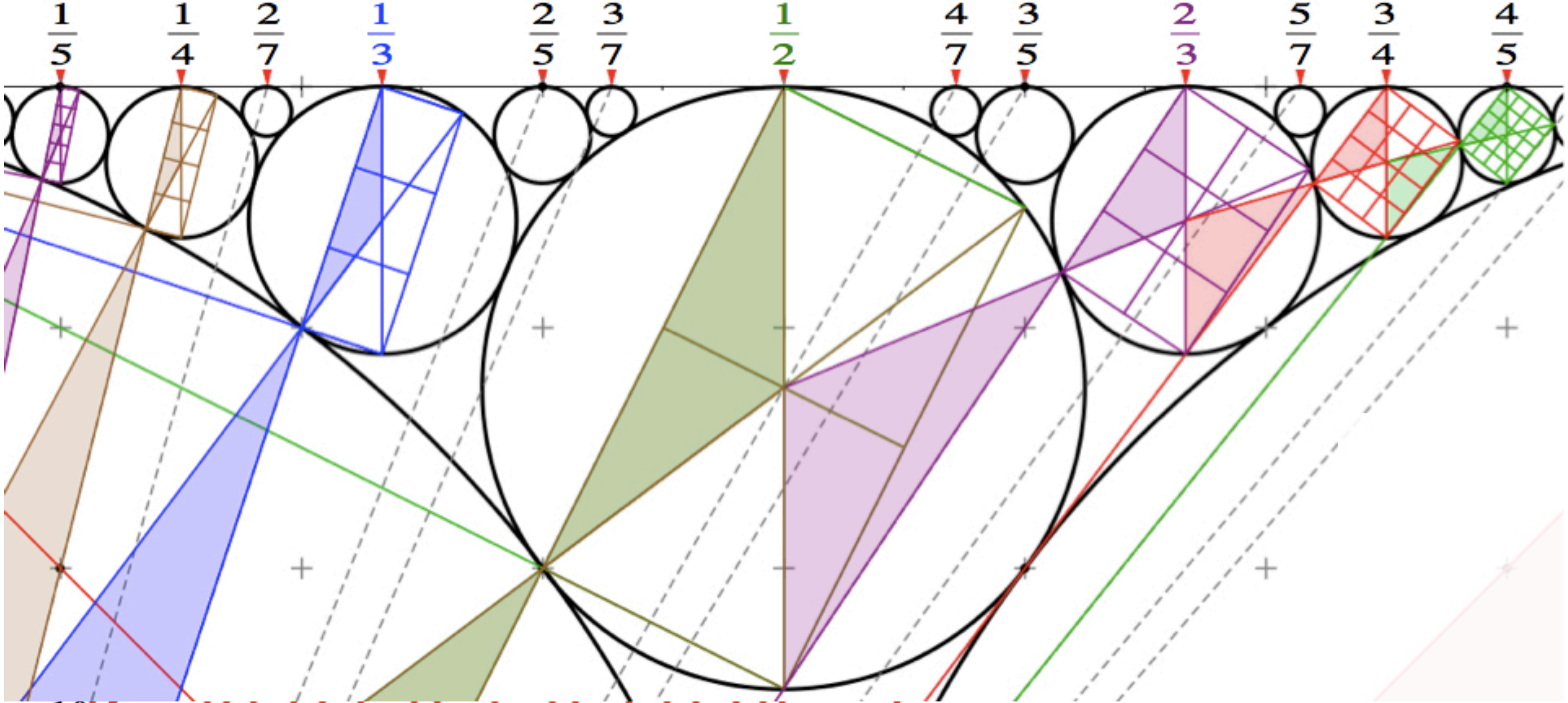


Thales Rectangles

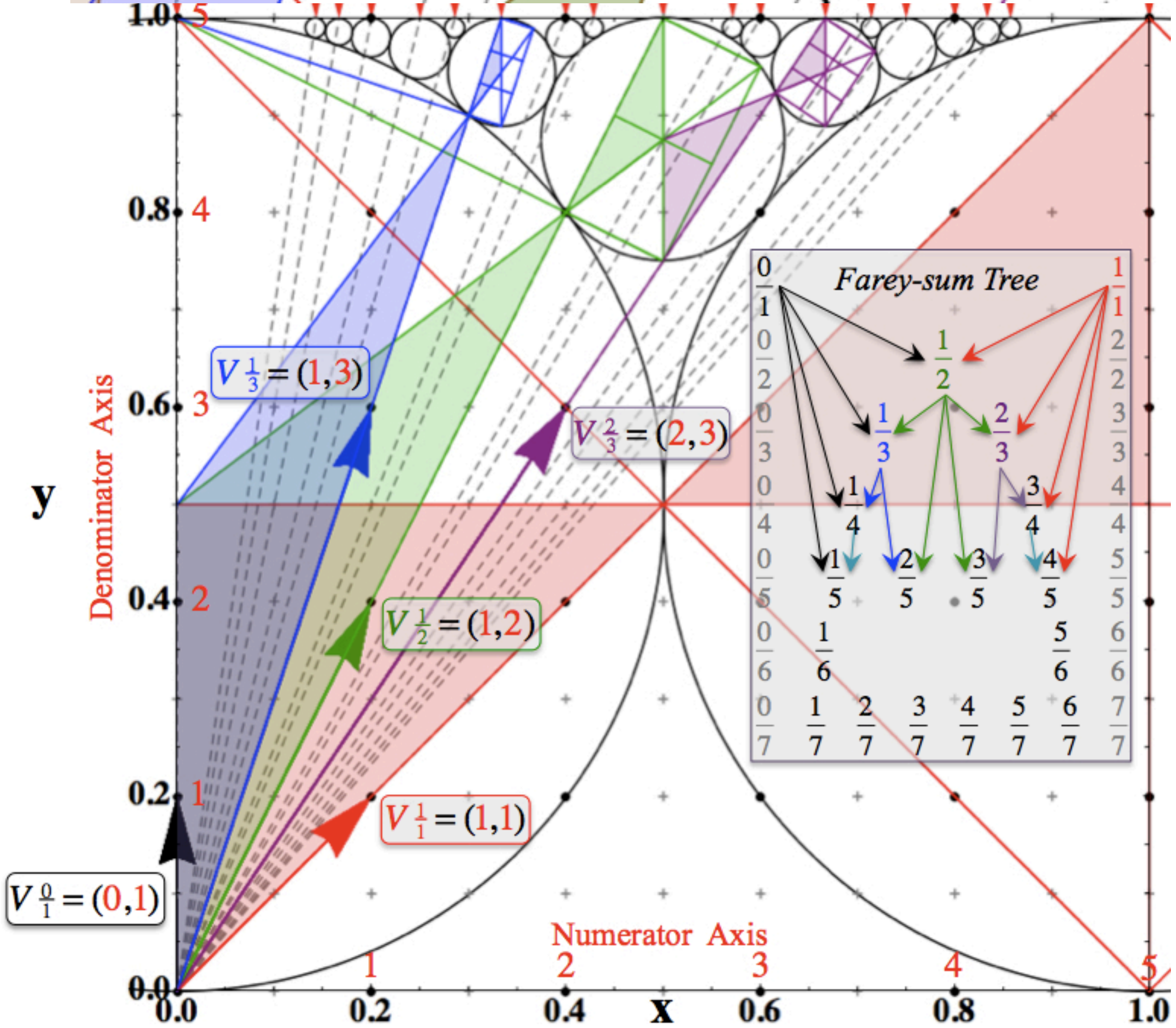
provide
analytic geometry
of
fractal structure

[Li, Harter, Chem.Phys.Letters (2015)]



“Quantized” Thales Rectangles

provide
analytic geometry
of
fractal structure



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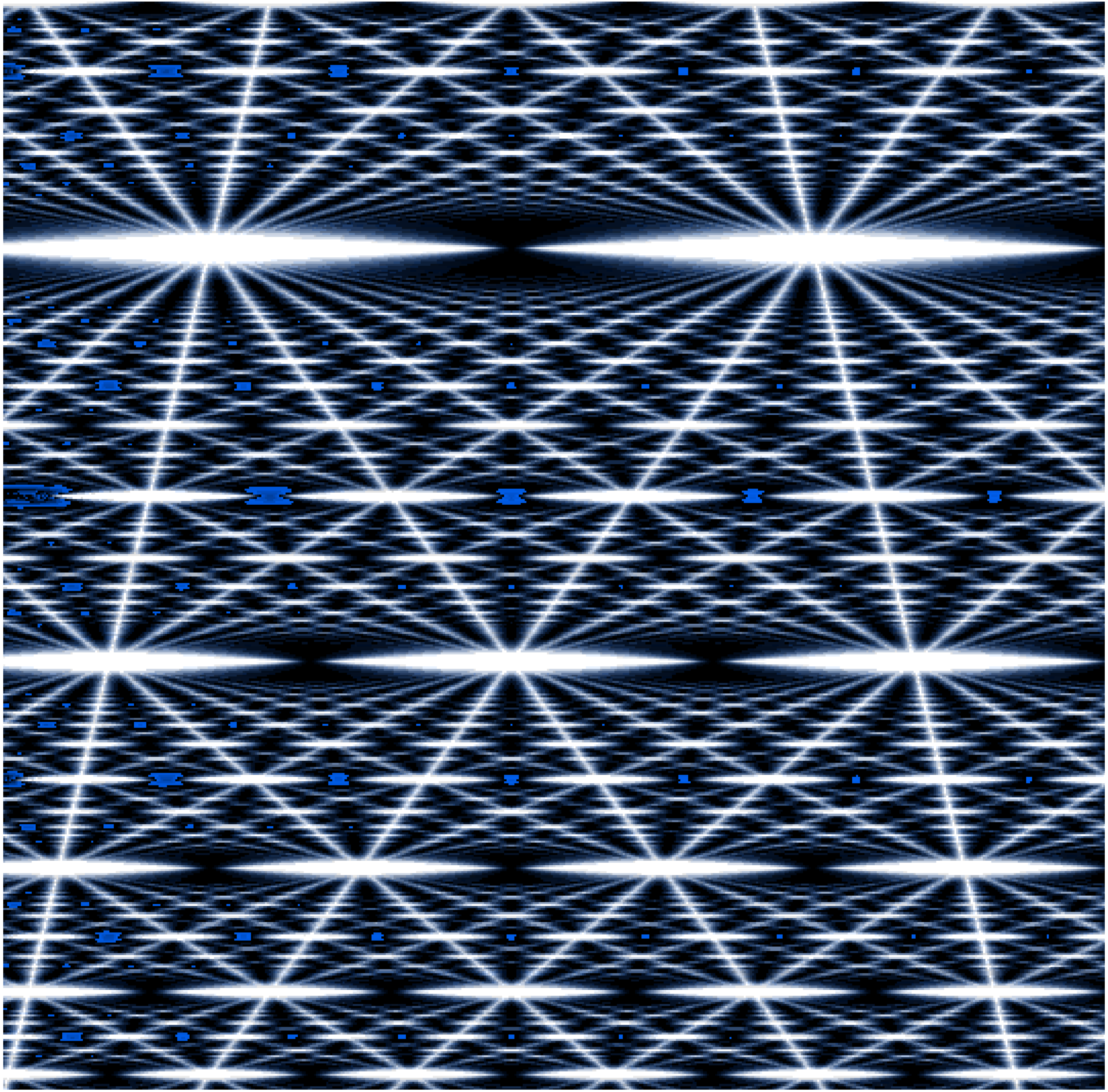
(Quantum computer simulation)

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



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