Molecules and Molecular Spectroscopy:

Learning about molecules from Quantum theory

and

Learning about Quantum theory from molecules

William G. Harter for Kennefict's Modern Physics class 3. 26 . 13

A sketch of modern molecular spectroscopy

The frequency hierarchy *Example of16μm spectra of CF_4*

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) 2^{nd} 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

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Wavepacket explodes! (Then revives)

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

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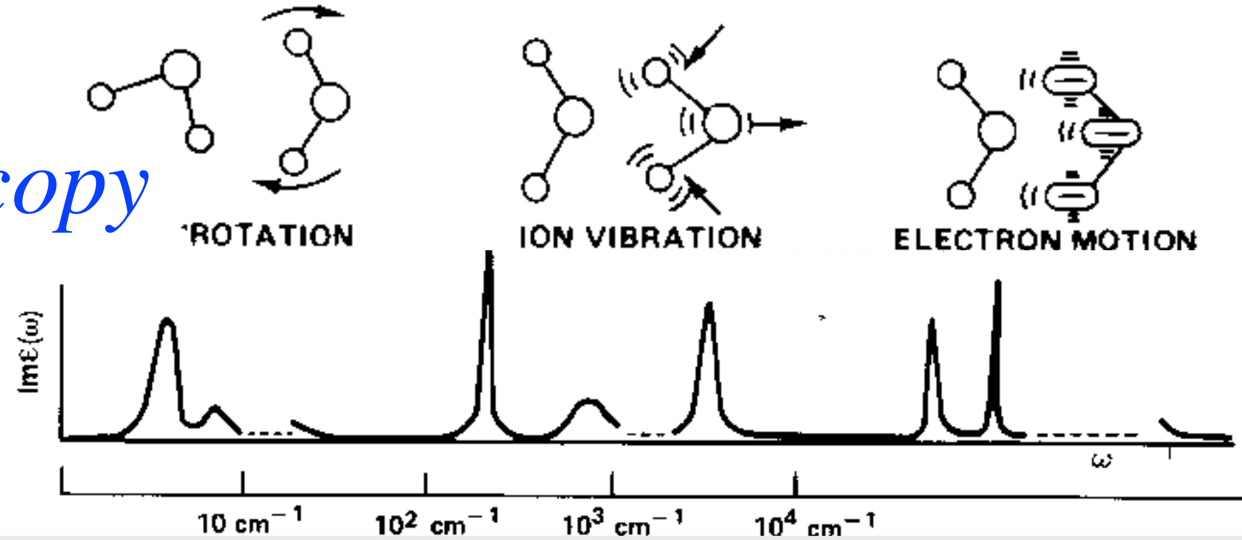
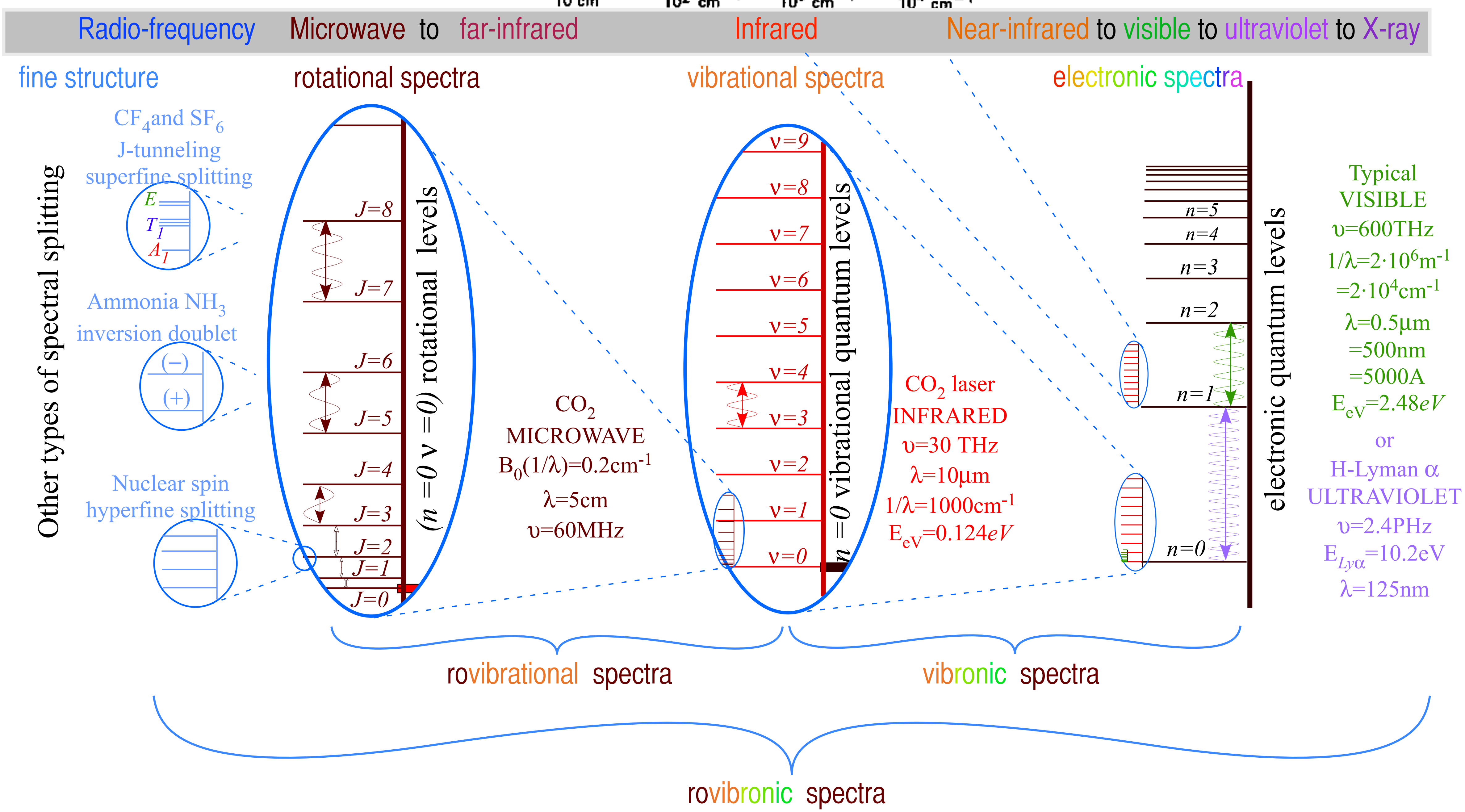


From Fig. 6.5.5.
Principles of Symmetry, Dynamics, and Spectroscopy
W. G. Harter, Wiley Interscience, NY (1993)

The frequency hierarchy



Spectral Quantities

Frequency υ
Hertz(sec^{-1})
THz $10^{12}s^{-1}$
GHz $10^{9}s^{-1}$
MHz $10^{6}s^{-1}$
kHz $10^{3}s^{-1}$

Wavelength λ
meters(m)
fm $10^{-15}m$
pm $10^{-12}m$
nm $10^{-9}m$
μm $10^{-6}m$
mm $10^{-3}m$
cm $10^{-2}m$
km $10^{3}m$

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

Energy $eh\upsilon$
electonVolts (eV)

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

W.G.Harter

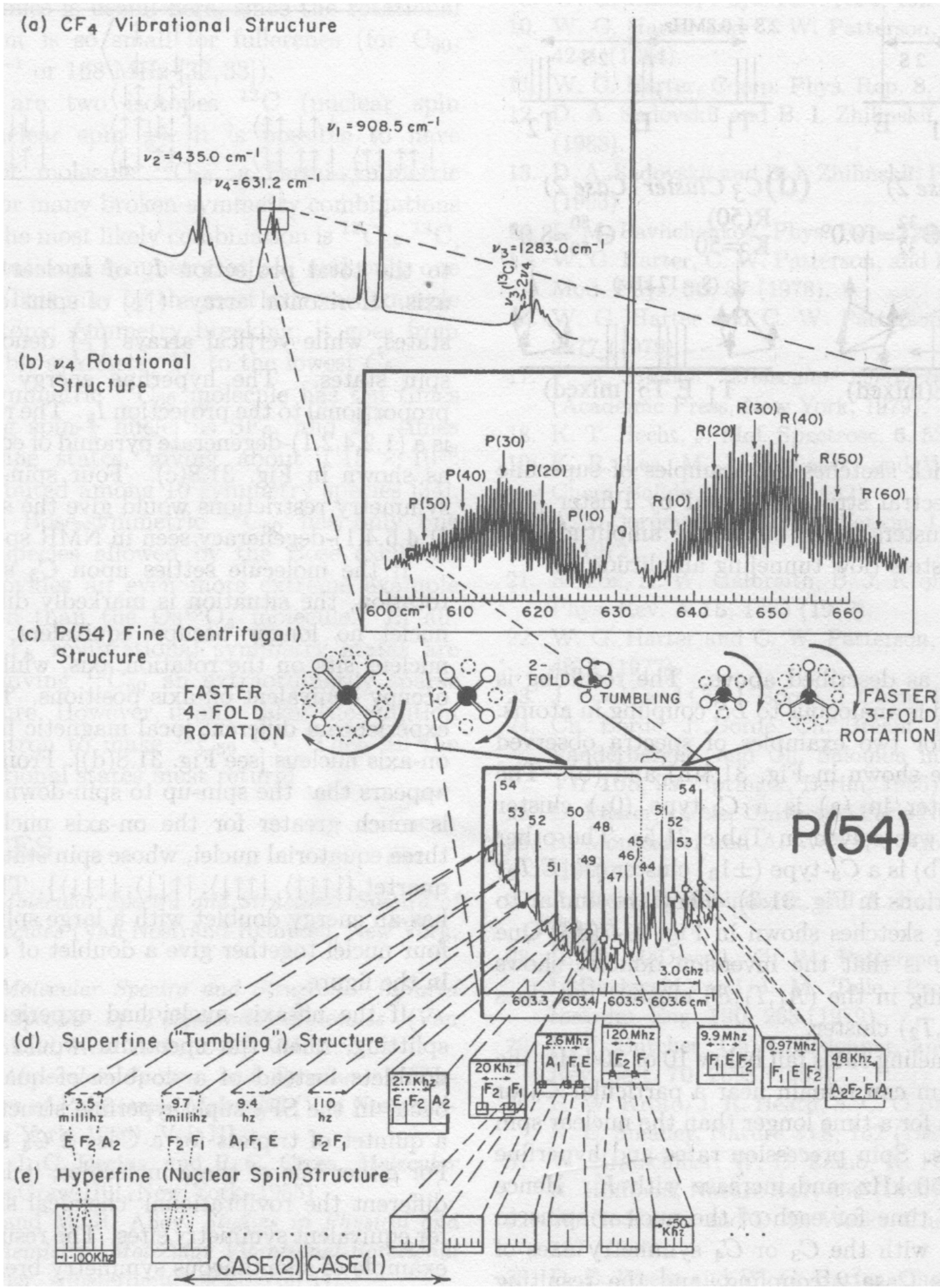
Ch. 31

Atomic, Molecular, & Optical Physics Handbook

Am. Int. of Physics

Gordon Drake Editor

(1996)



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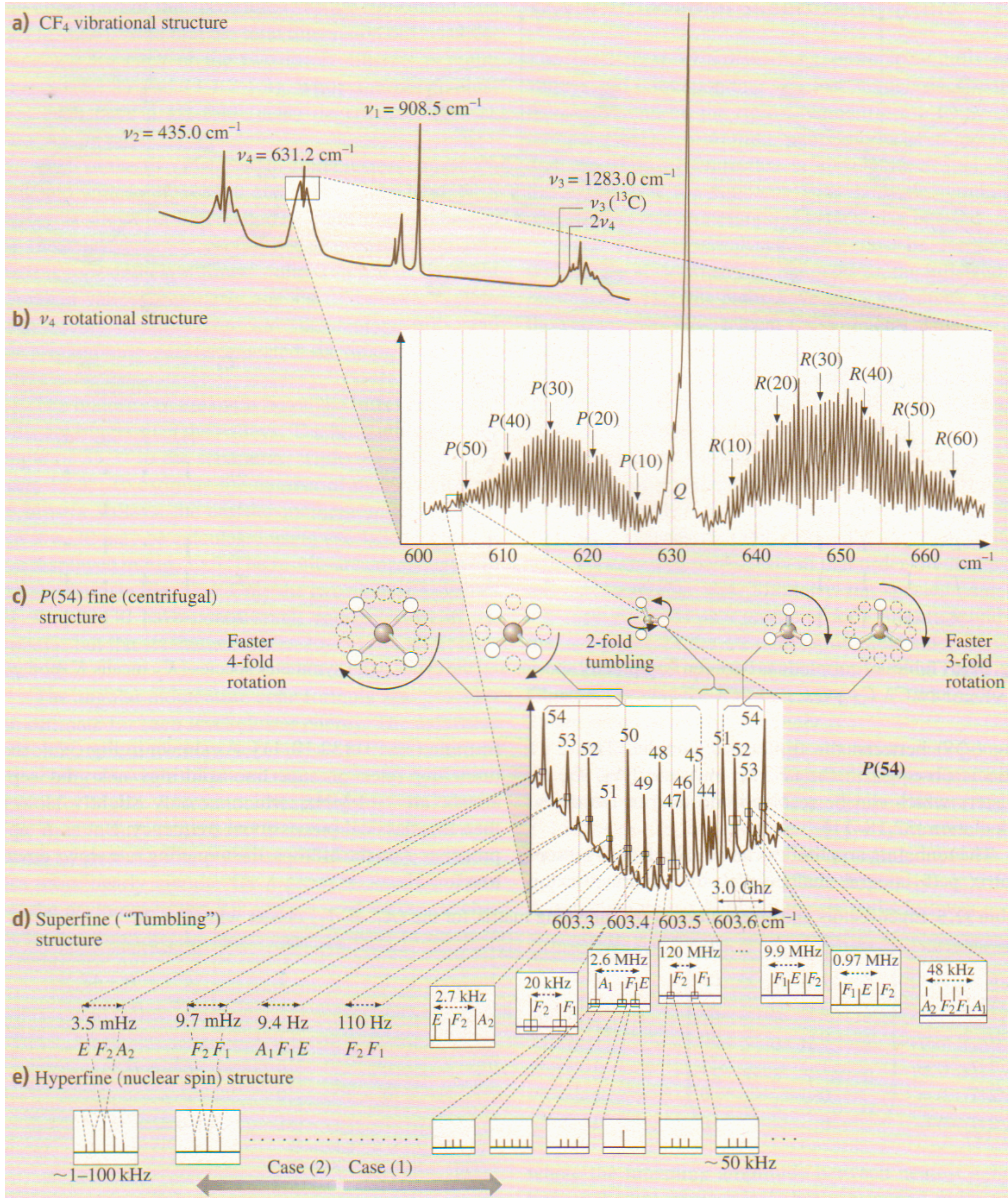
W.G.Harter

Fig. 32.7

Springer Handbook of Atomic, Molecular, & Optical Physics

Gordon Drake Editor (2005)



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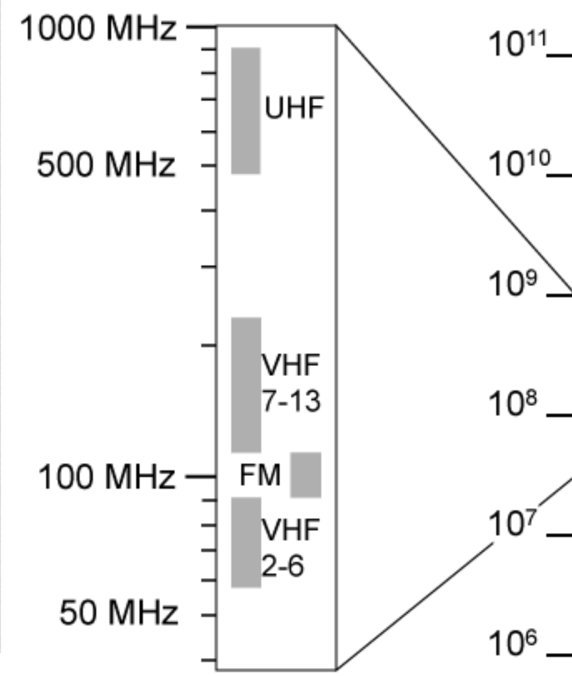
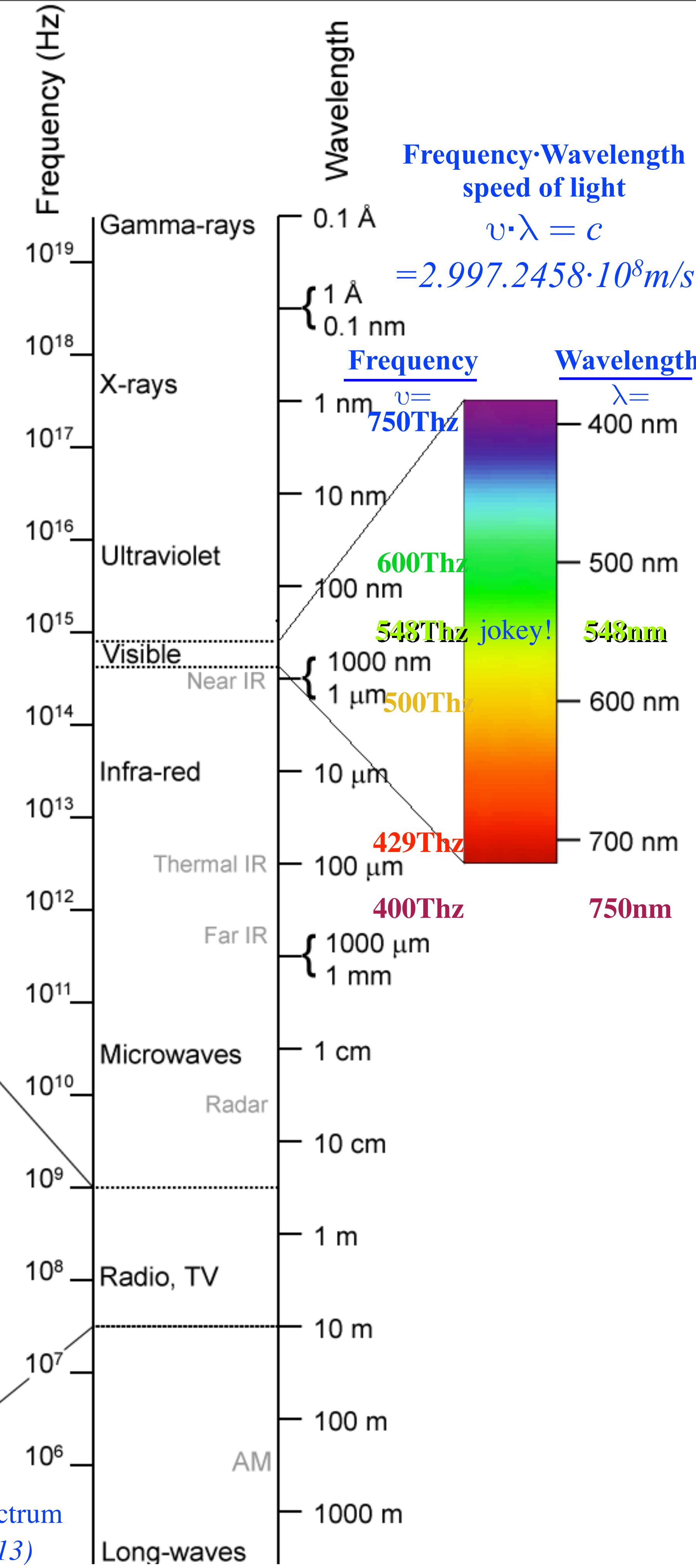
CLASS	FREQUENCY	WAVELENGTH	ENERGY
	300 EHz	1 pm	1.24 MeV
γ	30 EHz	10 pm	124 keV
HX	3 EHz	100 pm	12.4 keV
SX	300 PHz	1 nm	1.24 keV
	30 PHz	10 nm	124 eV
EUV	3 PHz	100 nm	12.4 eV
NUV	300 THz	1 μm	1.24 eV
NIR	30 THz	10 μm	124 meV
MIR	3 THz	100 μm	12.4 meV
FIR	300 GHz	1 mm	1.24 meV
EHF	30 GHz	1 cm	124 μeV
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}





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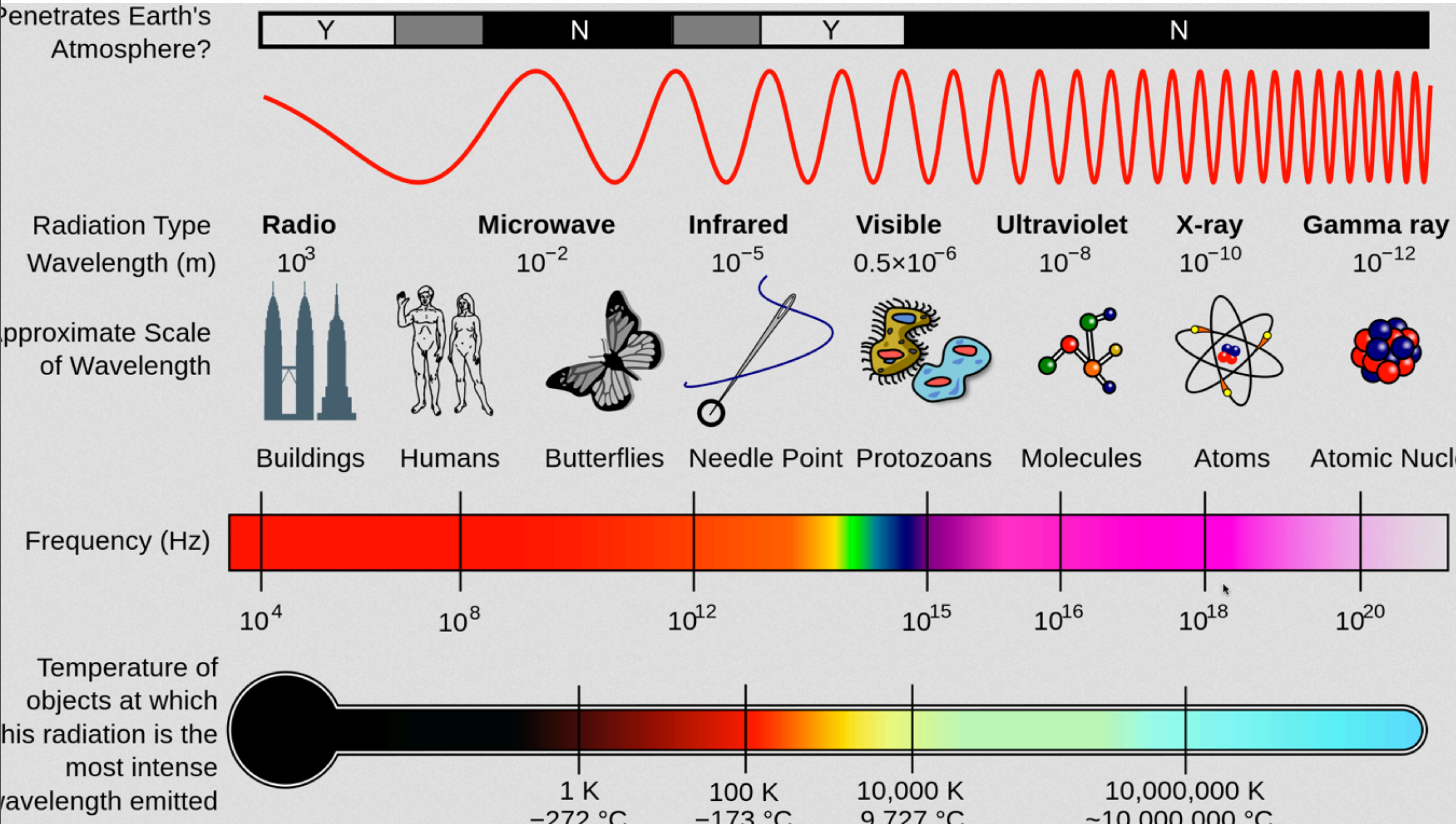
Units of frequency (Hz), wavelength (m), and energy (eV)



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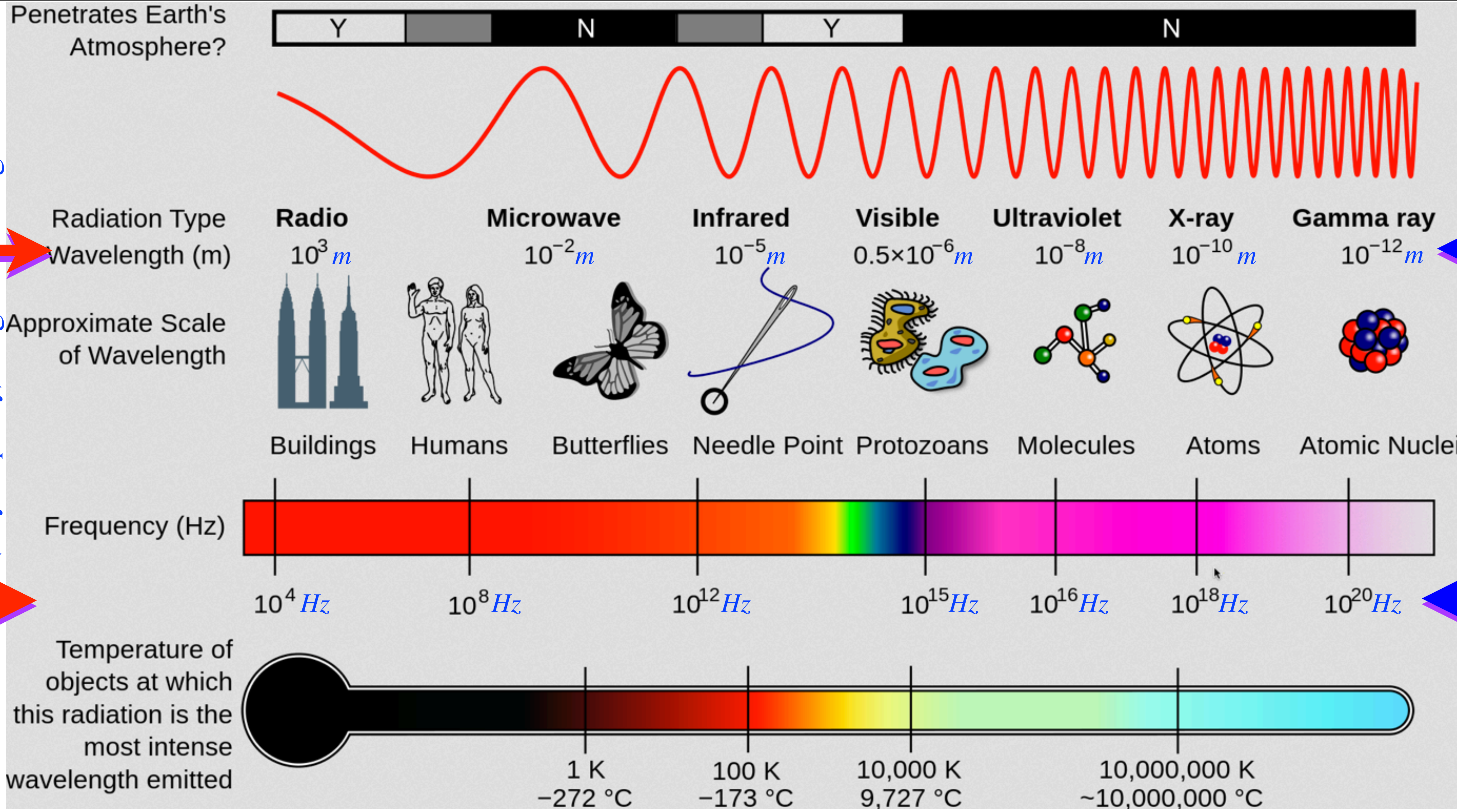
(Tiny frequency) Huge wavelength



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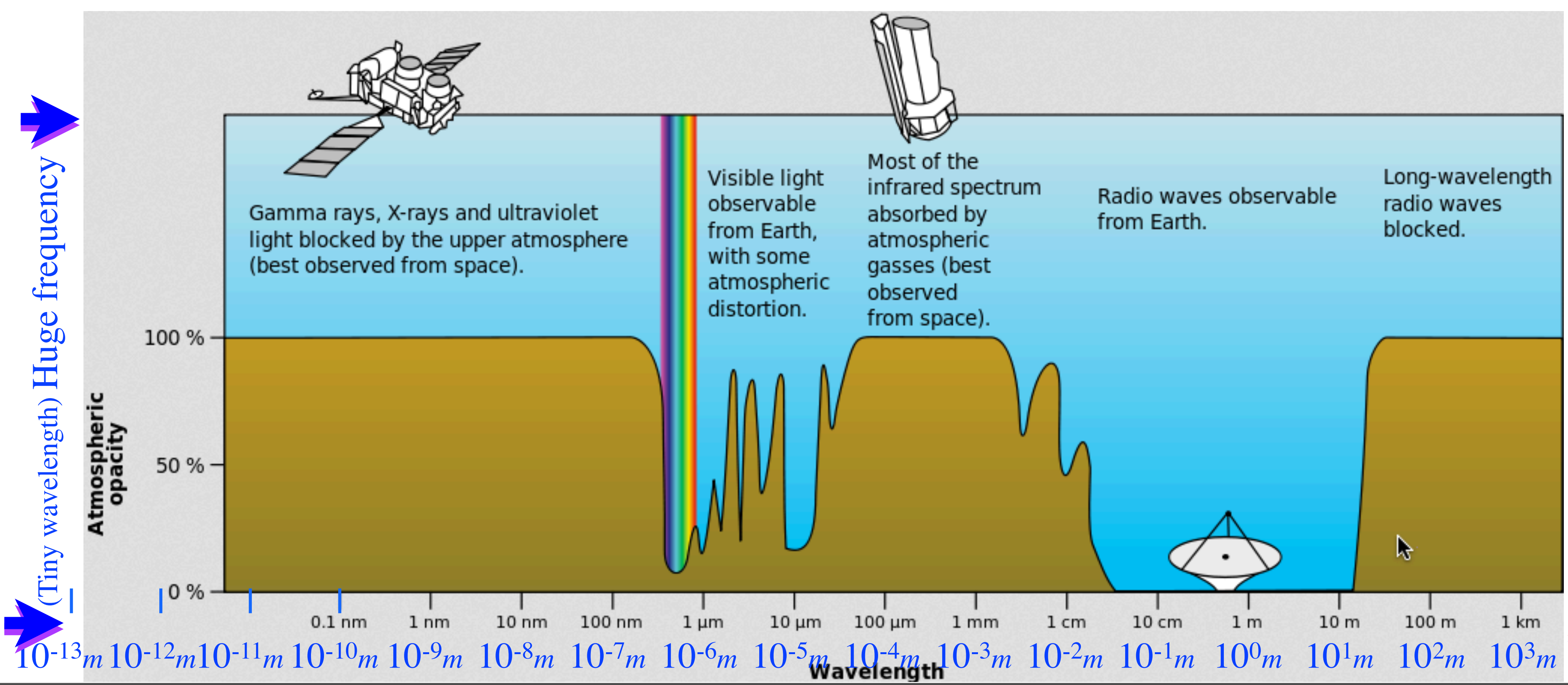

(Tiny frequency) Huge wavelength

Spectral windows in Earth atmosphere

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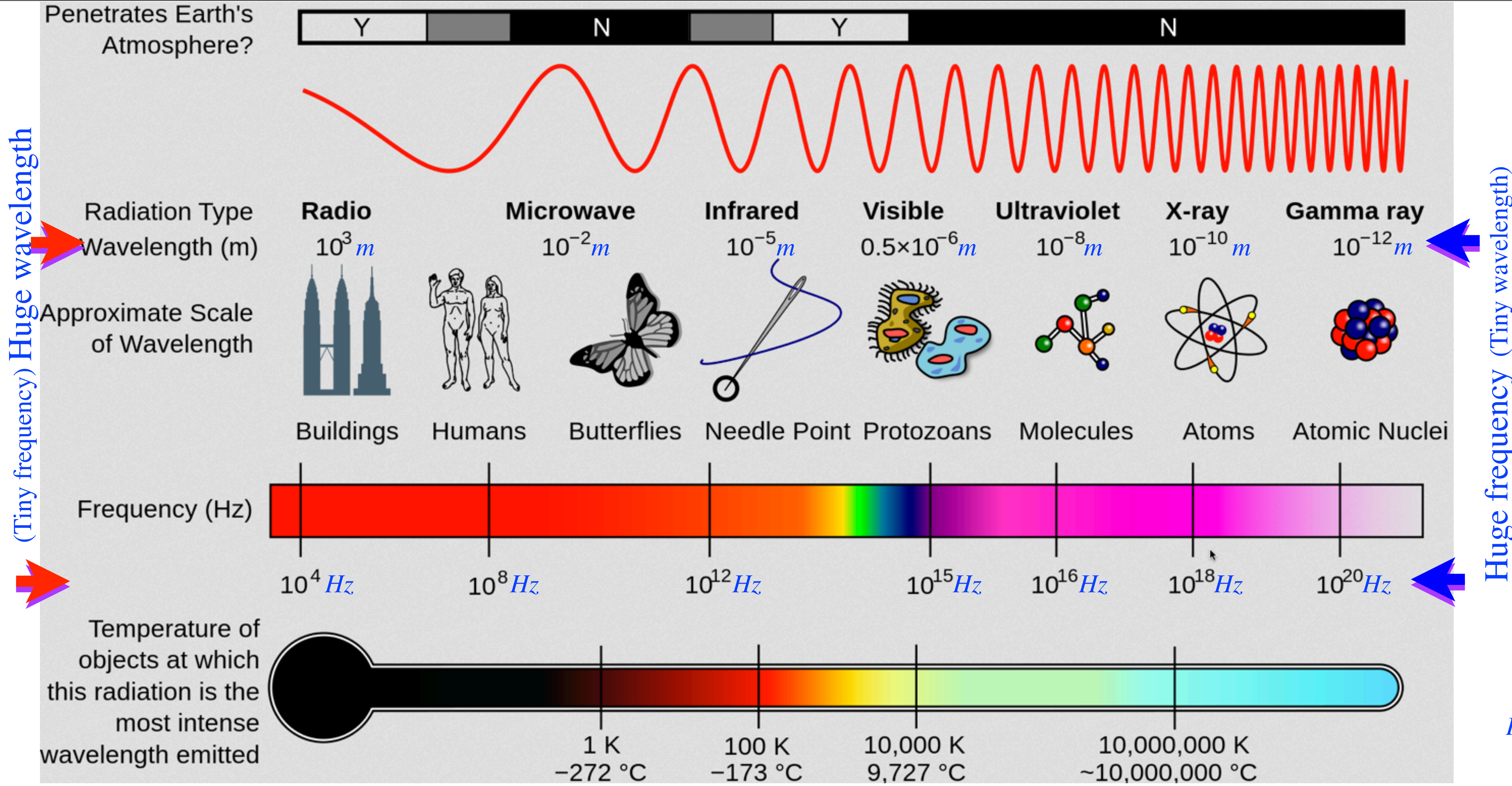

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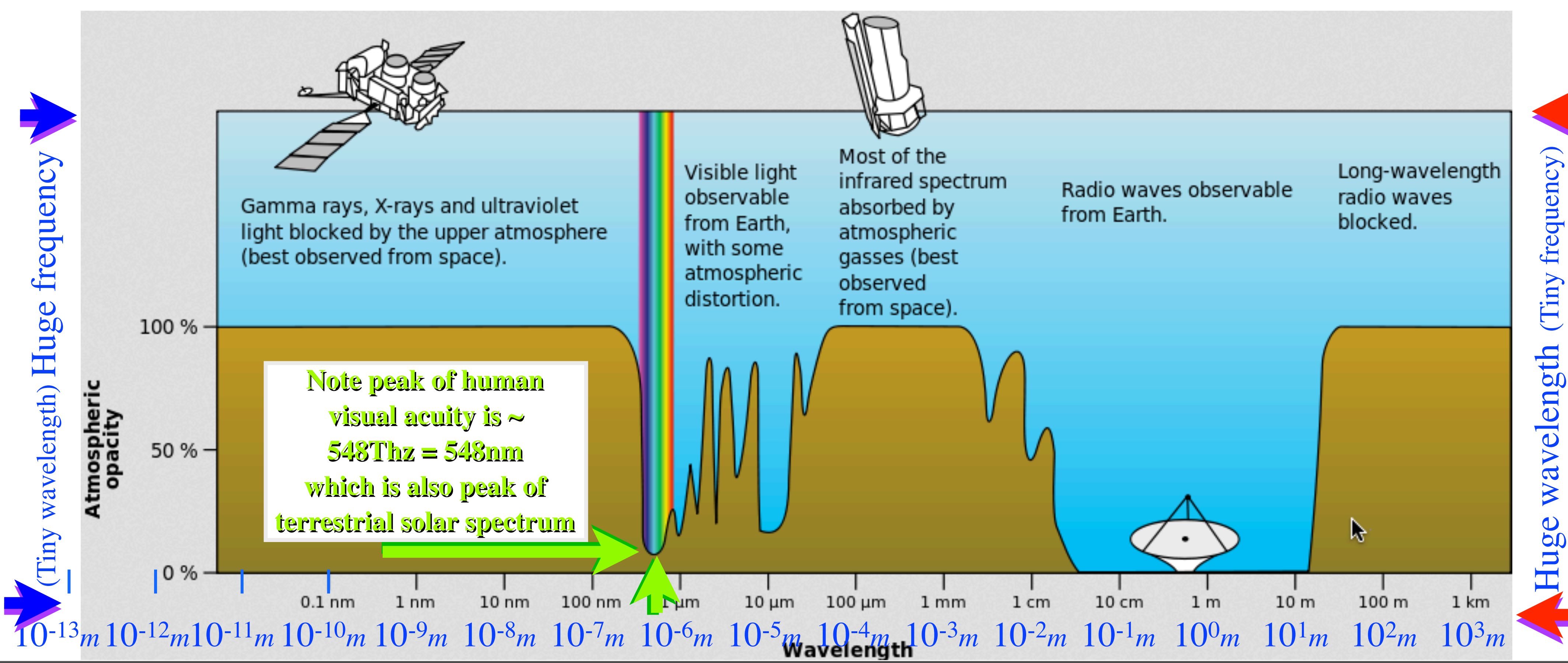

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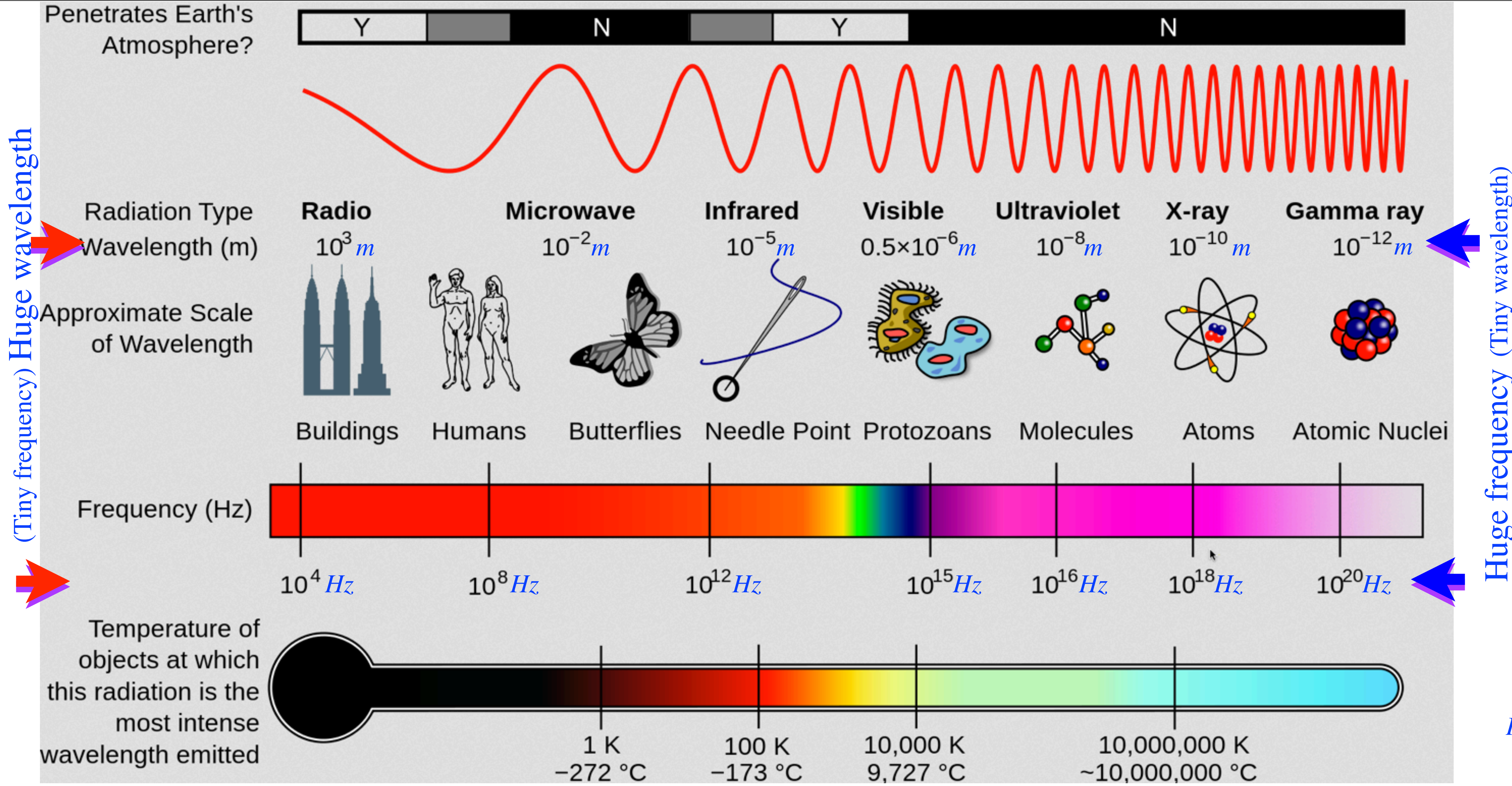

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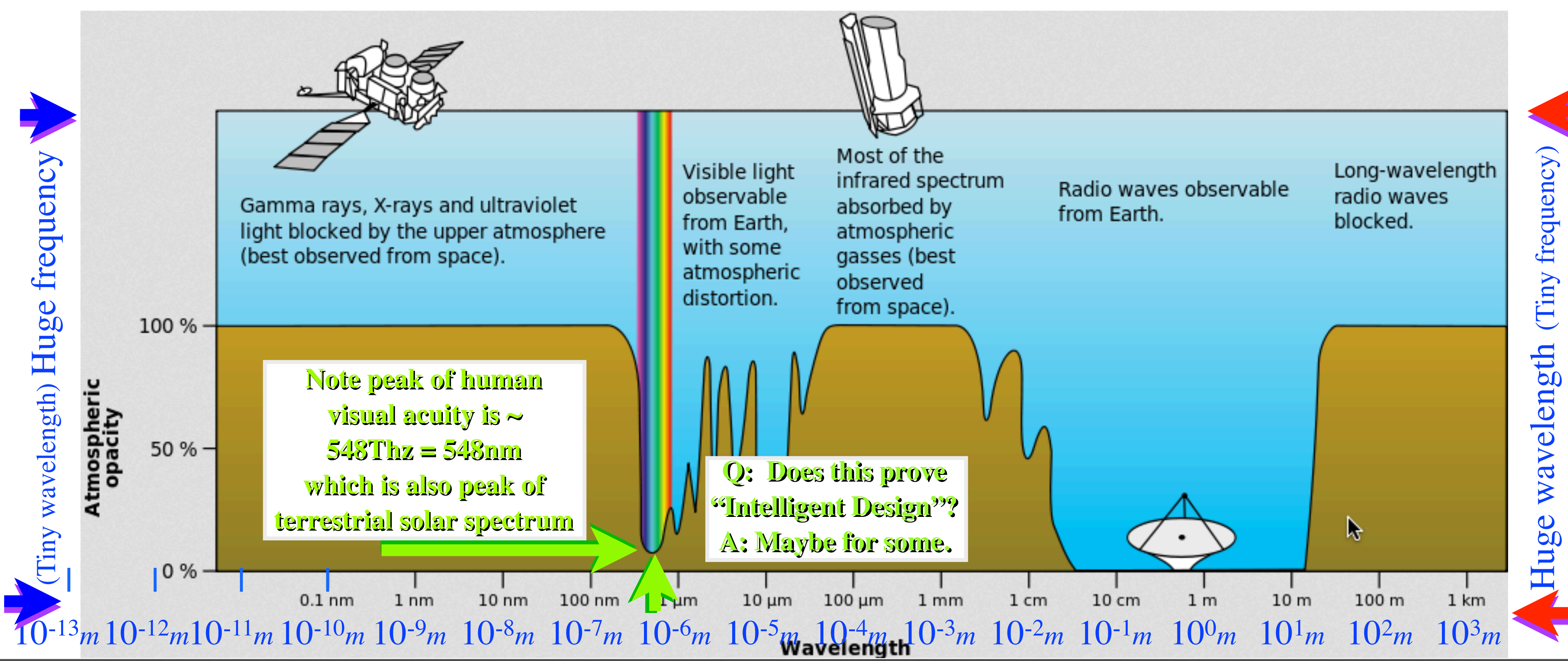

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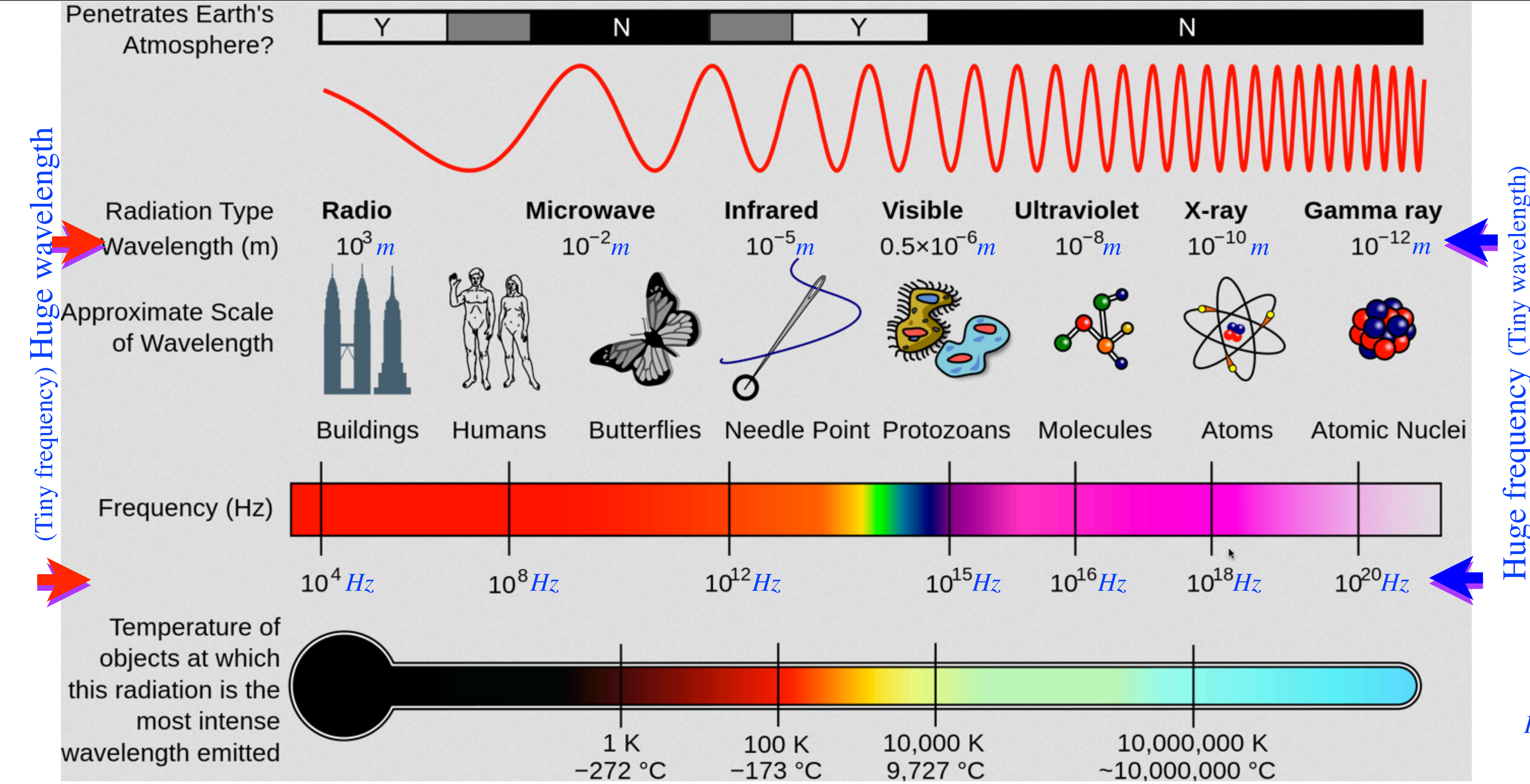

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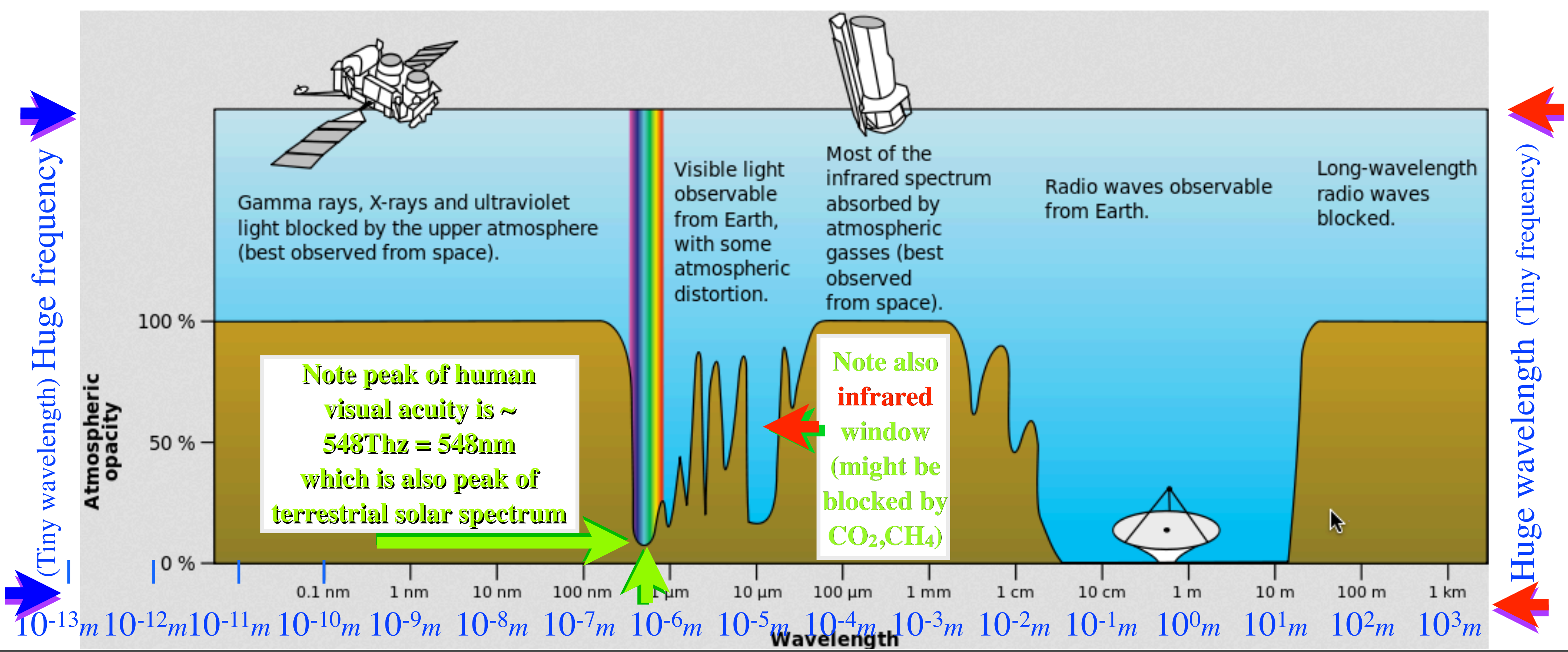

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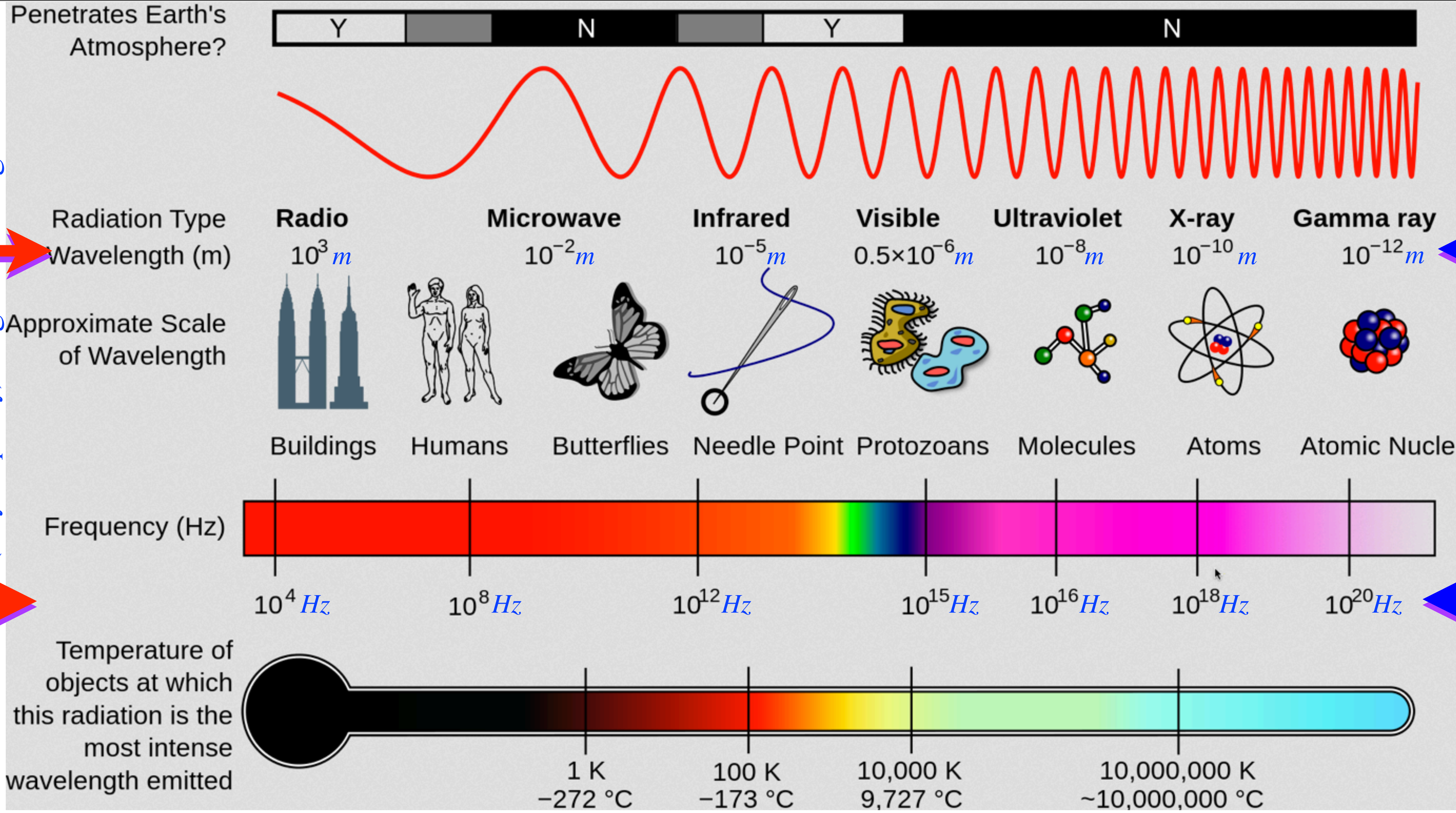

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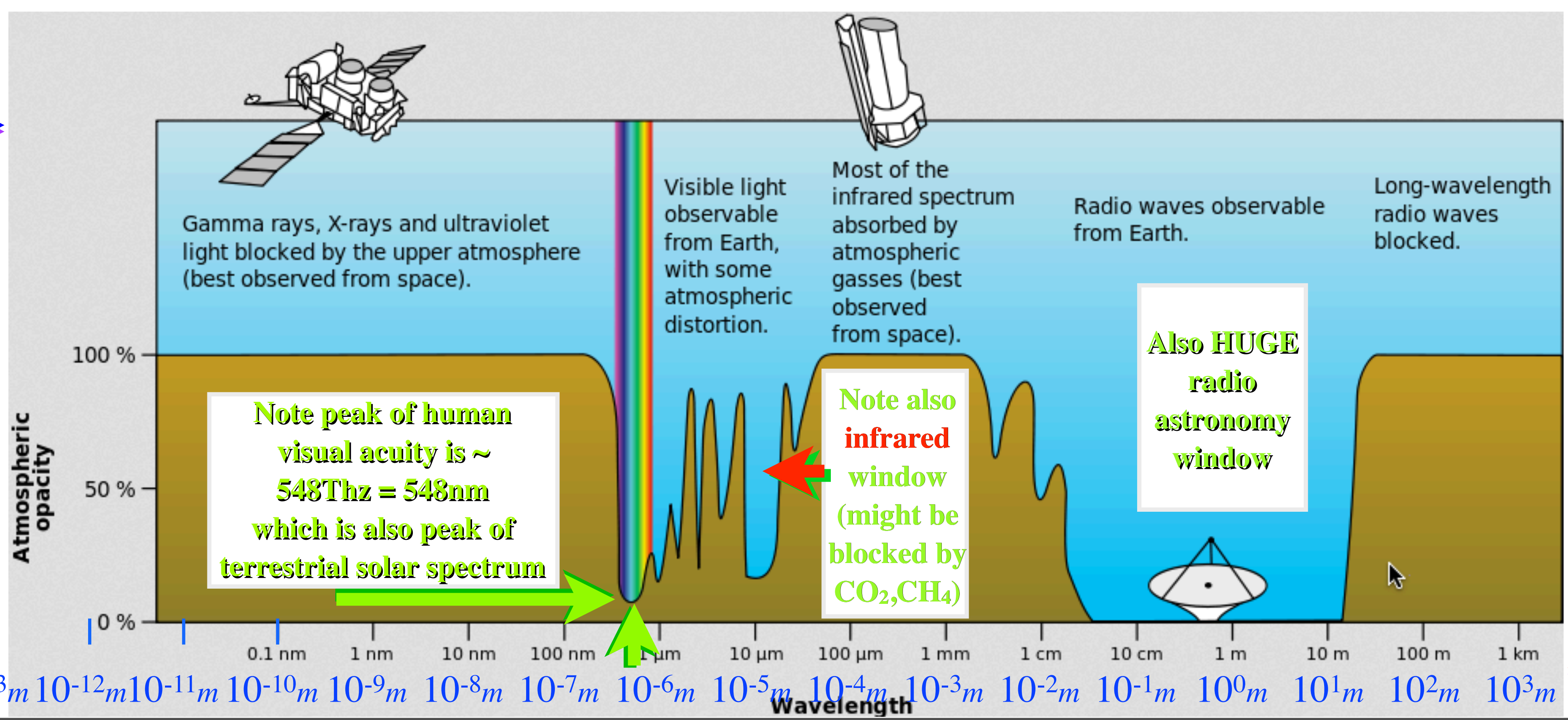

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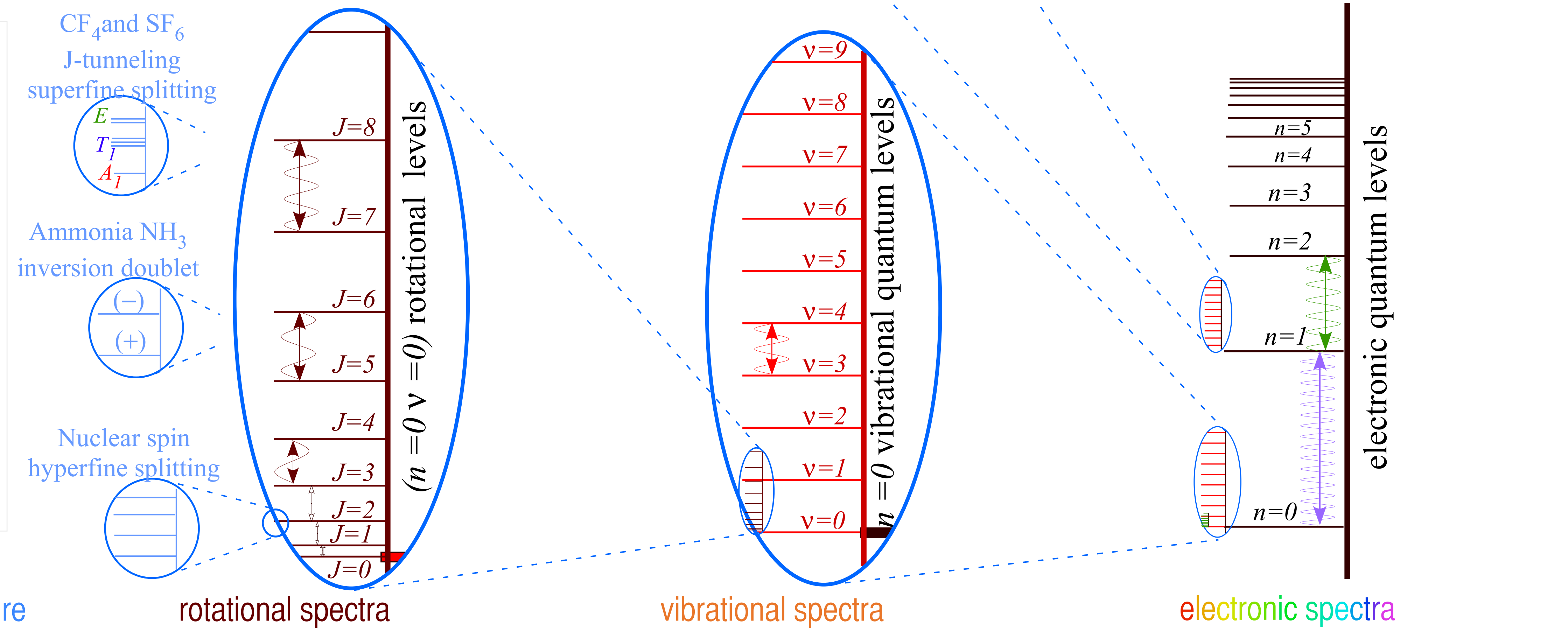
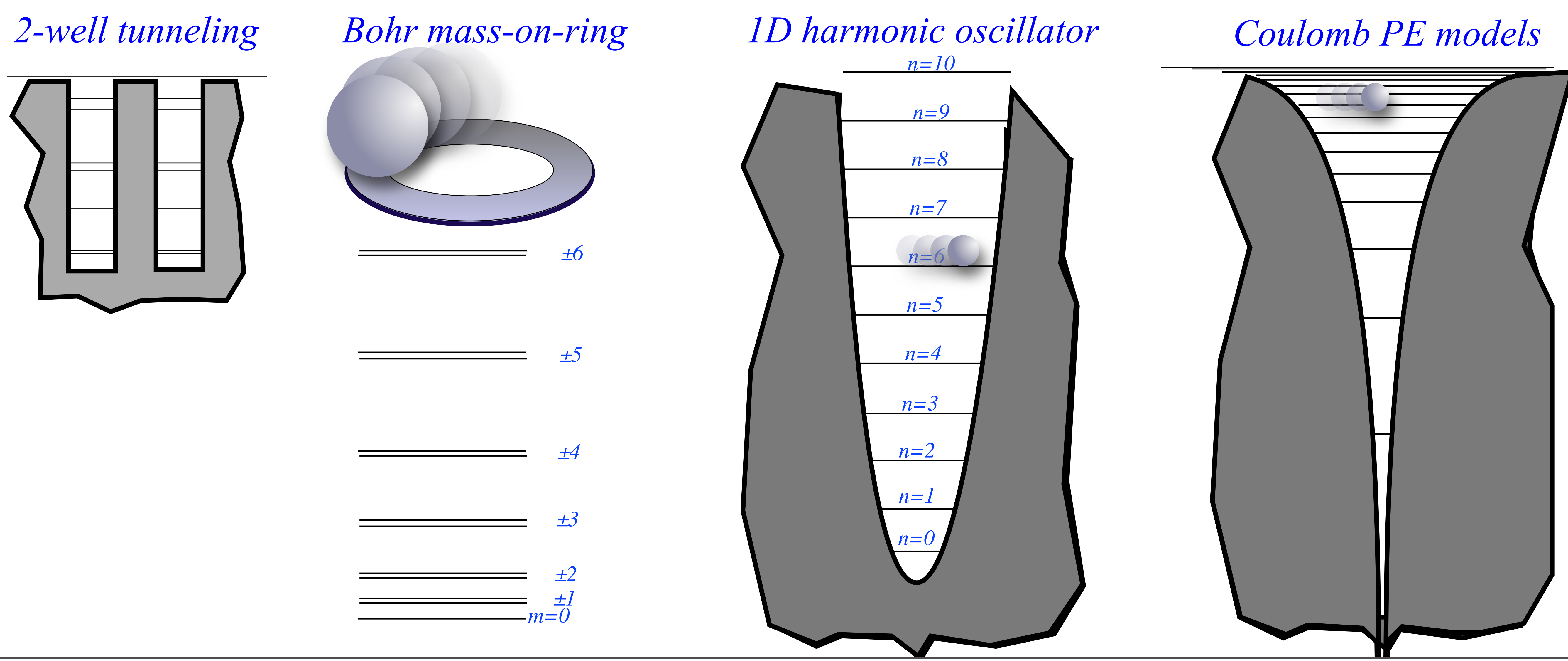
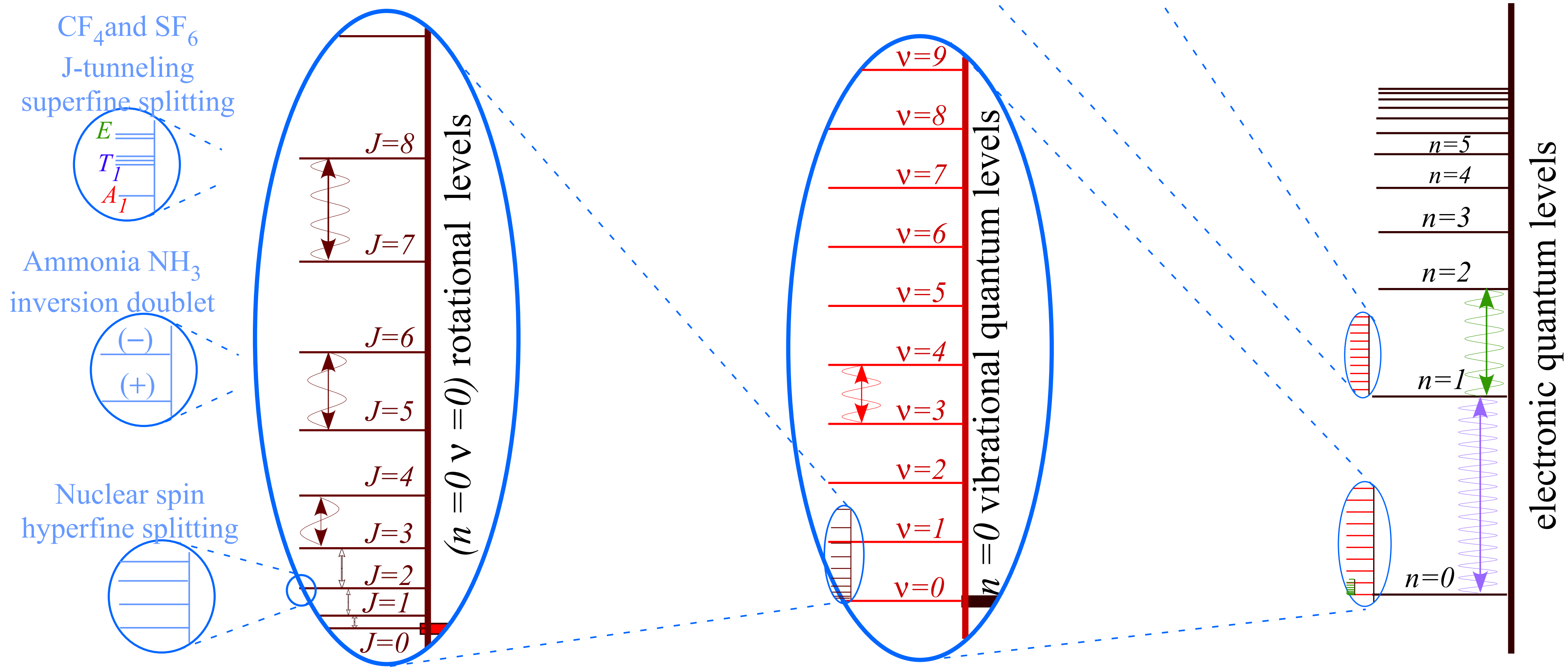




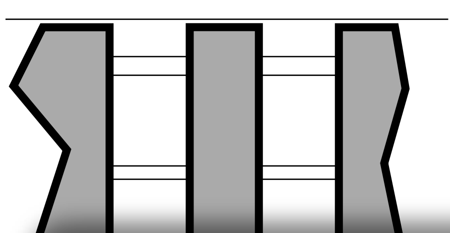
More Advanced Molecular Spectra Models

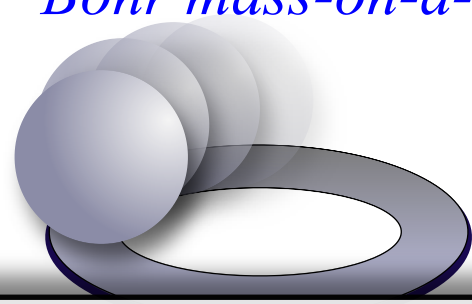
(Use symmetry group theory)

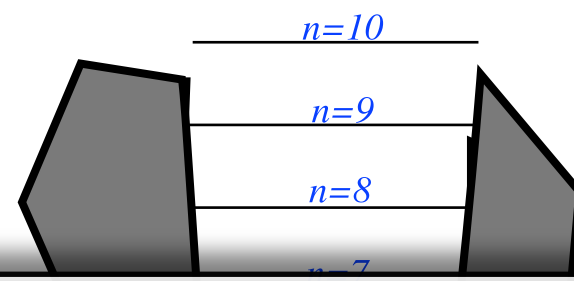


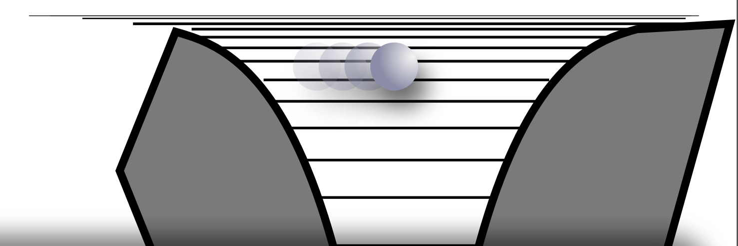
fine structure | rotational spectra | vibrational spectra | electronic spectra

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









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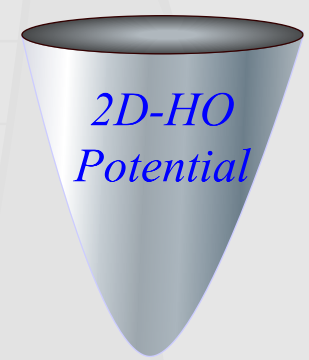
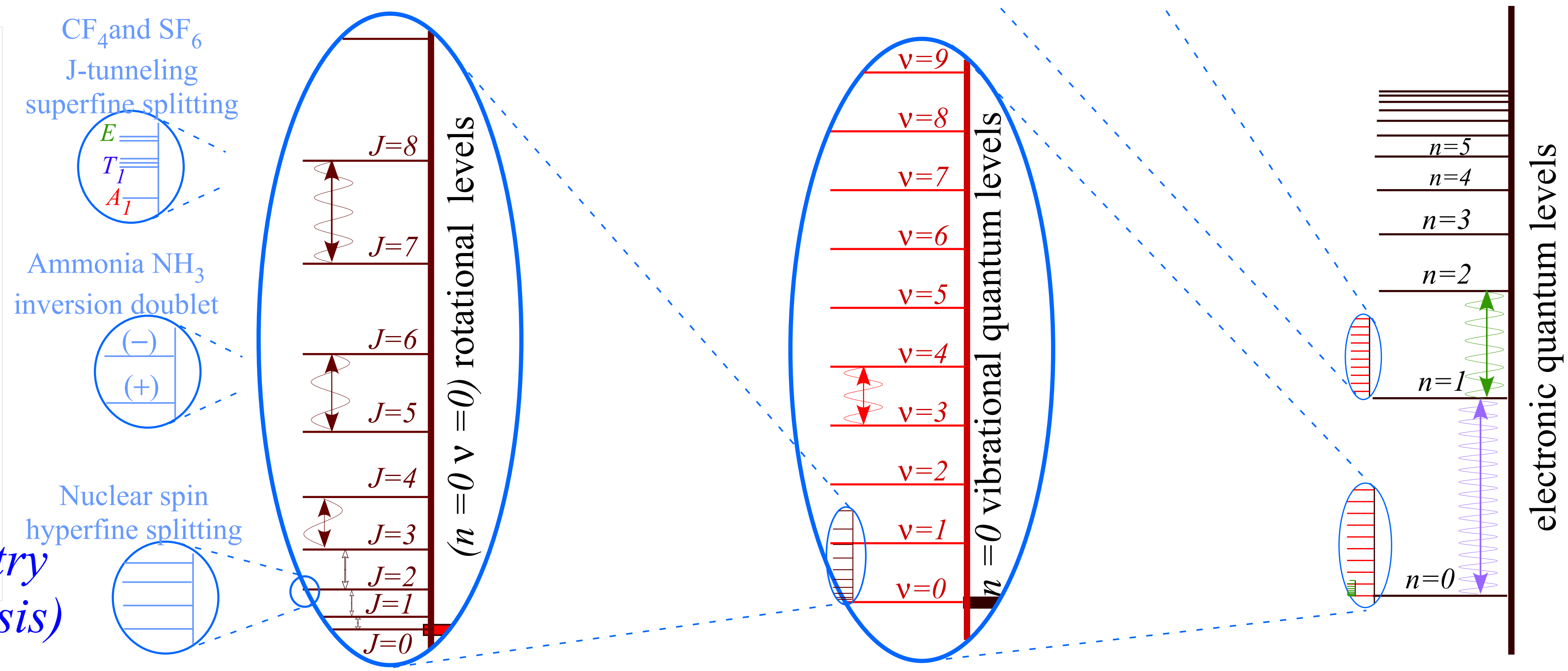
*U(m)*S$_n$ analysis of multi-electron states*



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

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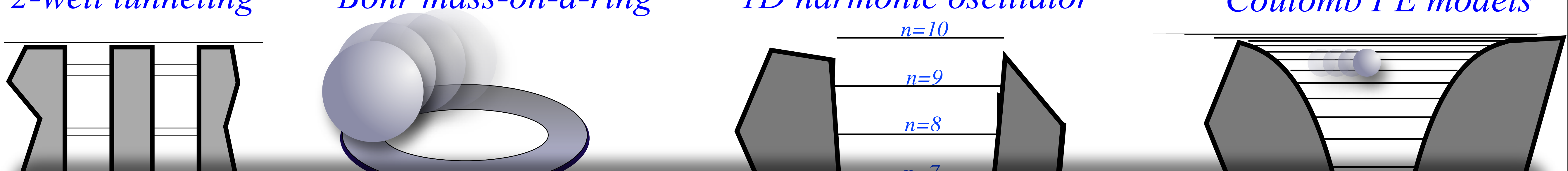

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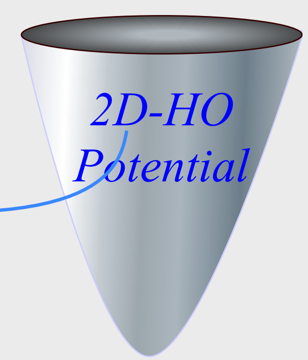

(closely connected)

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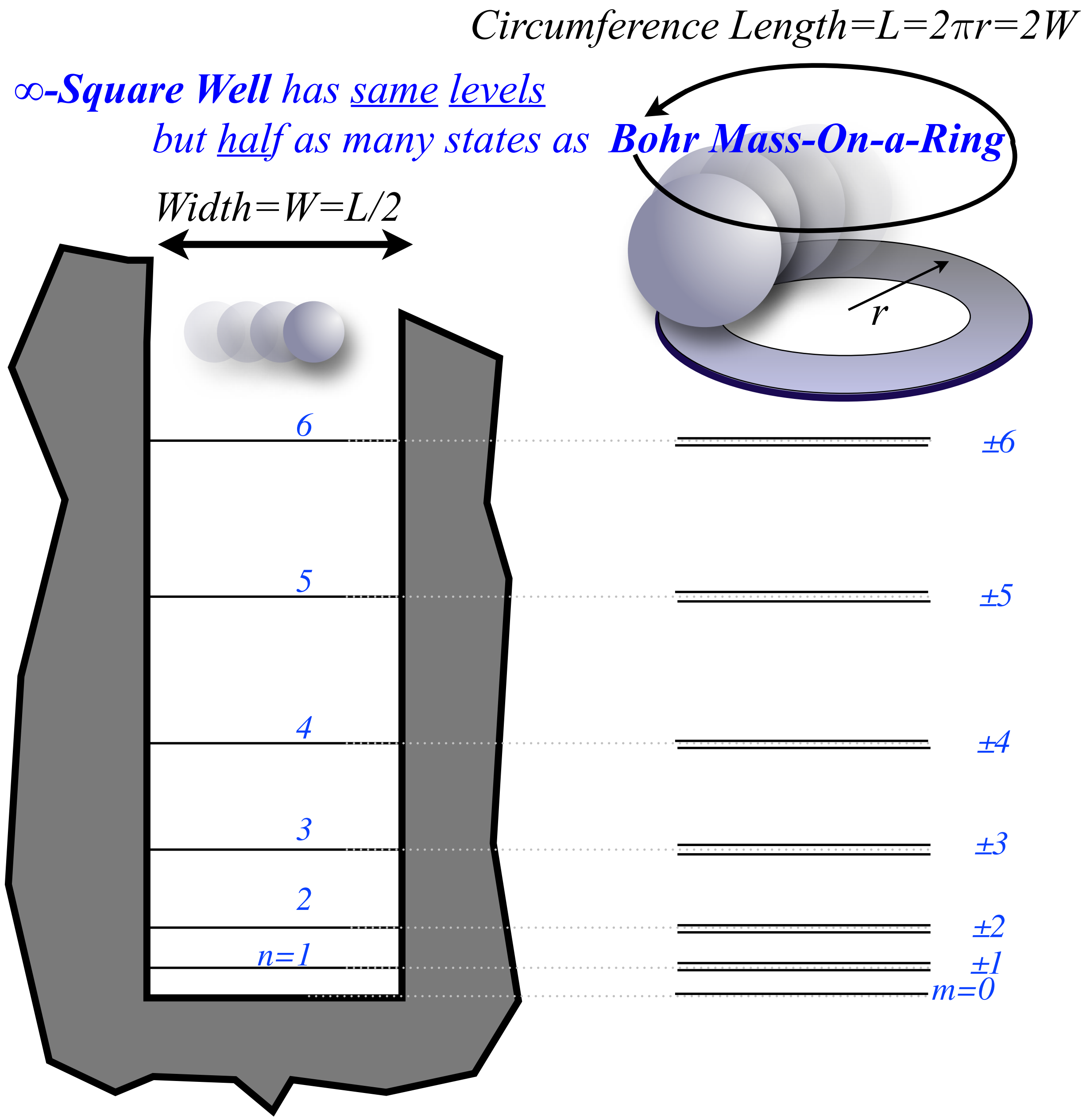
*∞-**Square Well** has same levels*
*but half as many states as **Bohr Mass-On-a-Ring***



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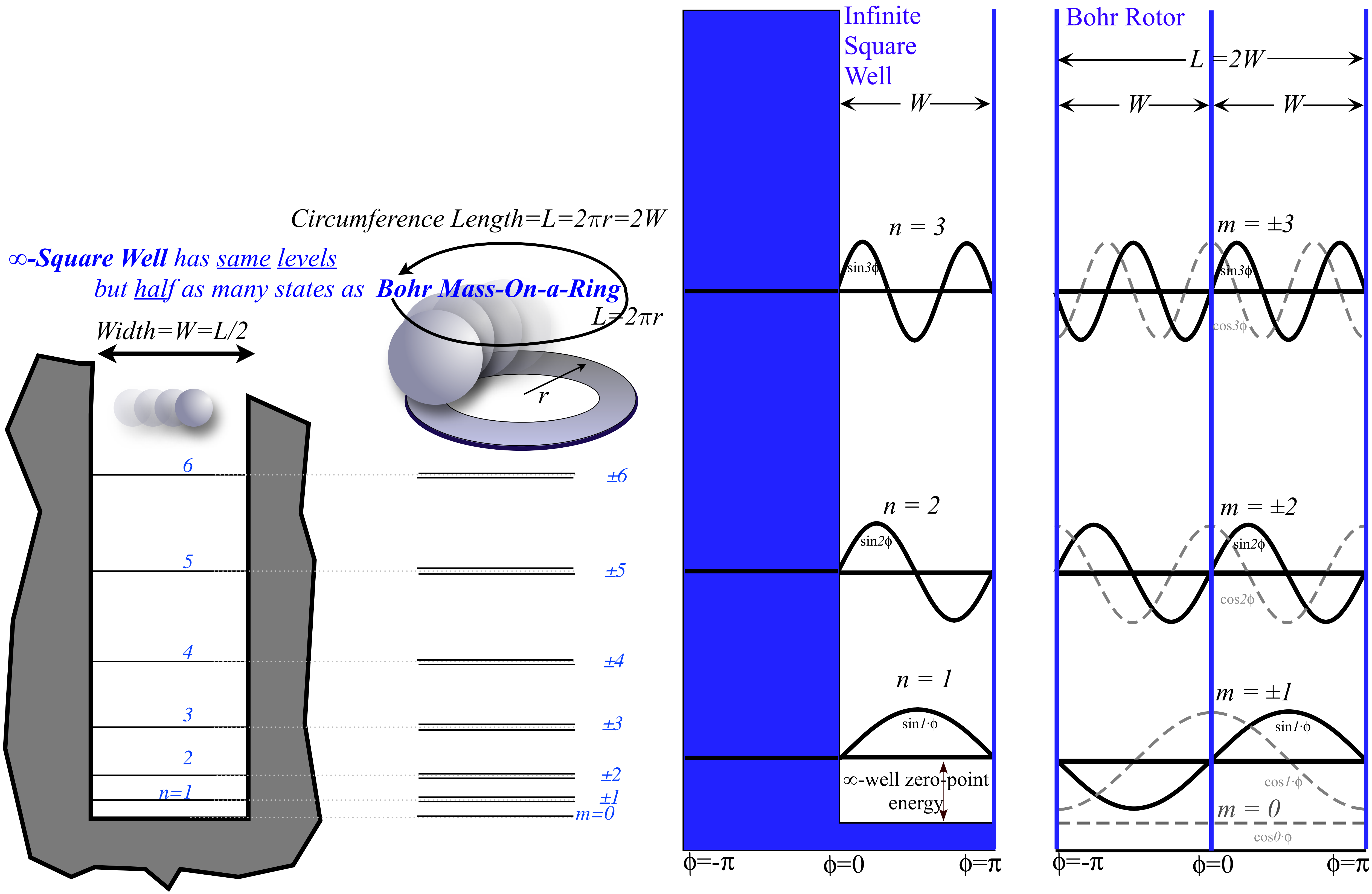

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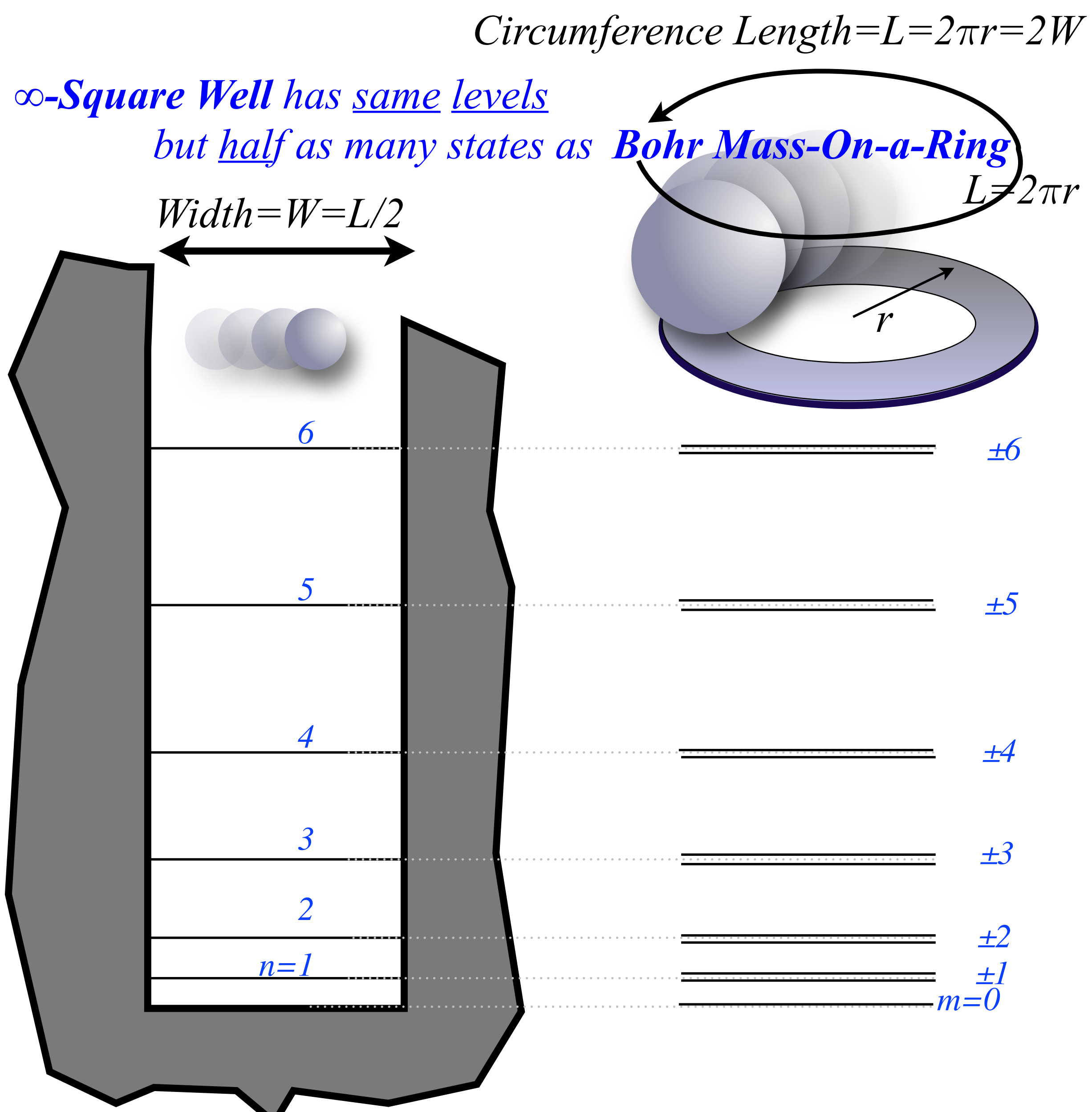
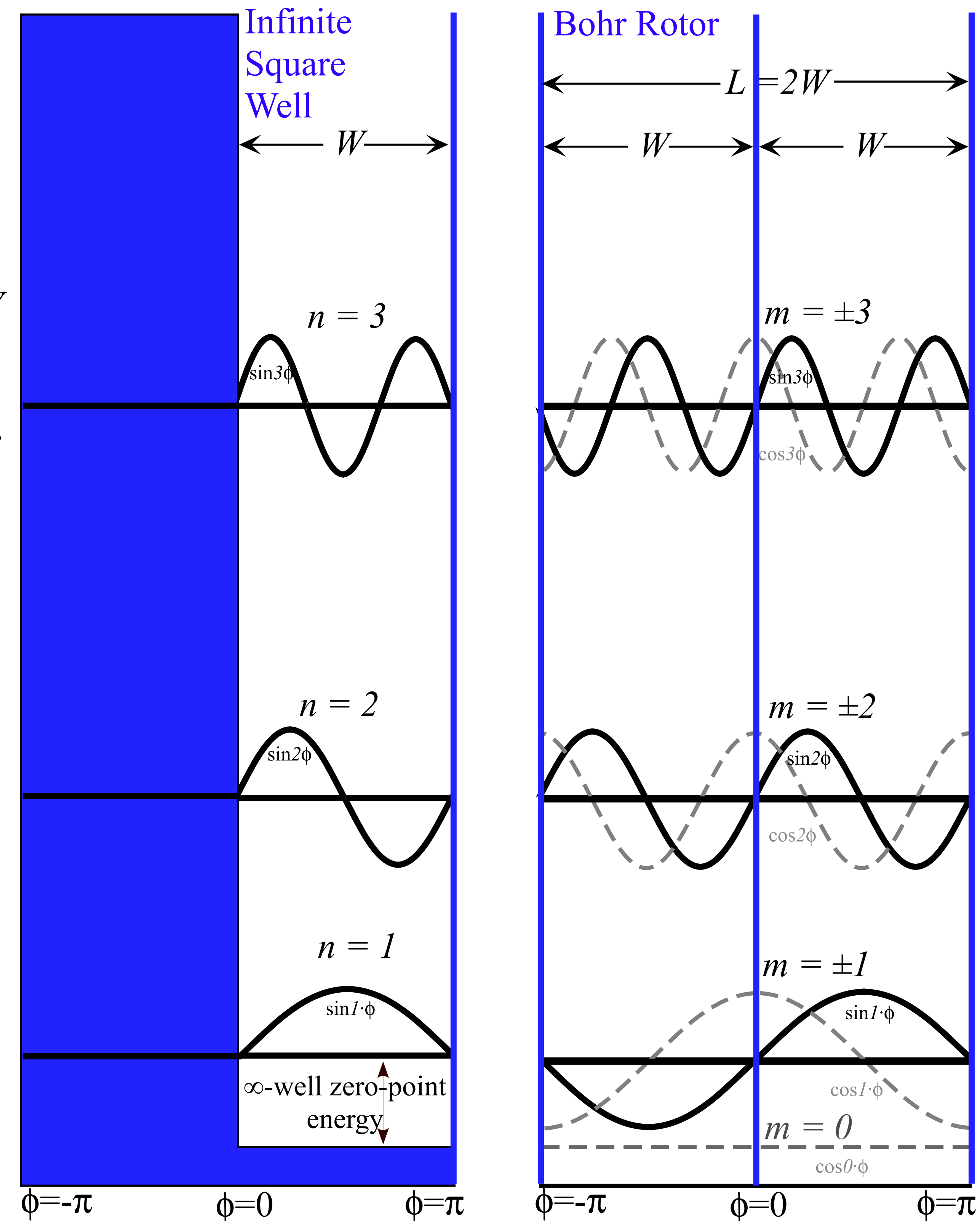
∞-Square Well *has only <u>sine</u> <u>standing</u> waves* $\psi_n = A\sin n\phi$

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



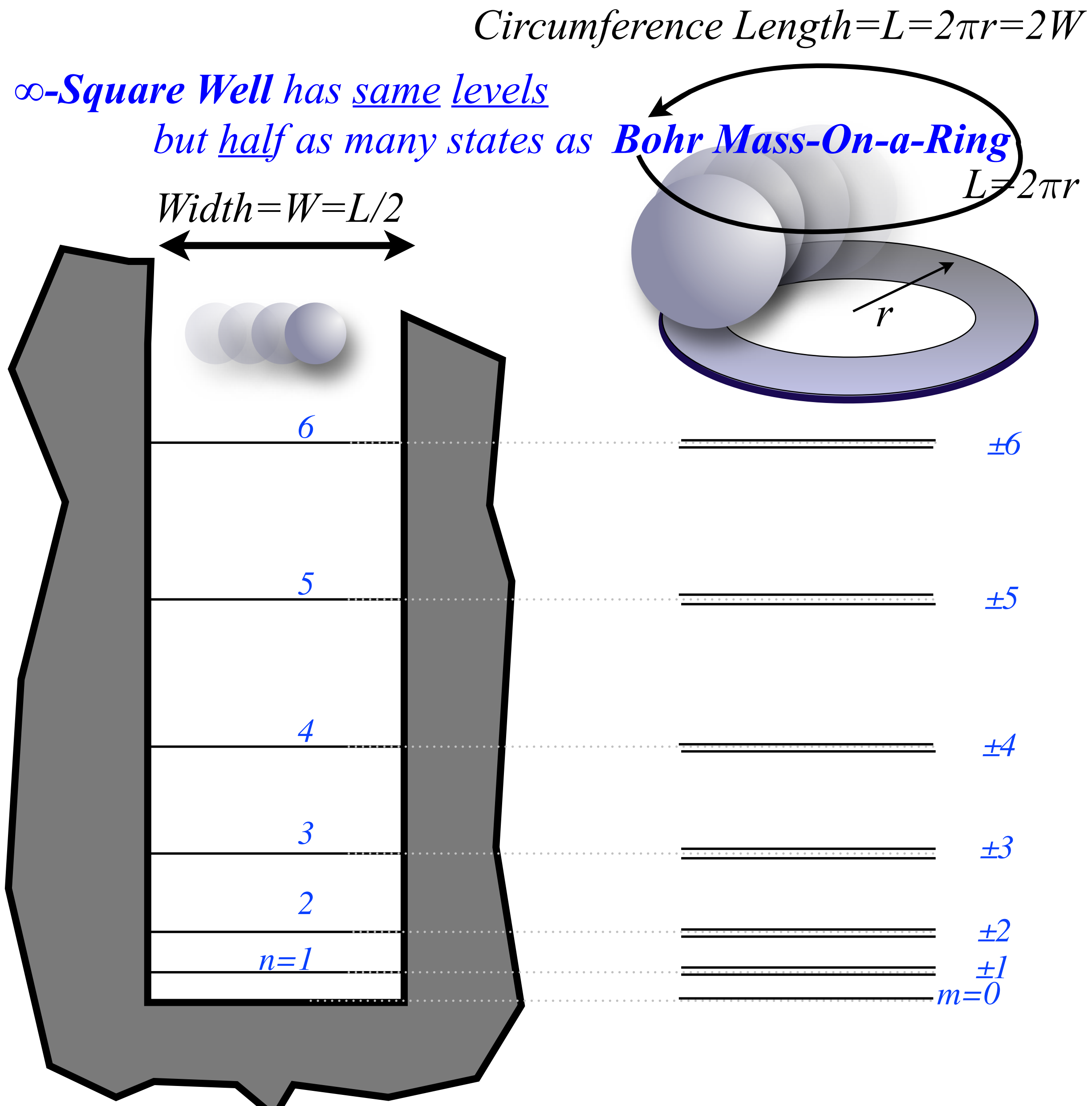


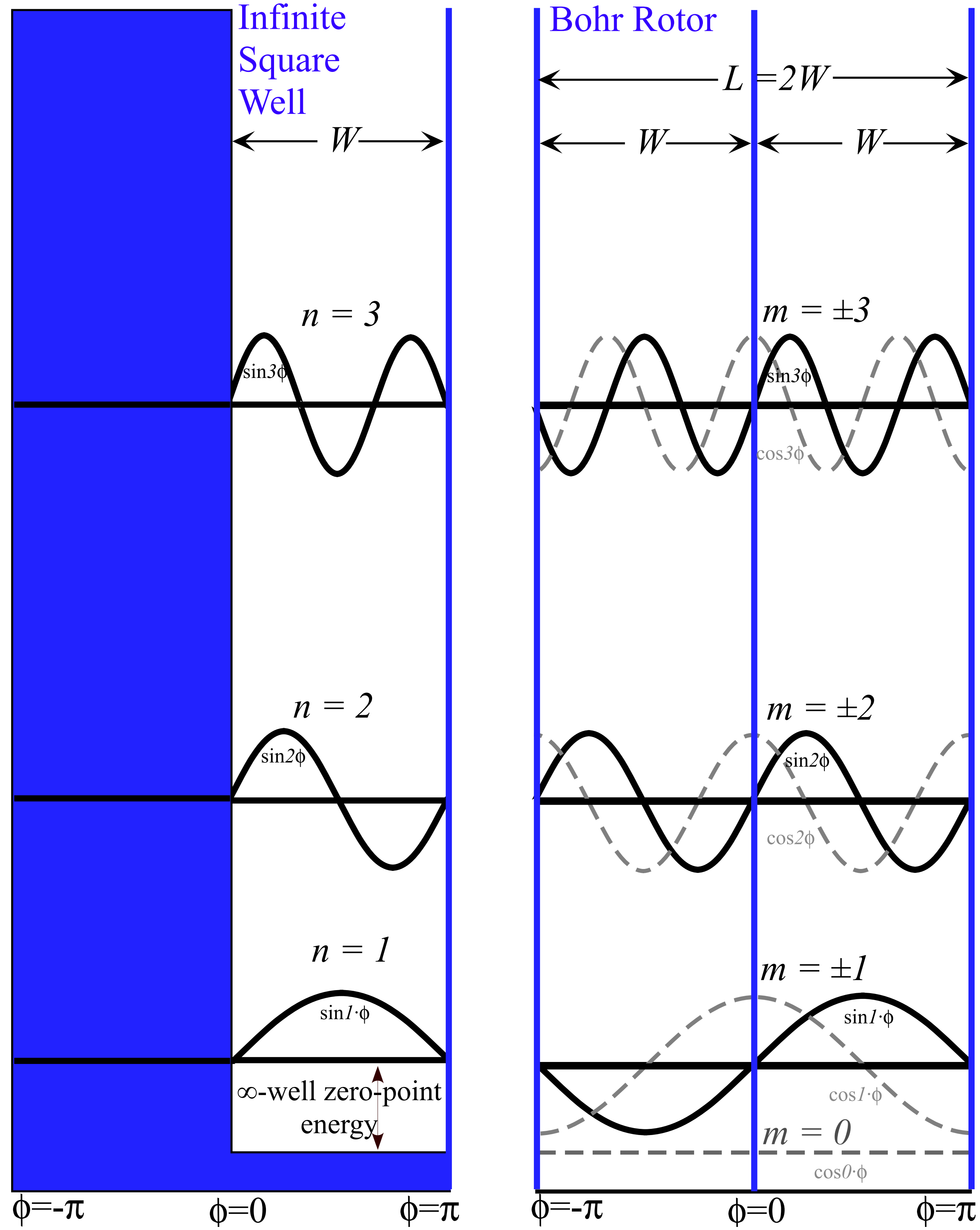
Bohr Mass-On-a-Ring *(model of rotation) and related* ***∞-Square Well*** *(model of quantum dots)*

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

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

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





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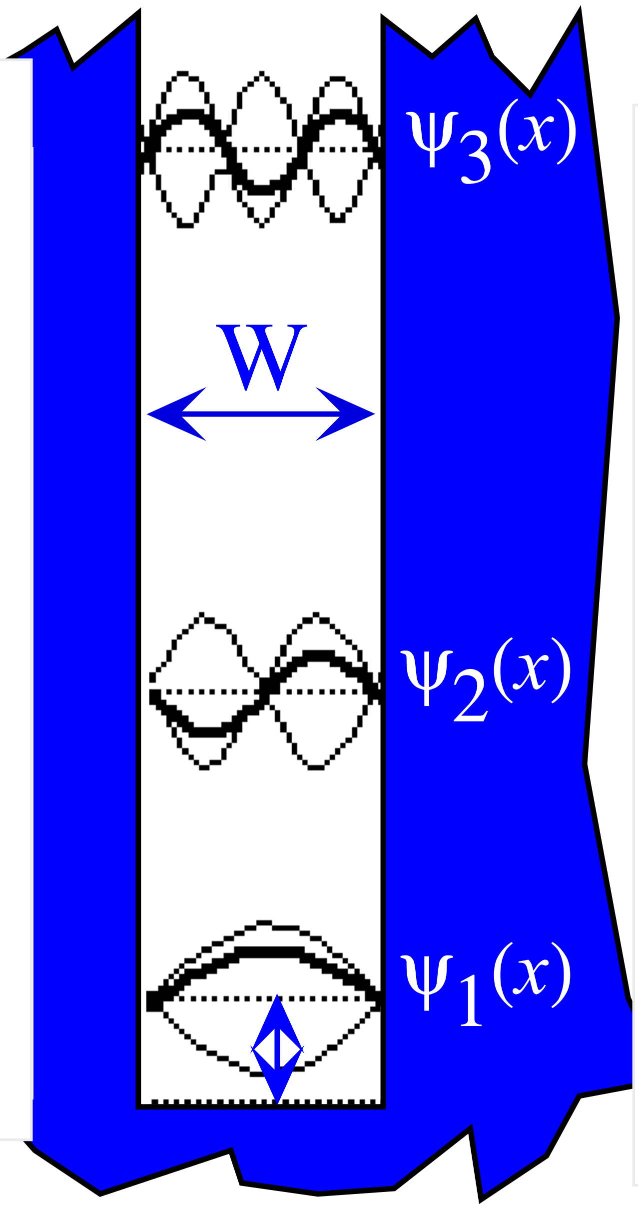
Standing wave $\langle x|\varepsilon_n\rangle = \psi_n(x) = A\sin(k_n x)$ *with boundary conditions* $kW = n\pi$ *or:* $k = n\pi/W$

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



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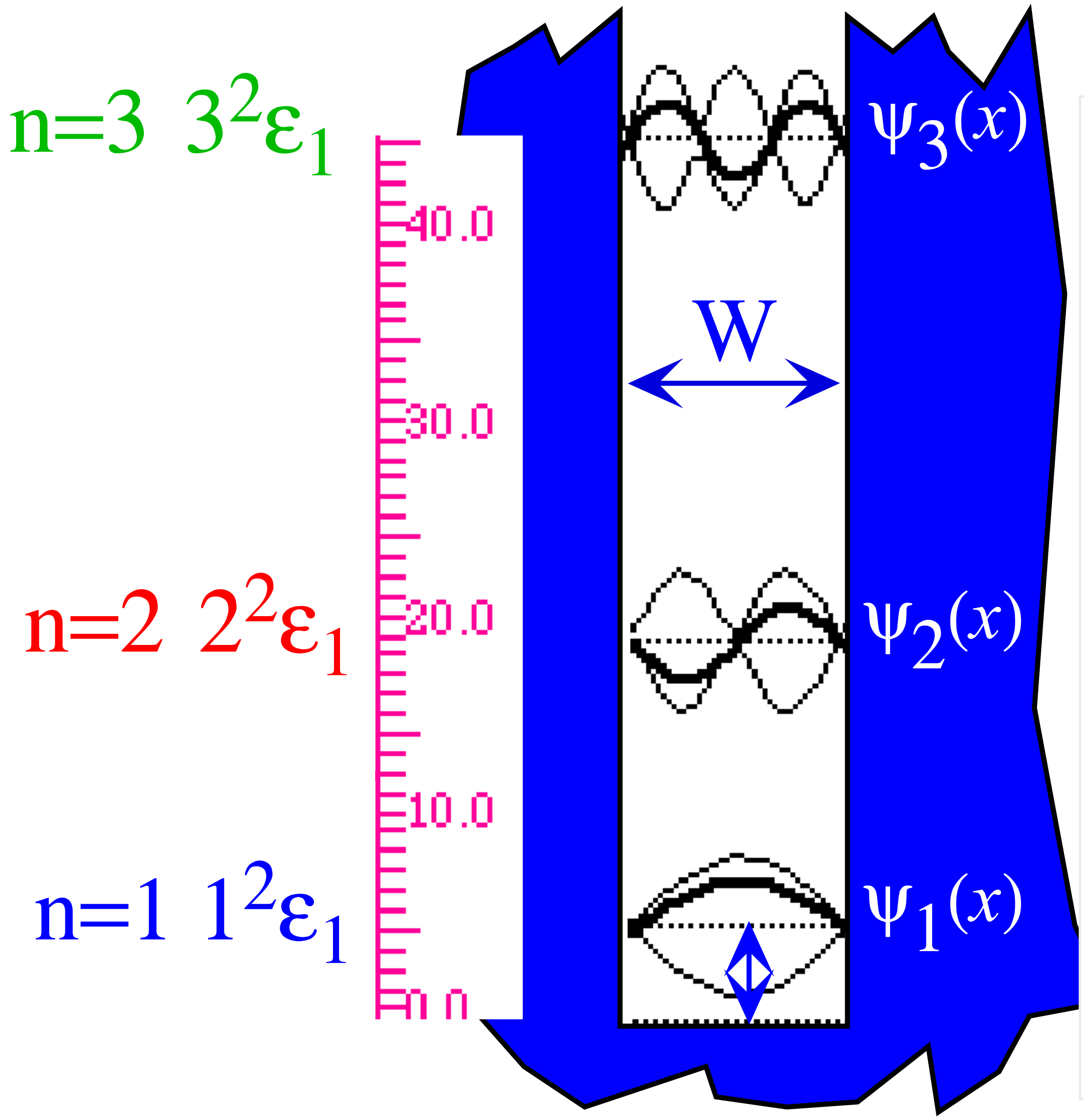
$$= A\sin\left(\frac{n\pi x}{W}\right) \quad (n=1,2,3,...\infty)$$

Gives energy levels:

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



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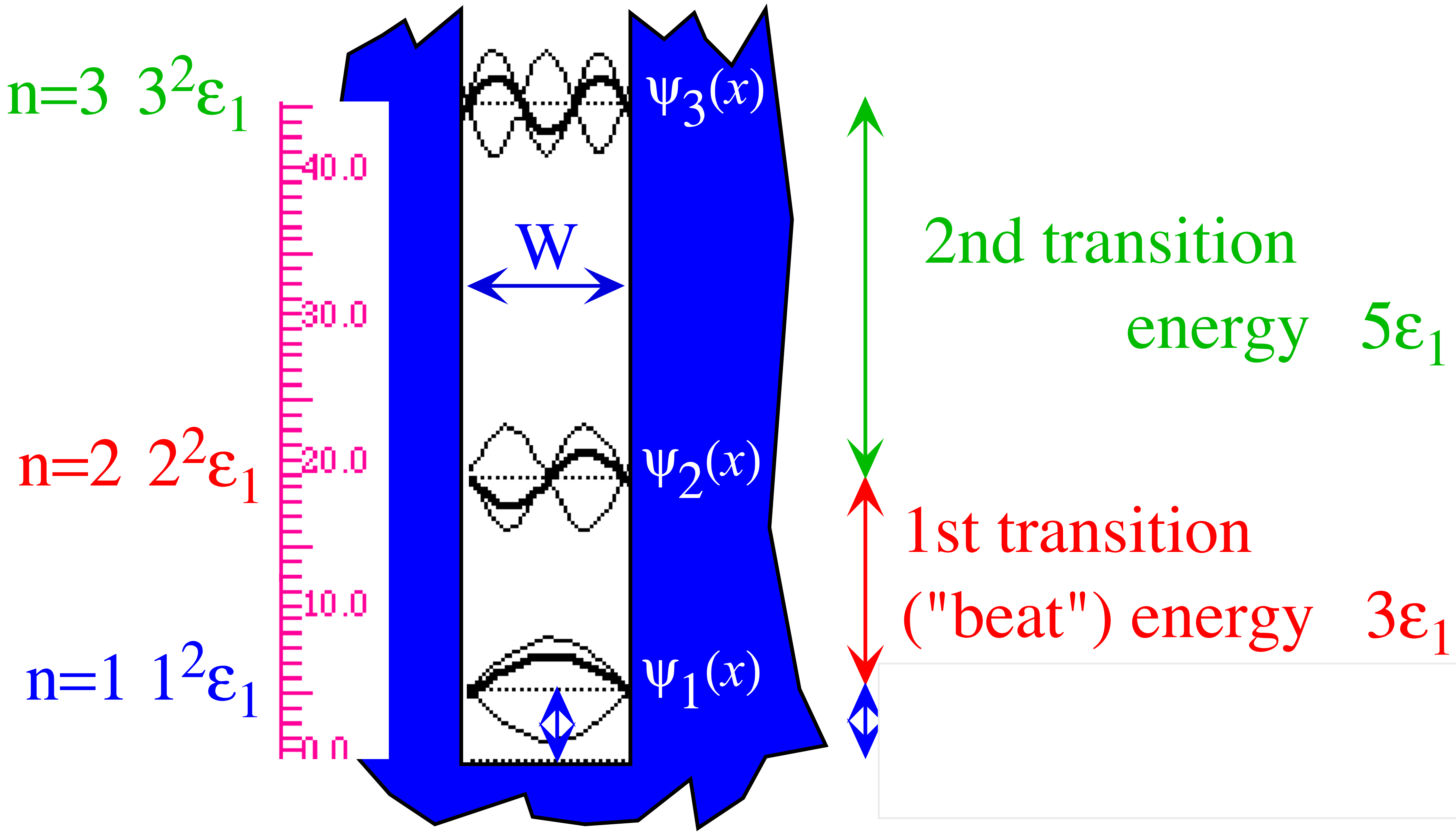

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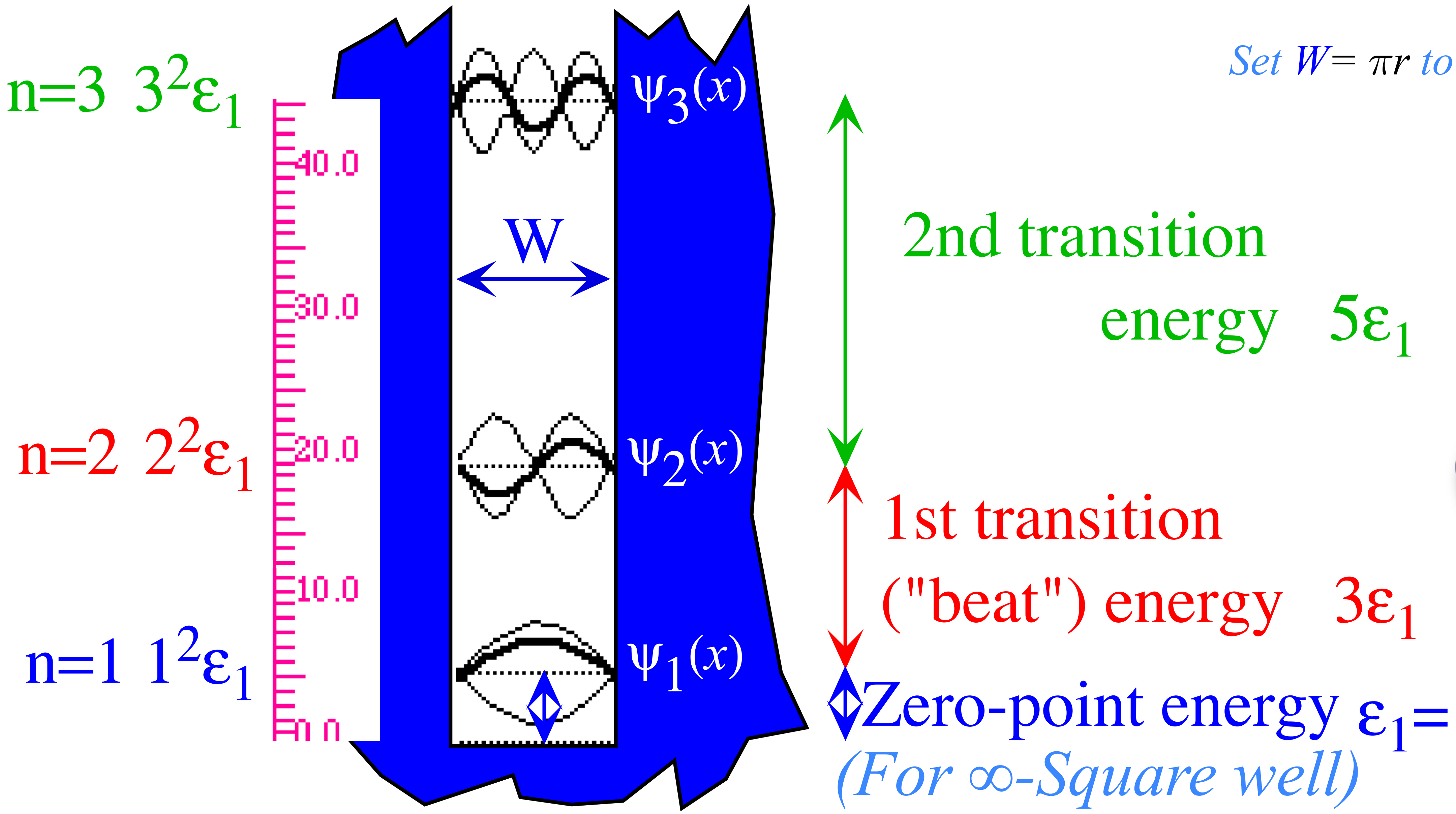
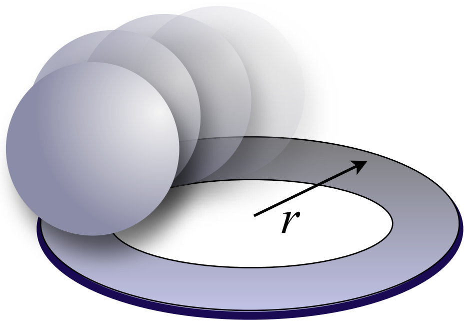
Set $W = \pi r$ *to get rotor energy:*





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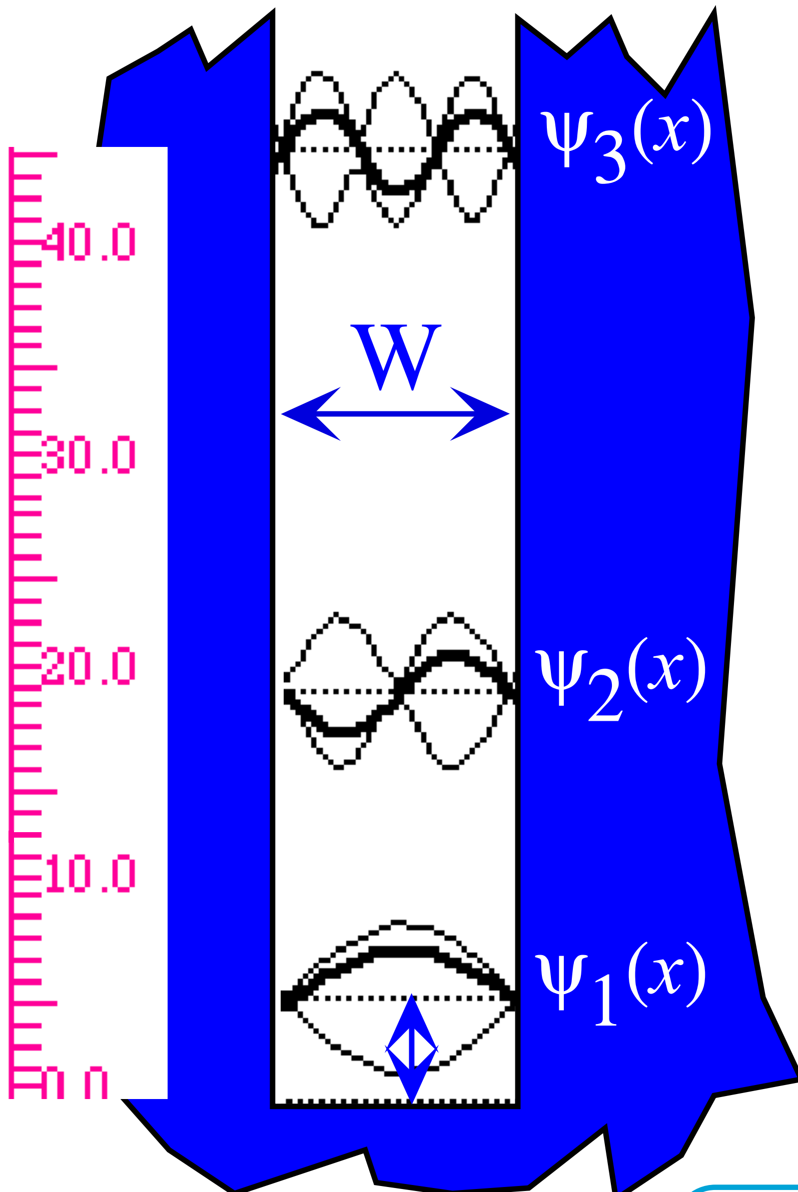
$$= \frac{h^2}{8M\pi^2 r^2}n^2 = \frac{\hbar^2}{2Mr^2}n^2 = \frac{\hbar^2}{2I}n^2$$

rotor energy for: $W = \pi r$

n=3 $3^2\varepsilon_1$

n=2 $2^2\varepsilon_1$

n=1 $1^2\varepsilon_1$

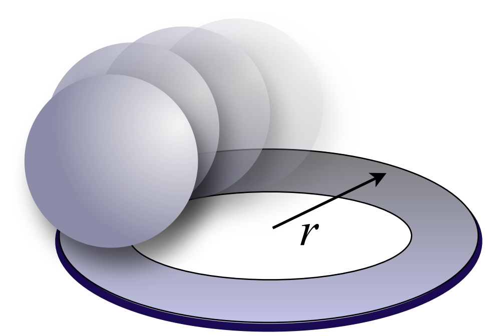


2nd transition energy $5\varepsilon_1$

1st transition ("beat") energy $3\varepsilon_1$

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

(For ∞-Square well)



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

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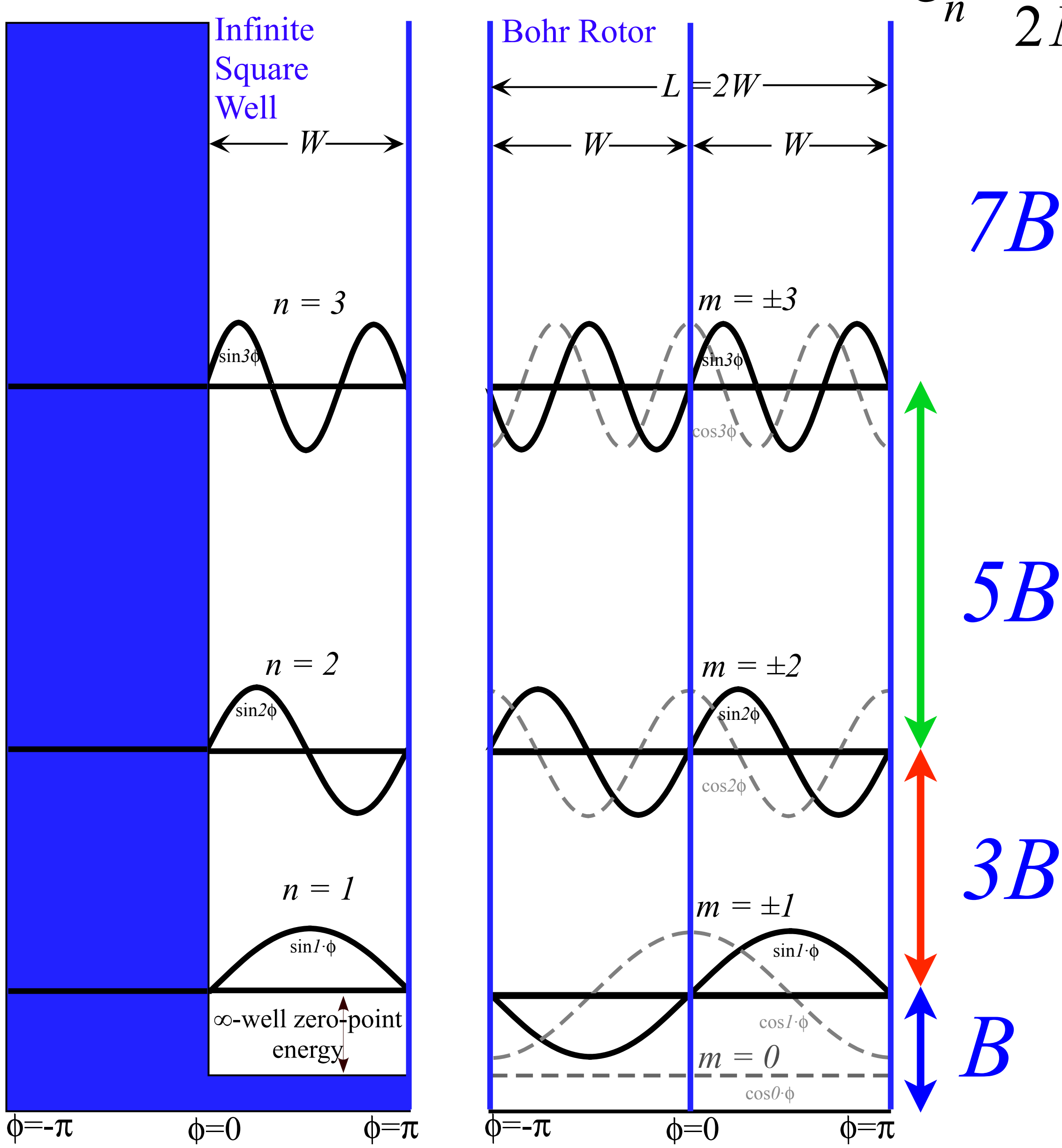

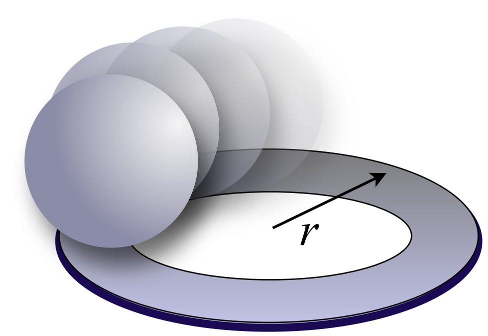

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The frequency hierarchy   Example of16μm spectra of CF_4

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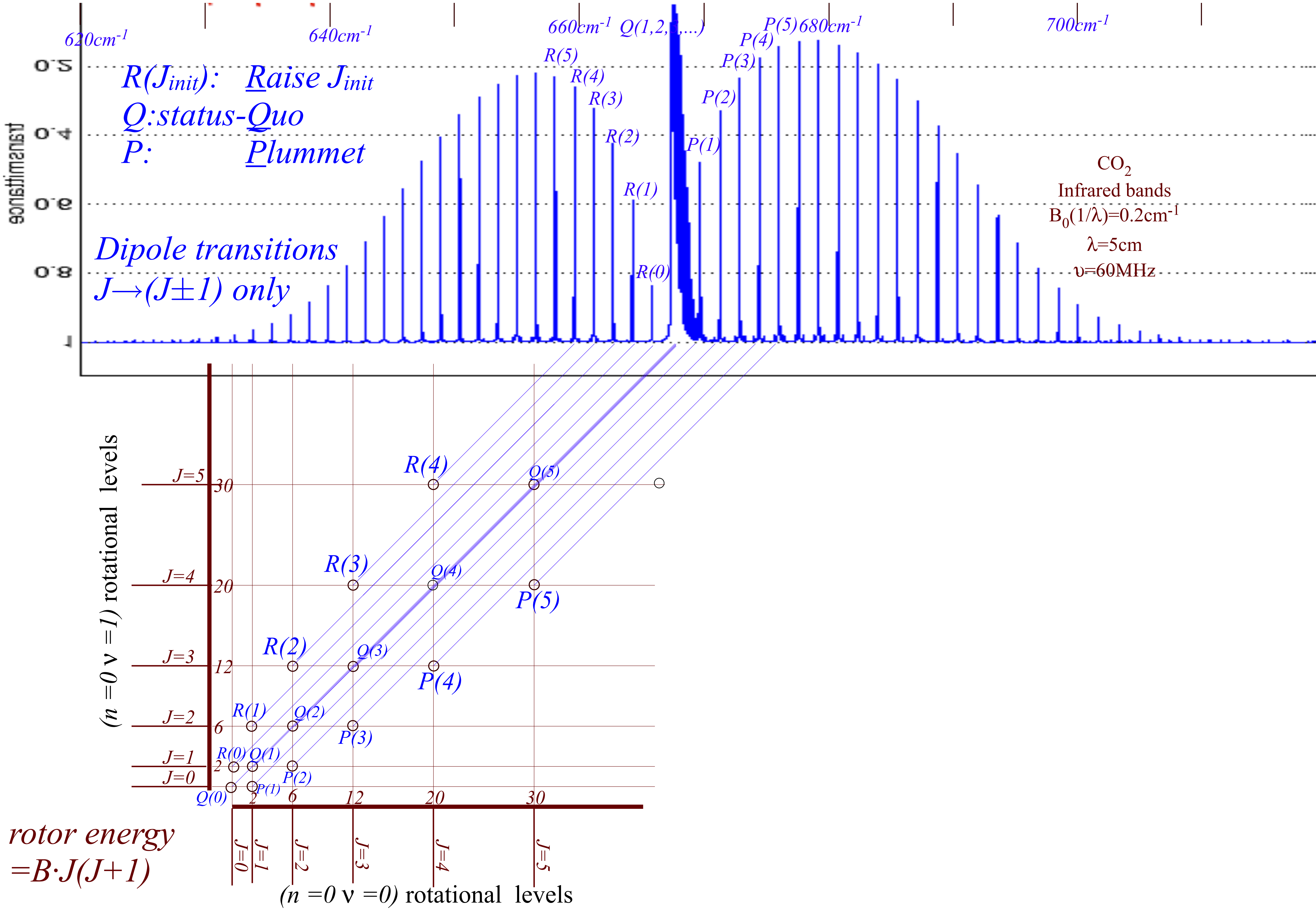

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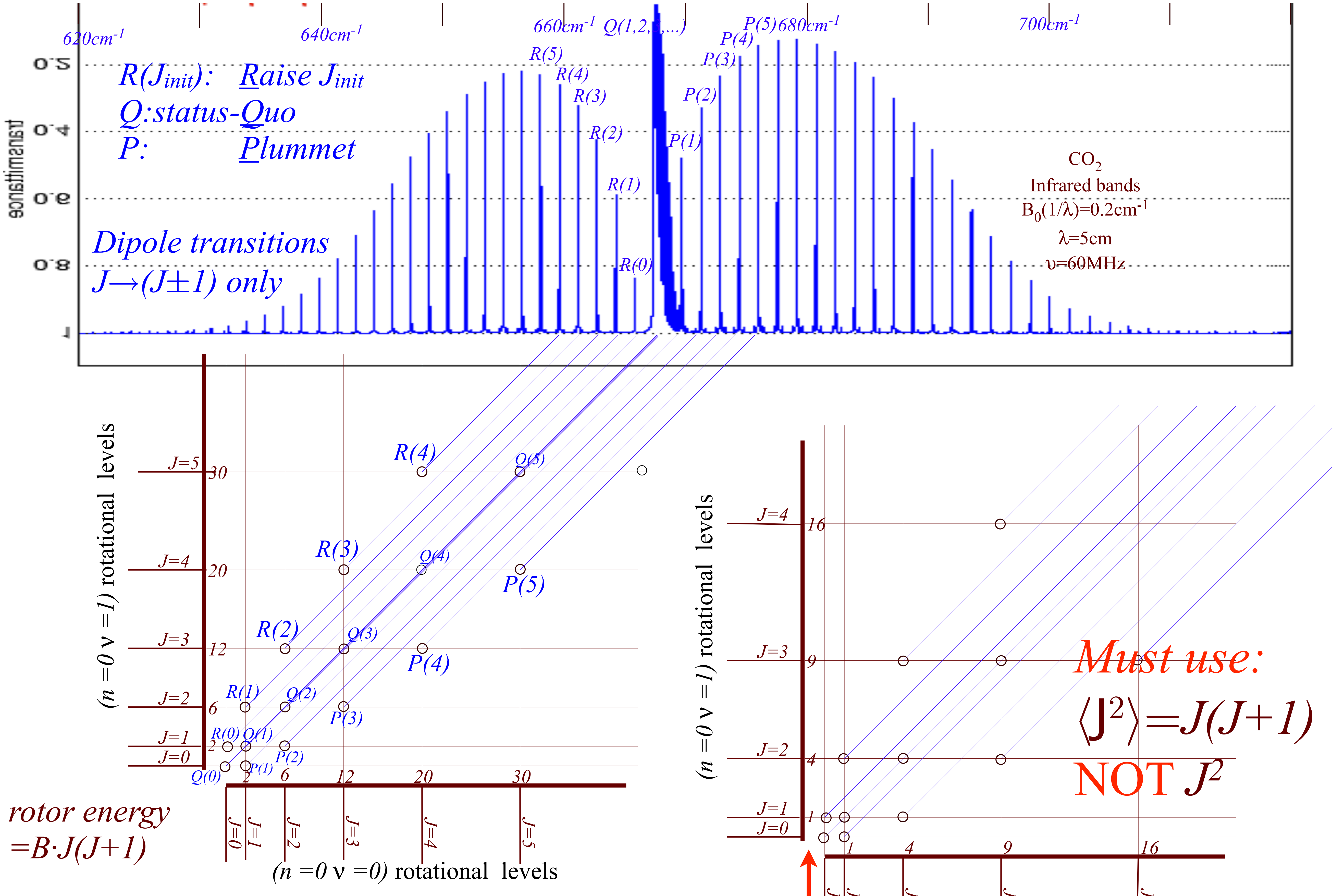

What does NOT work: rotor energy $=B\cdot J^2$

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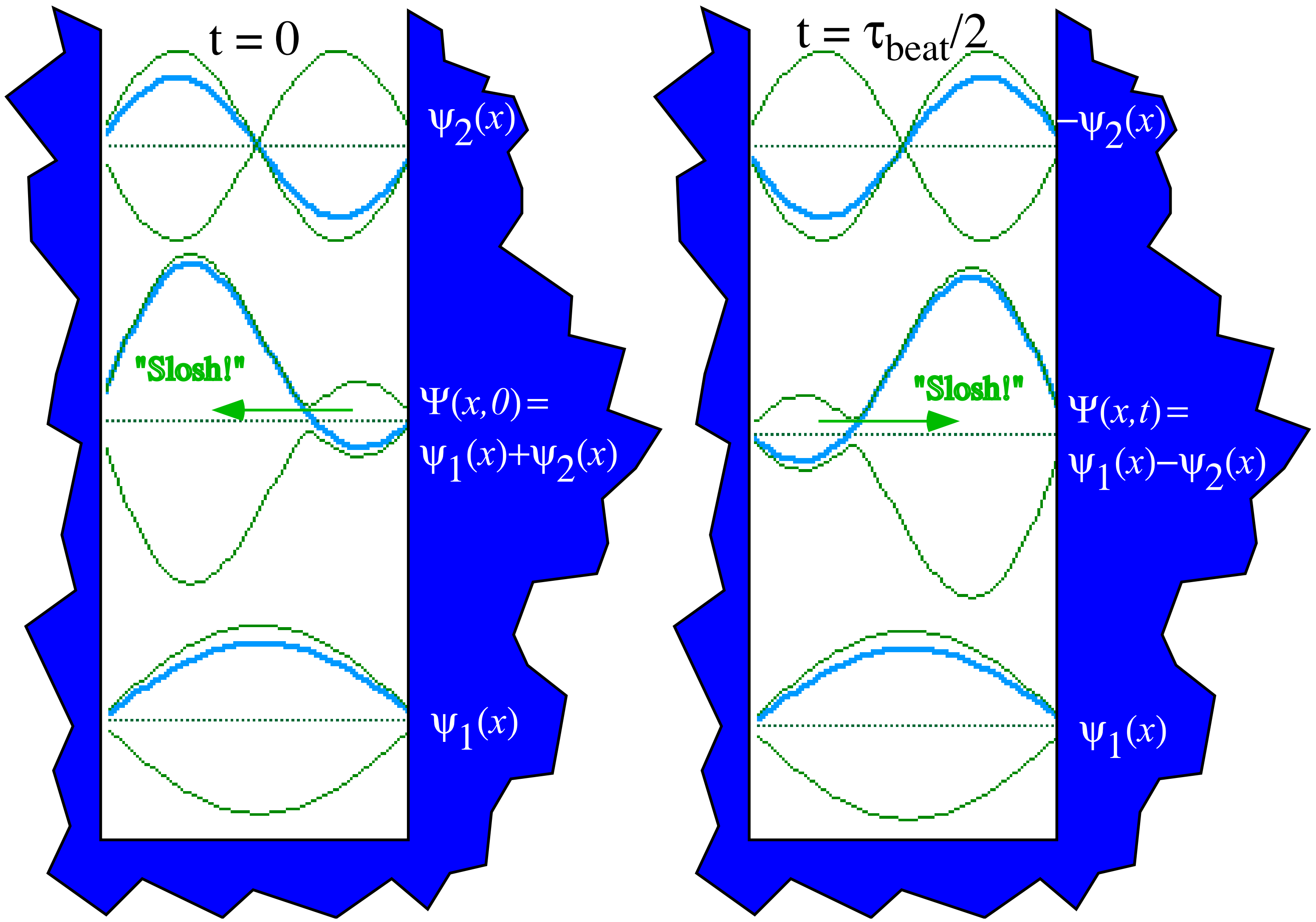

"Sloshing" charge acts like dipole antenna broadcasting linear polarized radiation*

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

Or receives (Depending on relative phase)

Quantum dynamics of ∞-Square well and Bohr rotor
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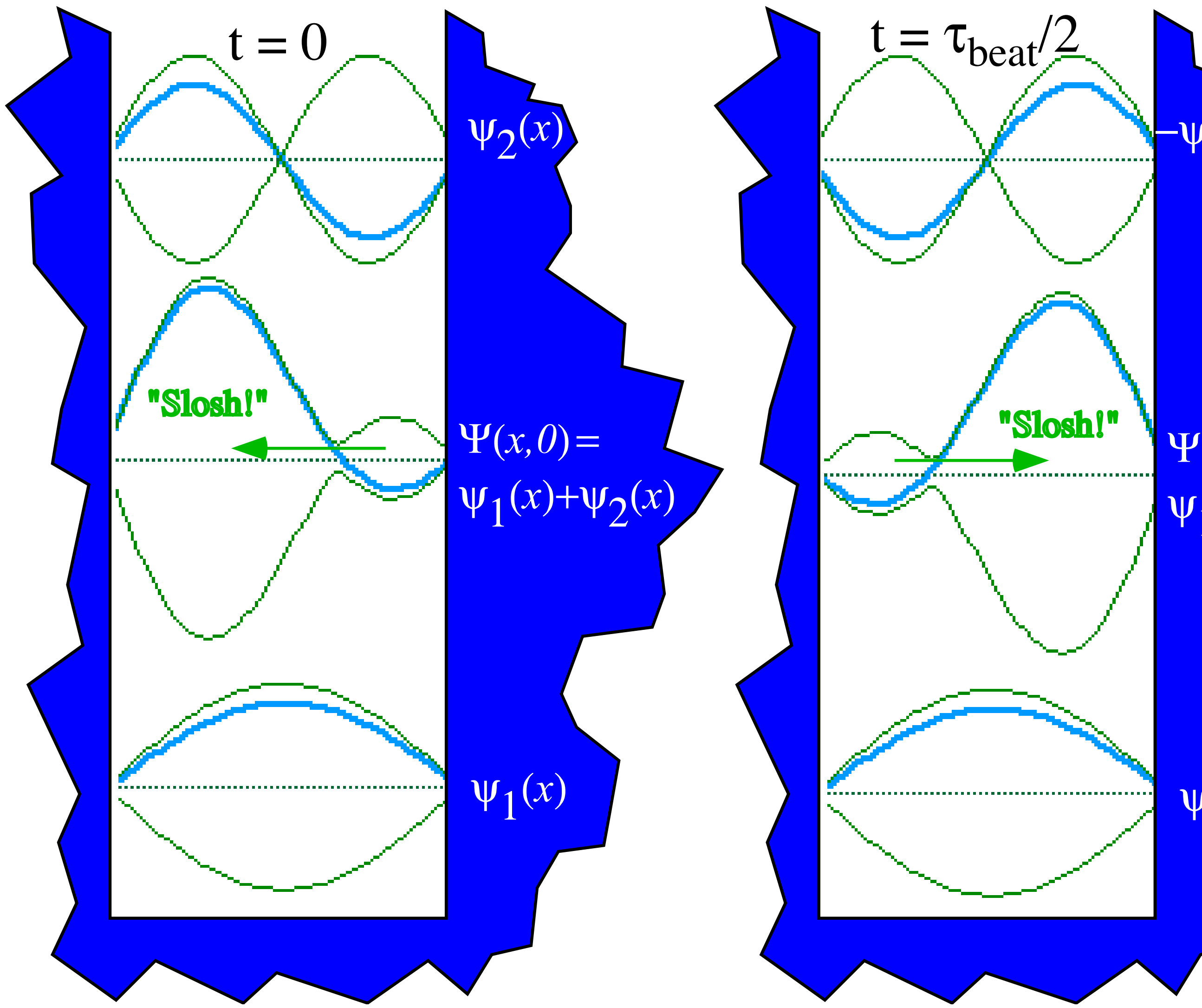
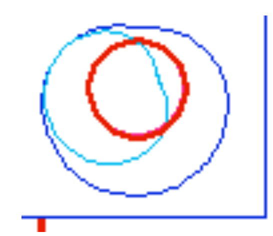
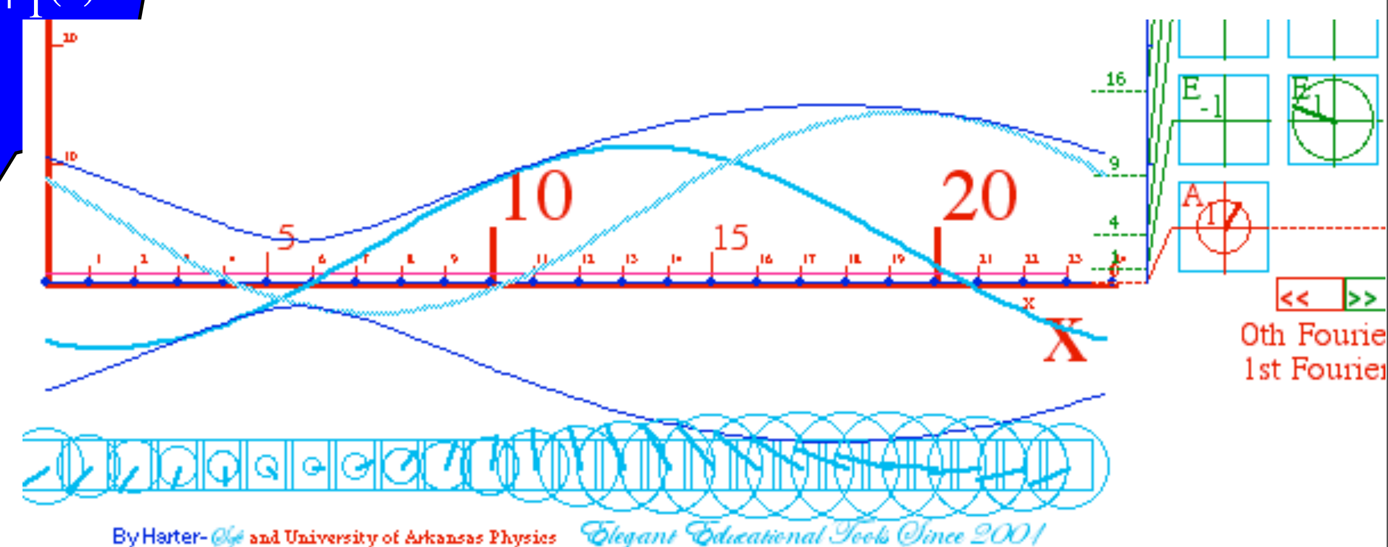


Rotating charge broadcasts circularly polarized radiation*





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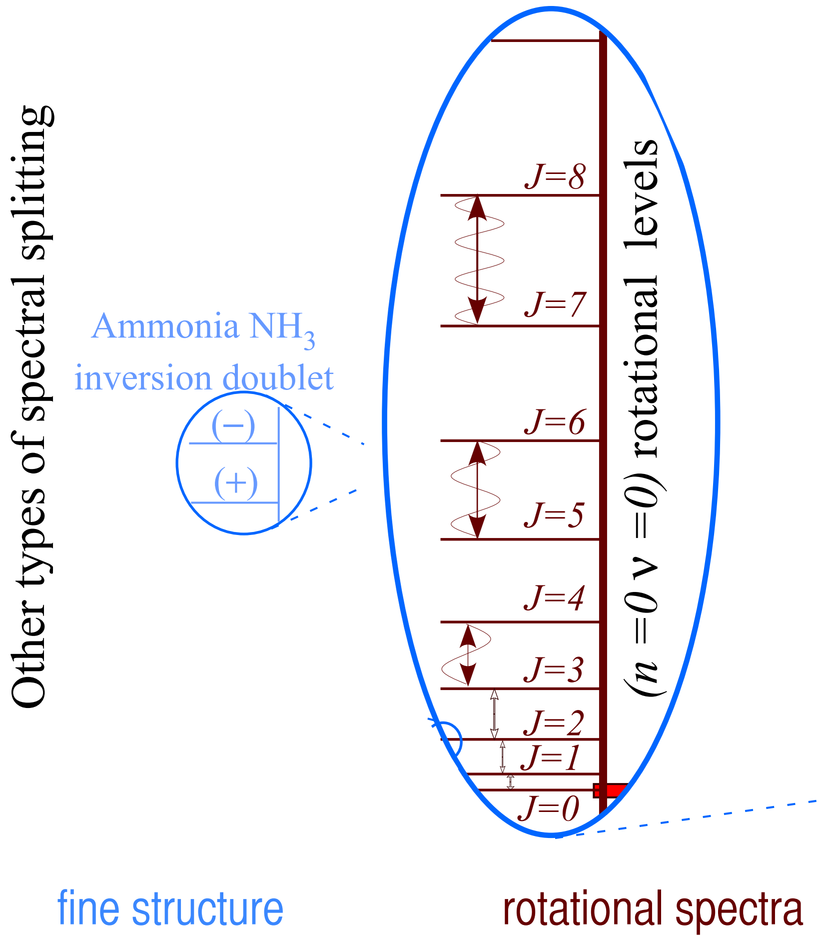
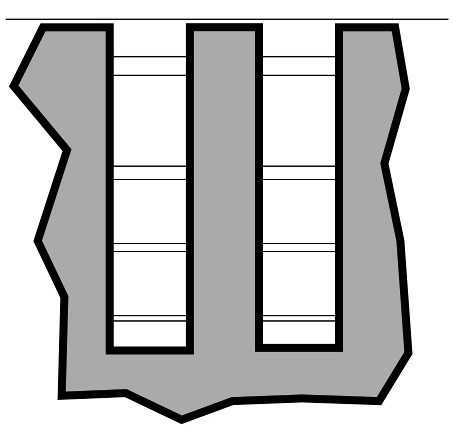


2-well tunneling



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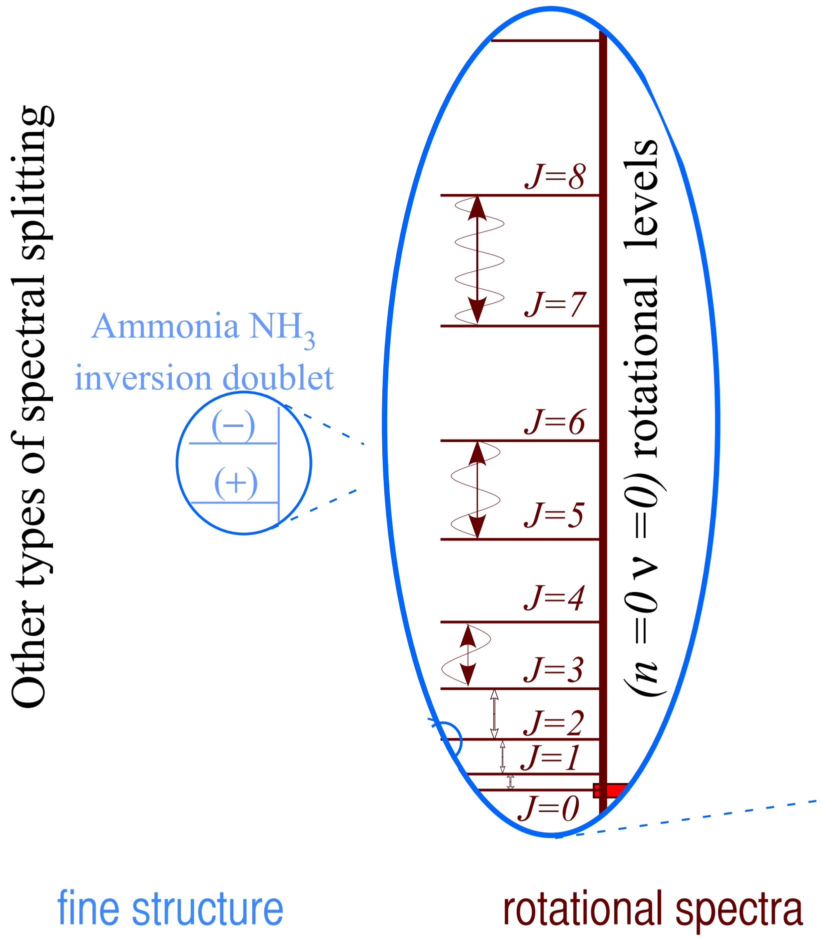
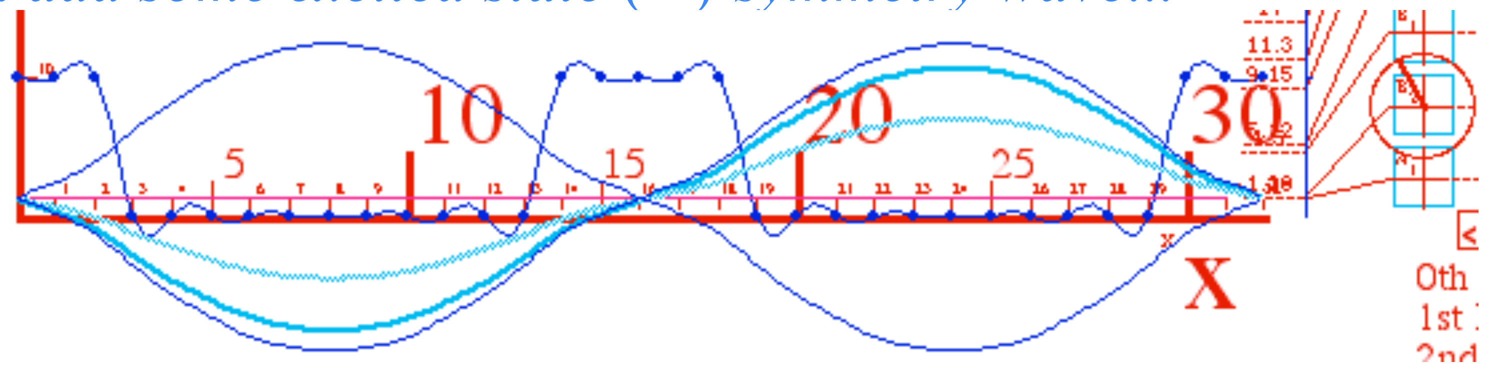
If you add some excited state (−)-symmetry wave...





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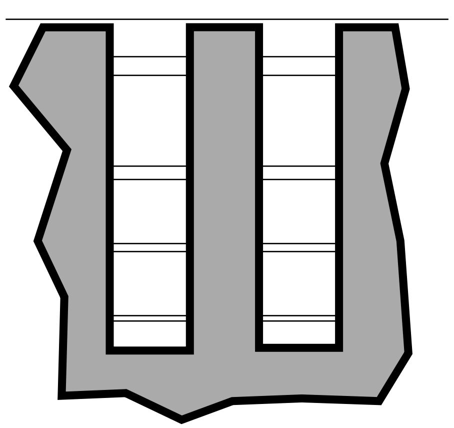

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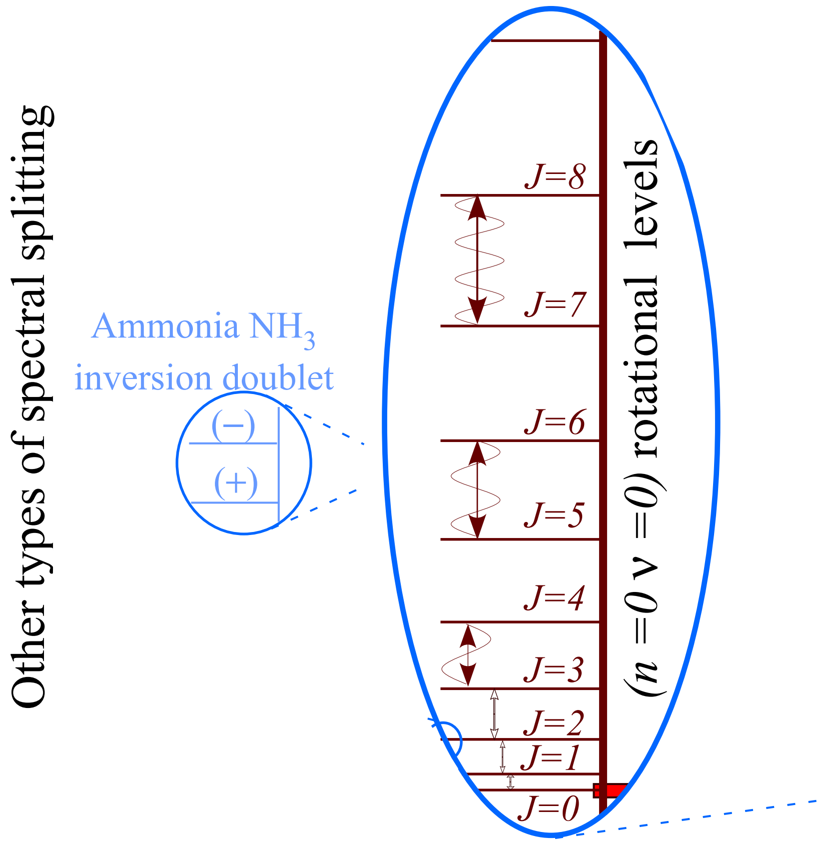

fine structure rotational spectra

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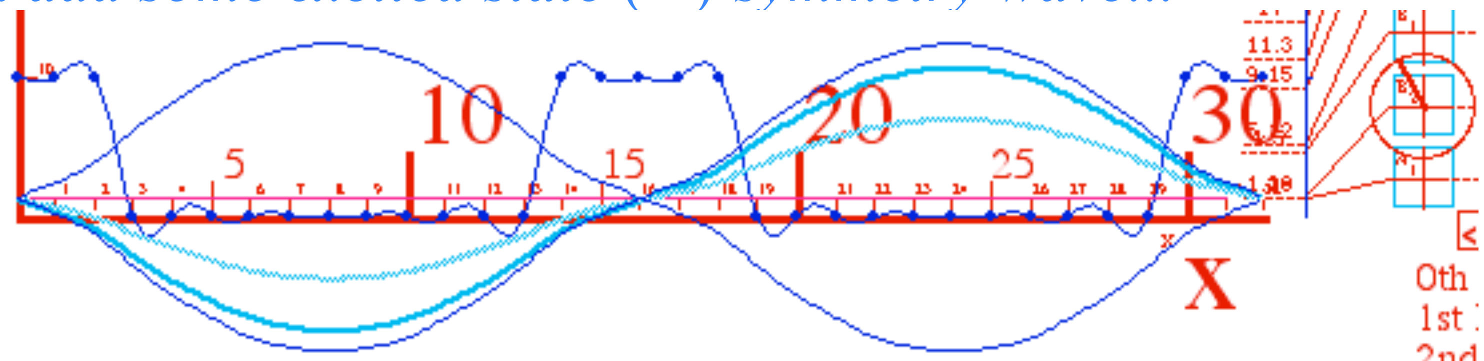
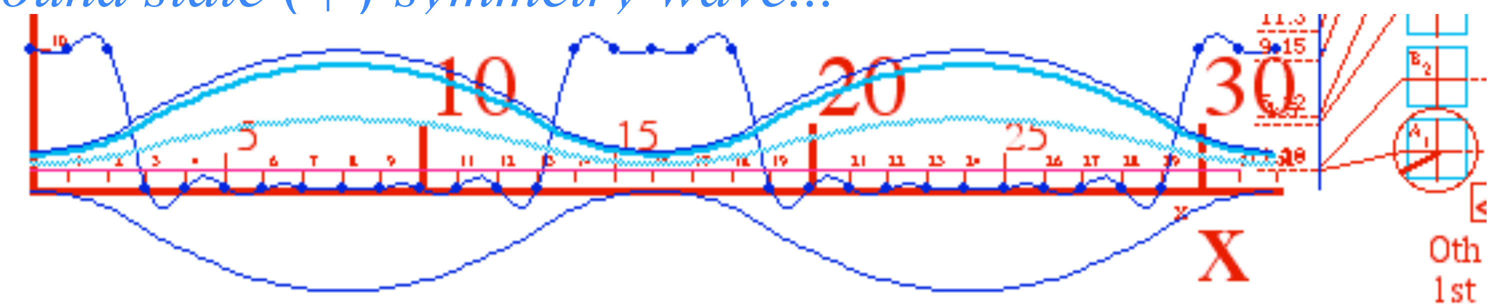


...to ground state (+)-symmetry wave...



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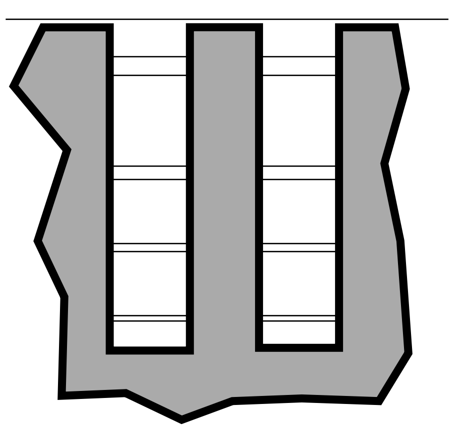

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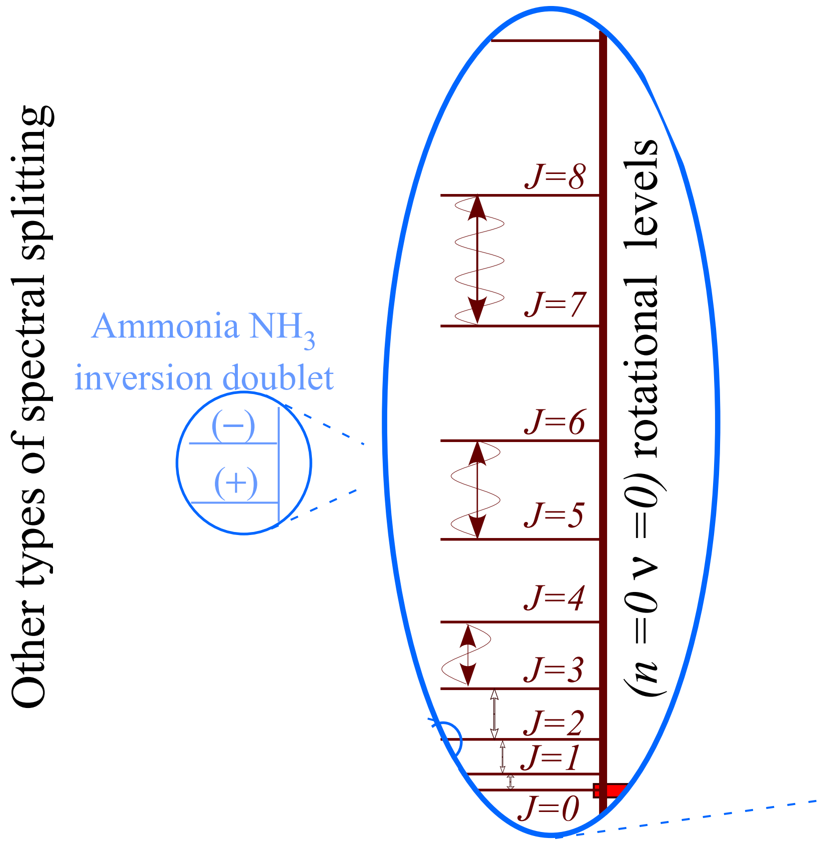
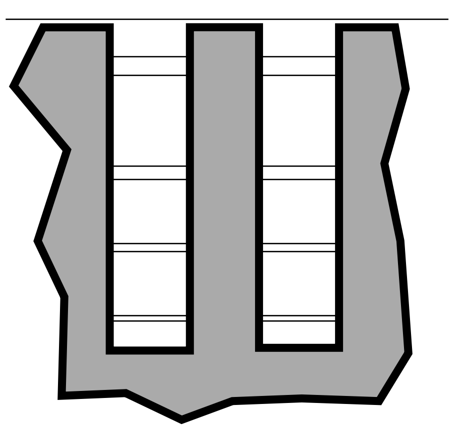


fine structure

rotational spectra

2-well tunneling



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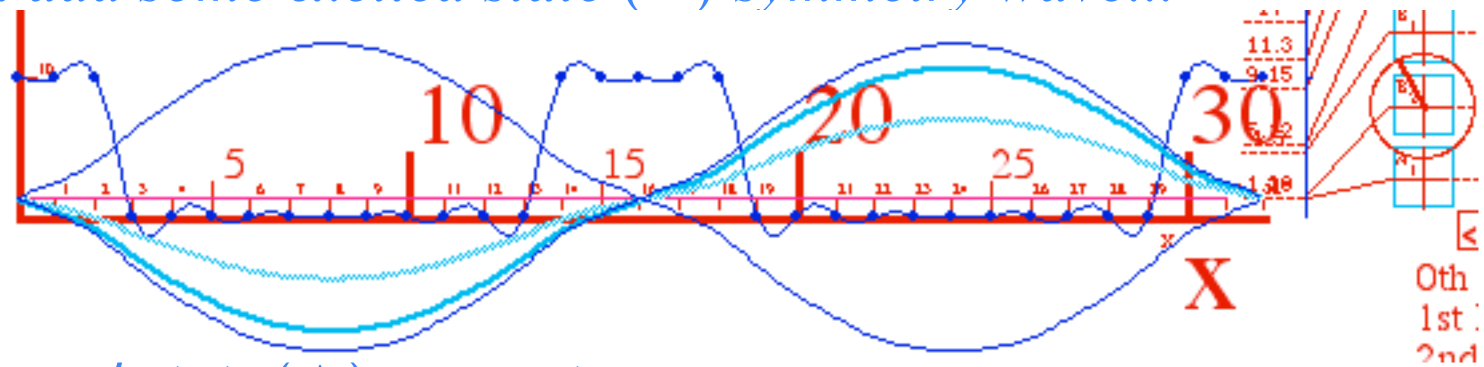

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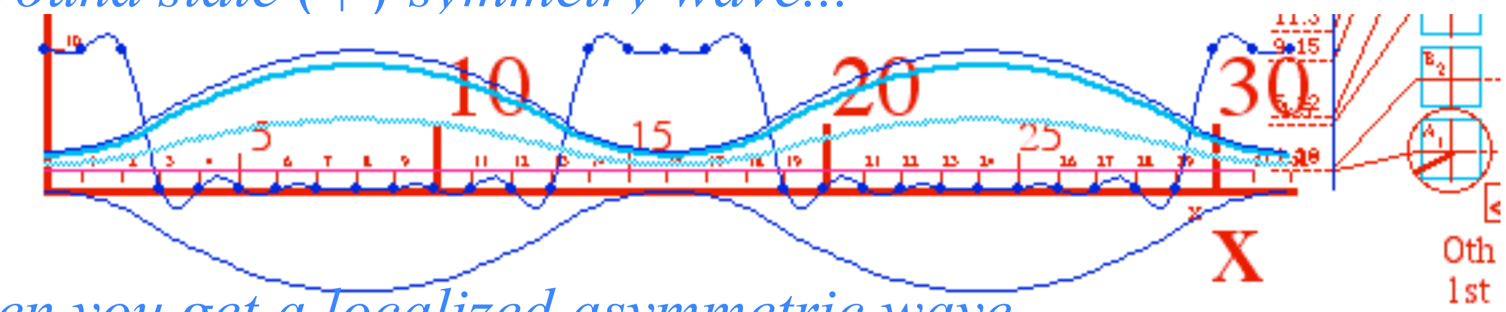
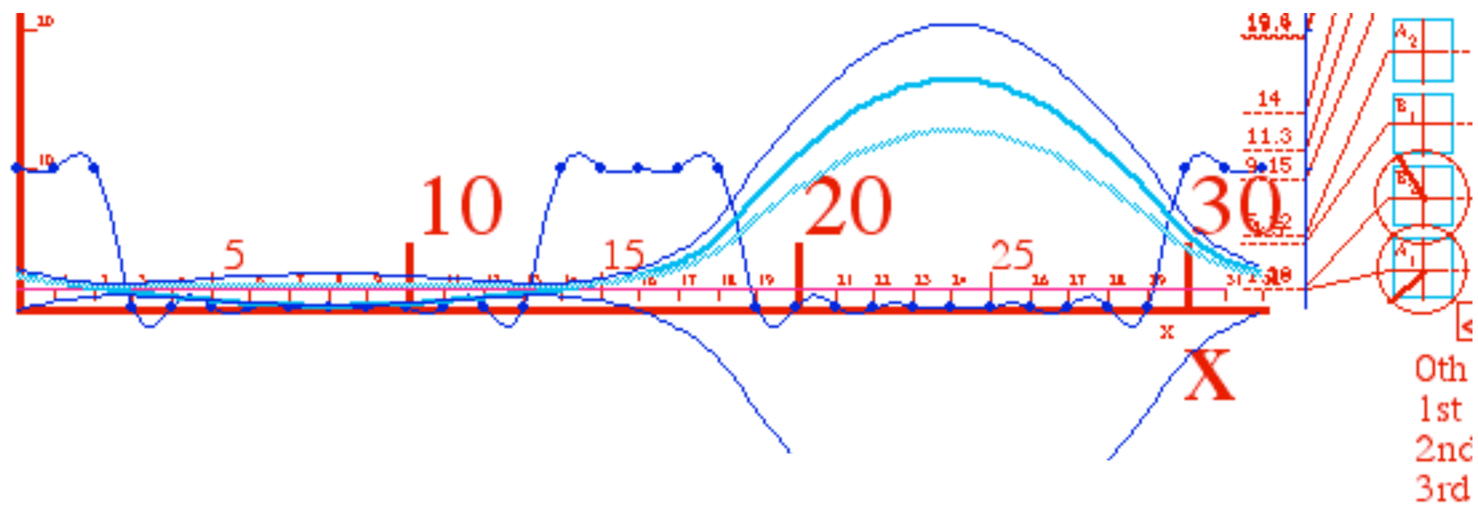


...then you get a localized asymmetric wave...



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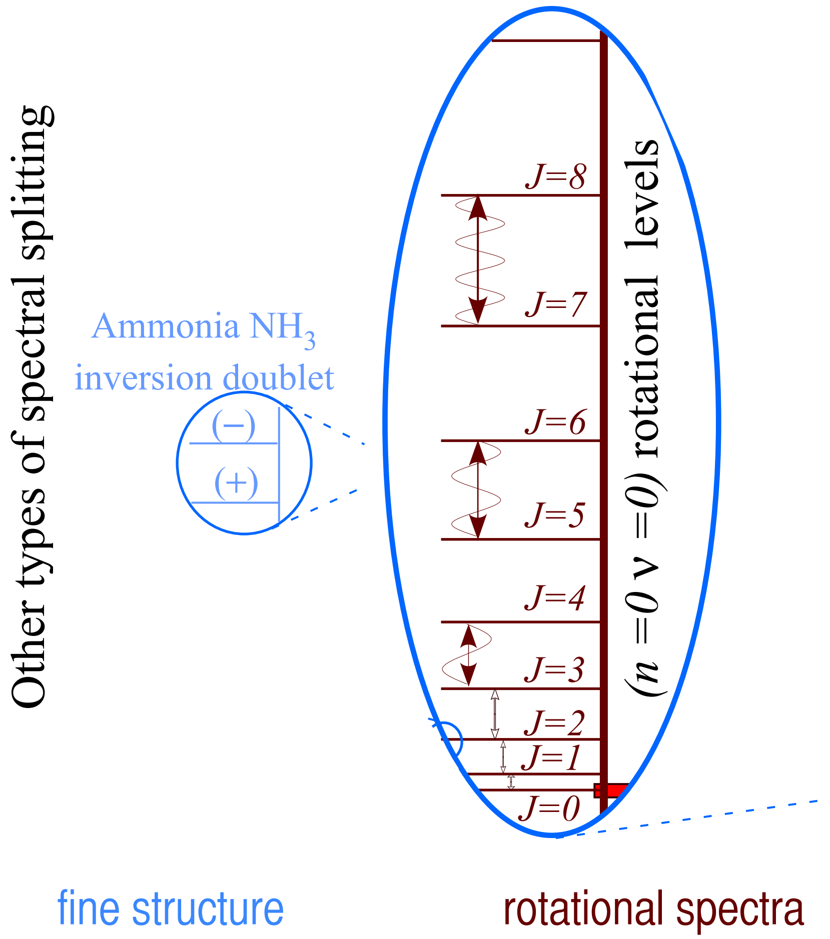

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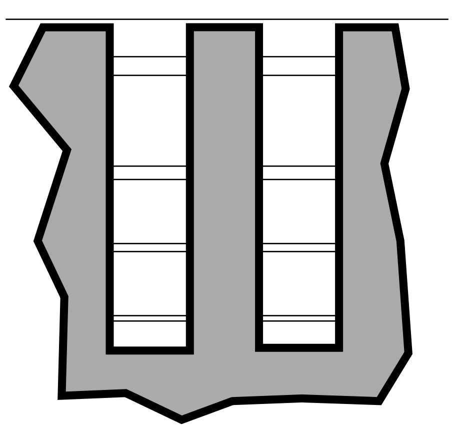

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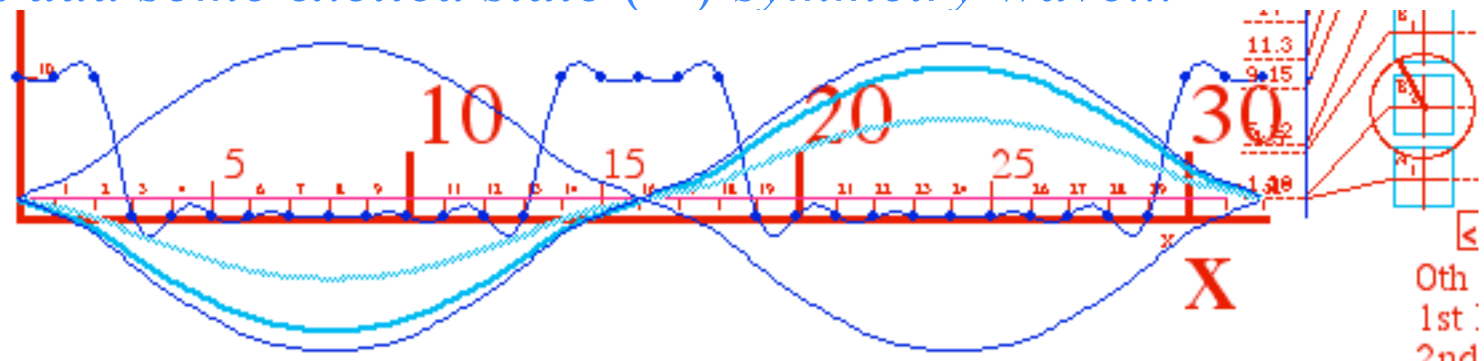

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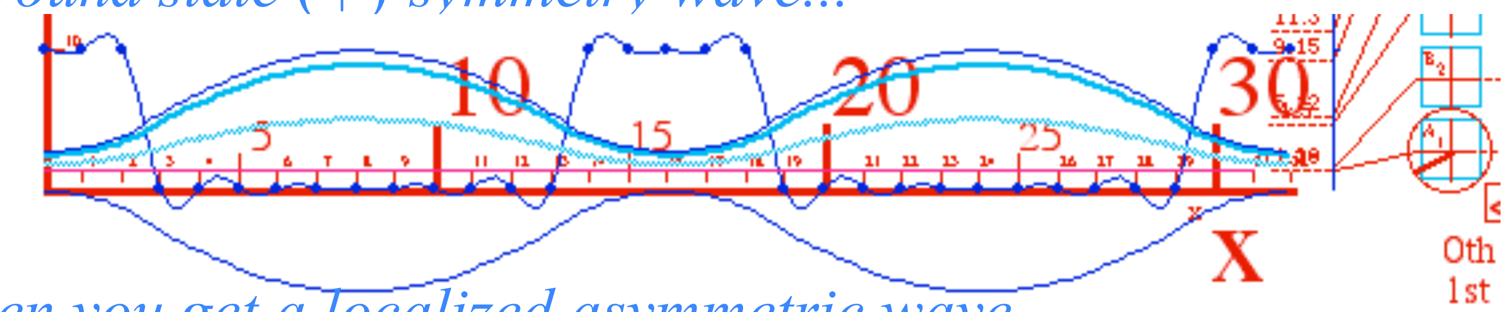

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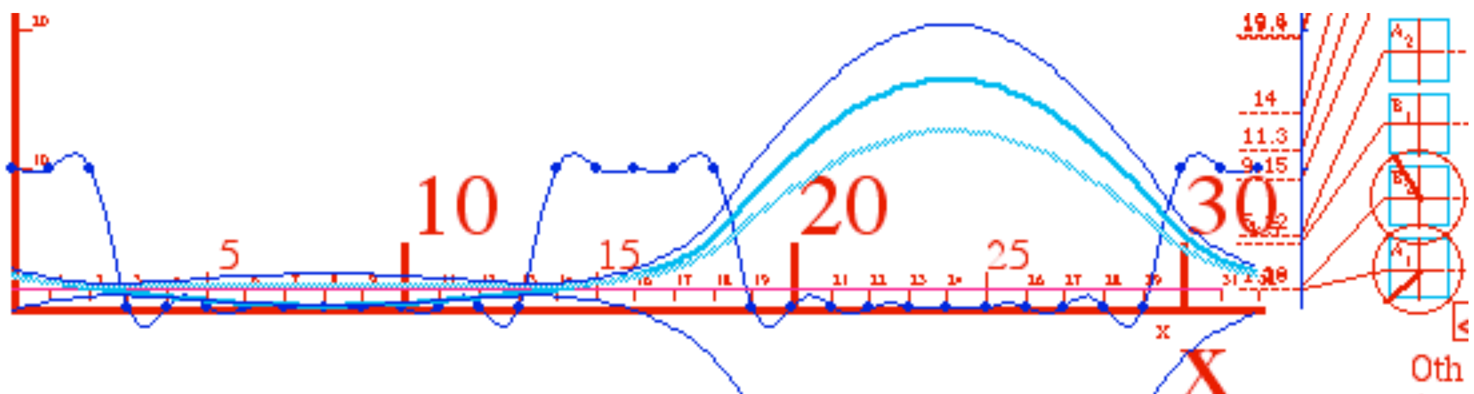
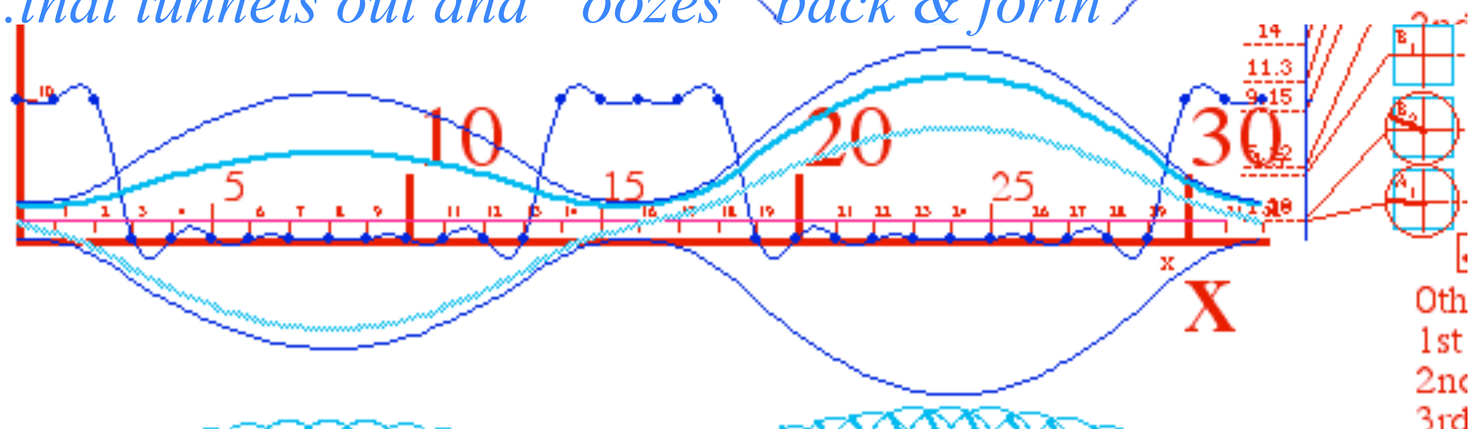


...that tunnels out and "oozes" back & forth



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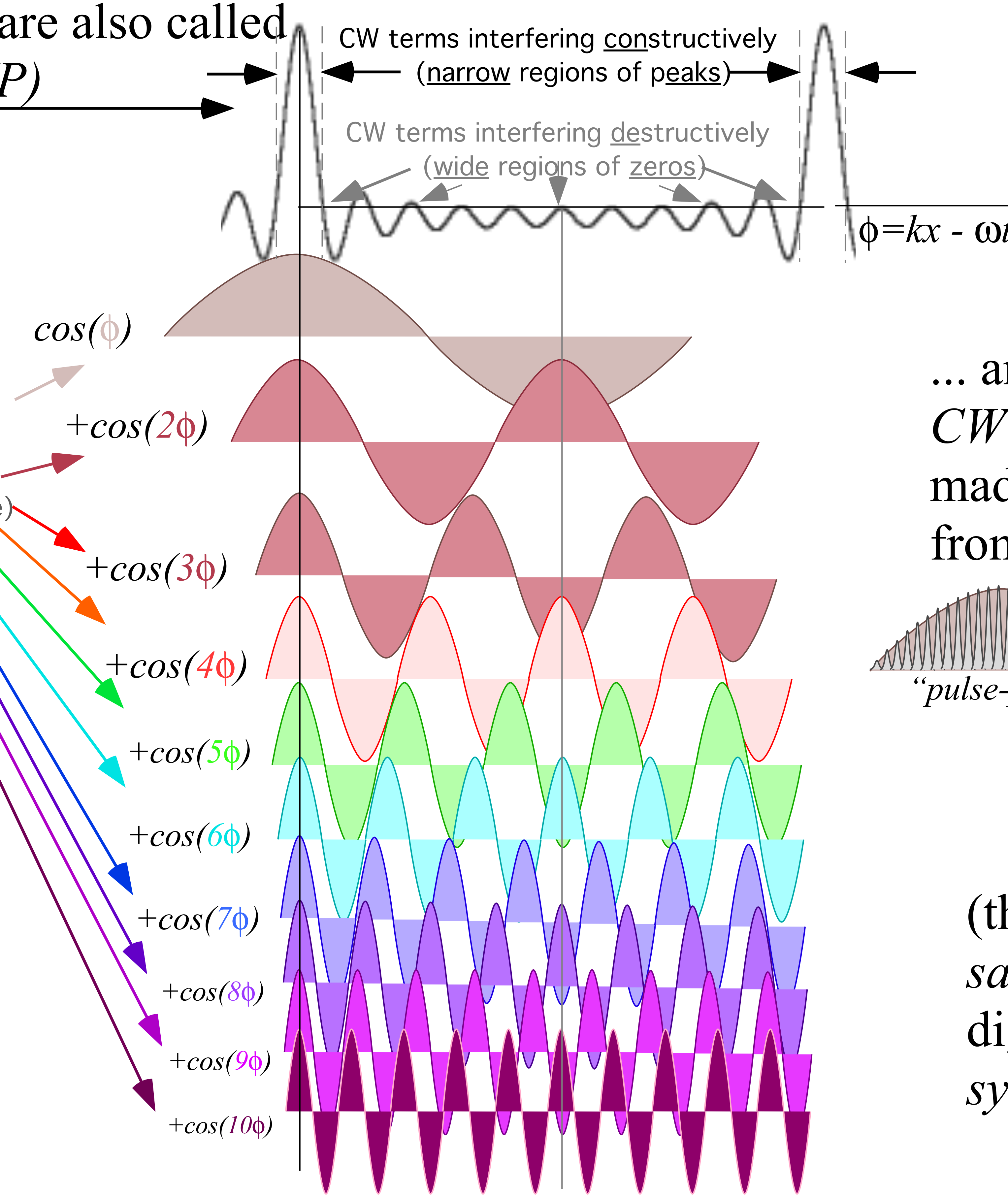
A lesson in quantum interference

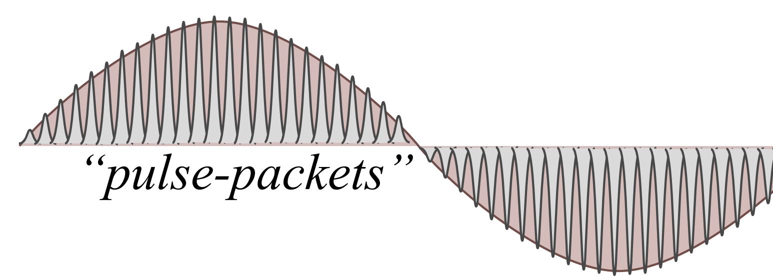
PulseWave forms are also called *Wave Packets (WP)* since they are interfering sums of many *CW* terms

(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 ...



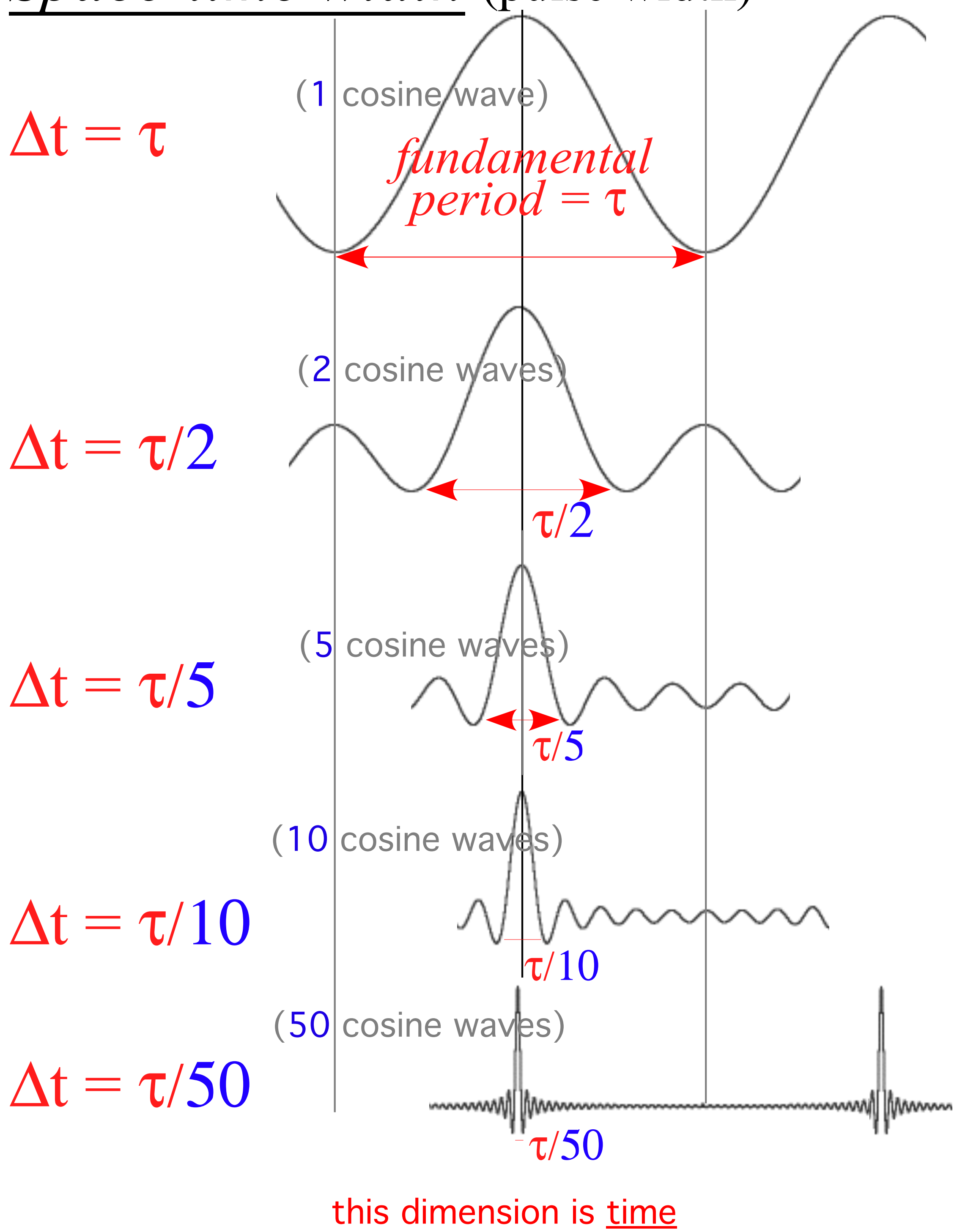
(this is digital *sampling* or digital-to-analog *synthesis*.)

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

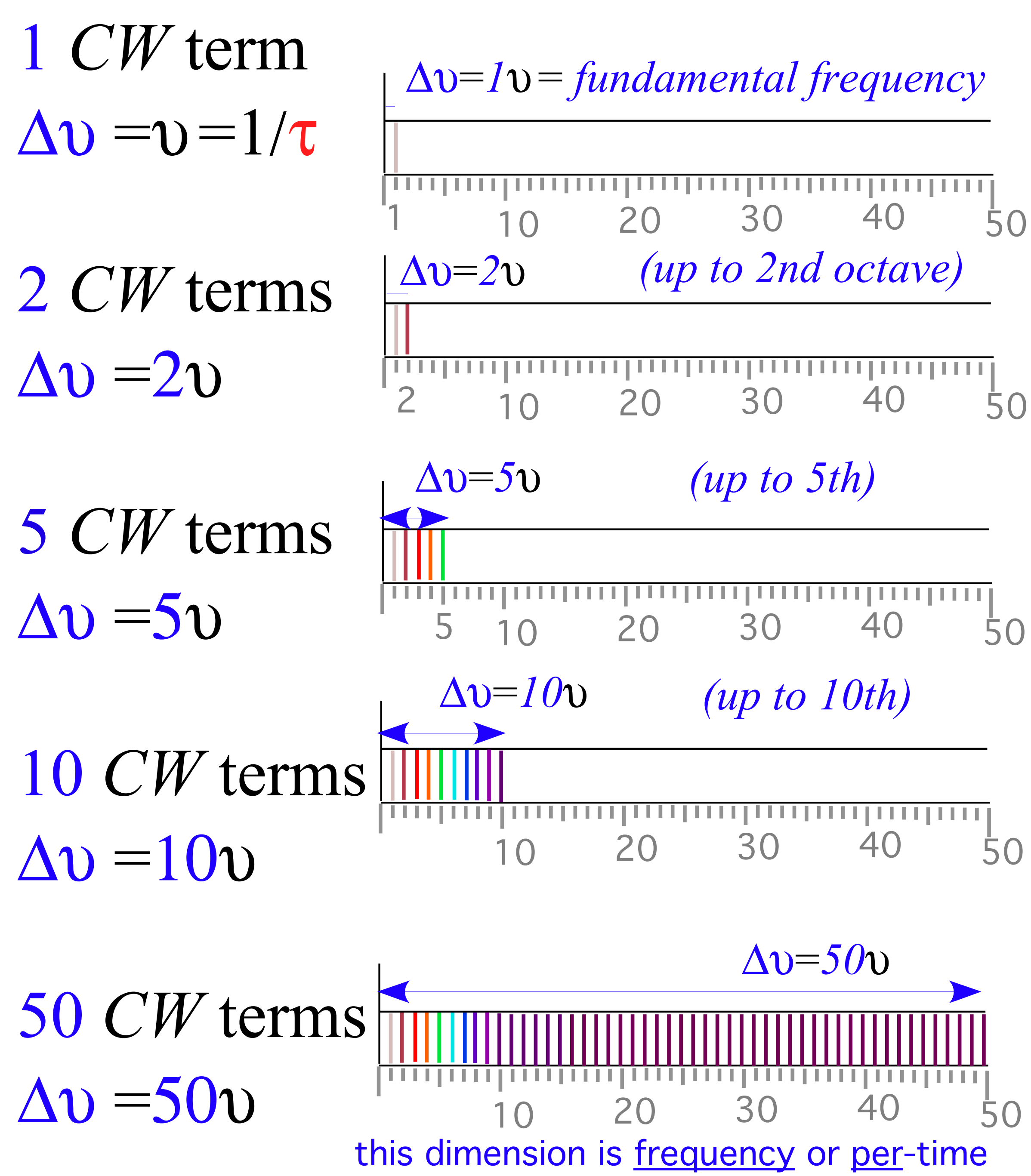
A lesson in quantum interference

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

Space-time width (pulse width)



Spectral width (harmonic frequency range)



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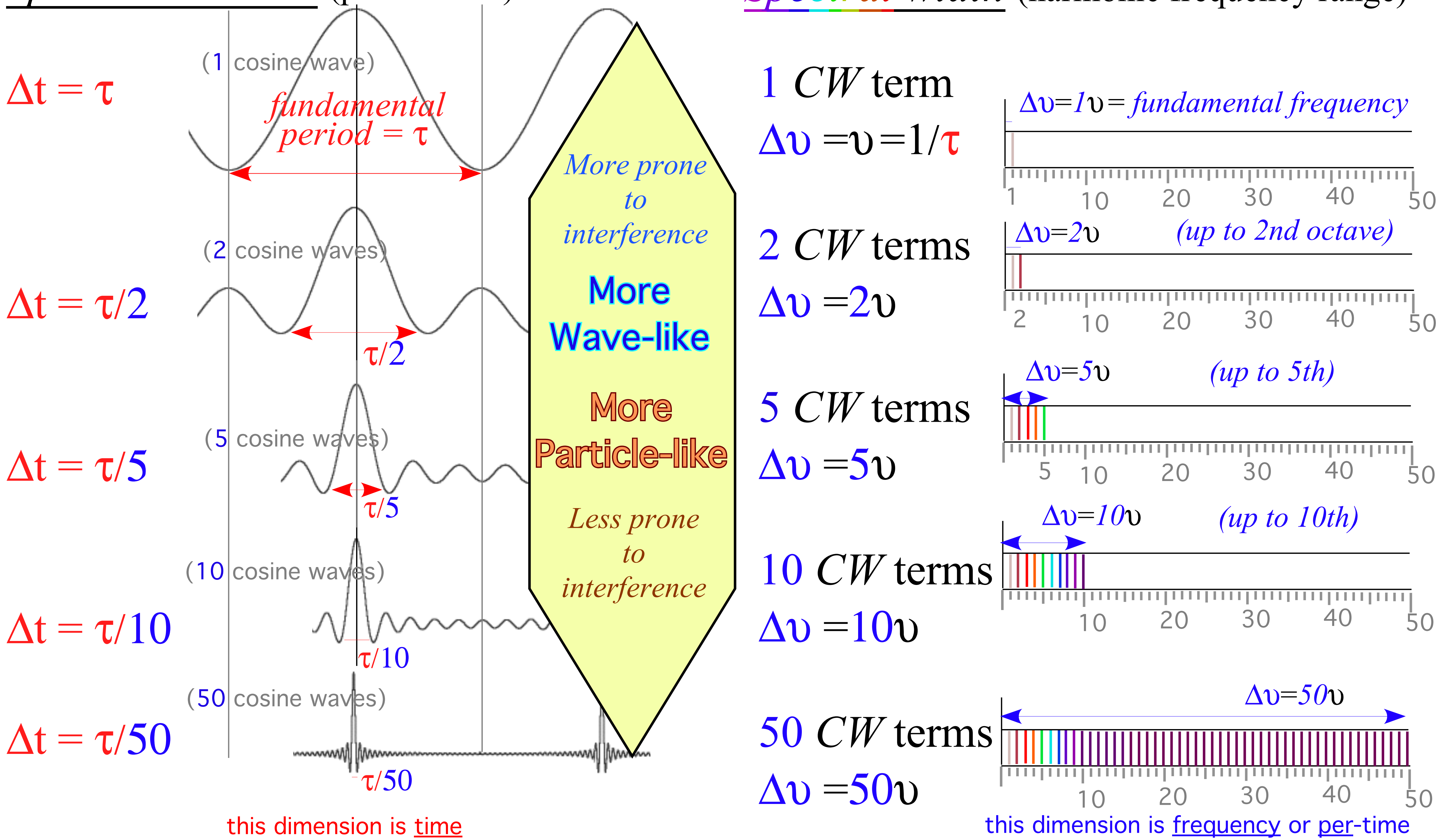
Space-time width (pulse width) | *Spectral width* (harmonic frequency range)



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

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

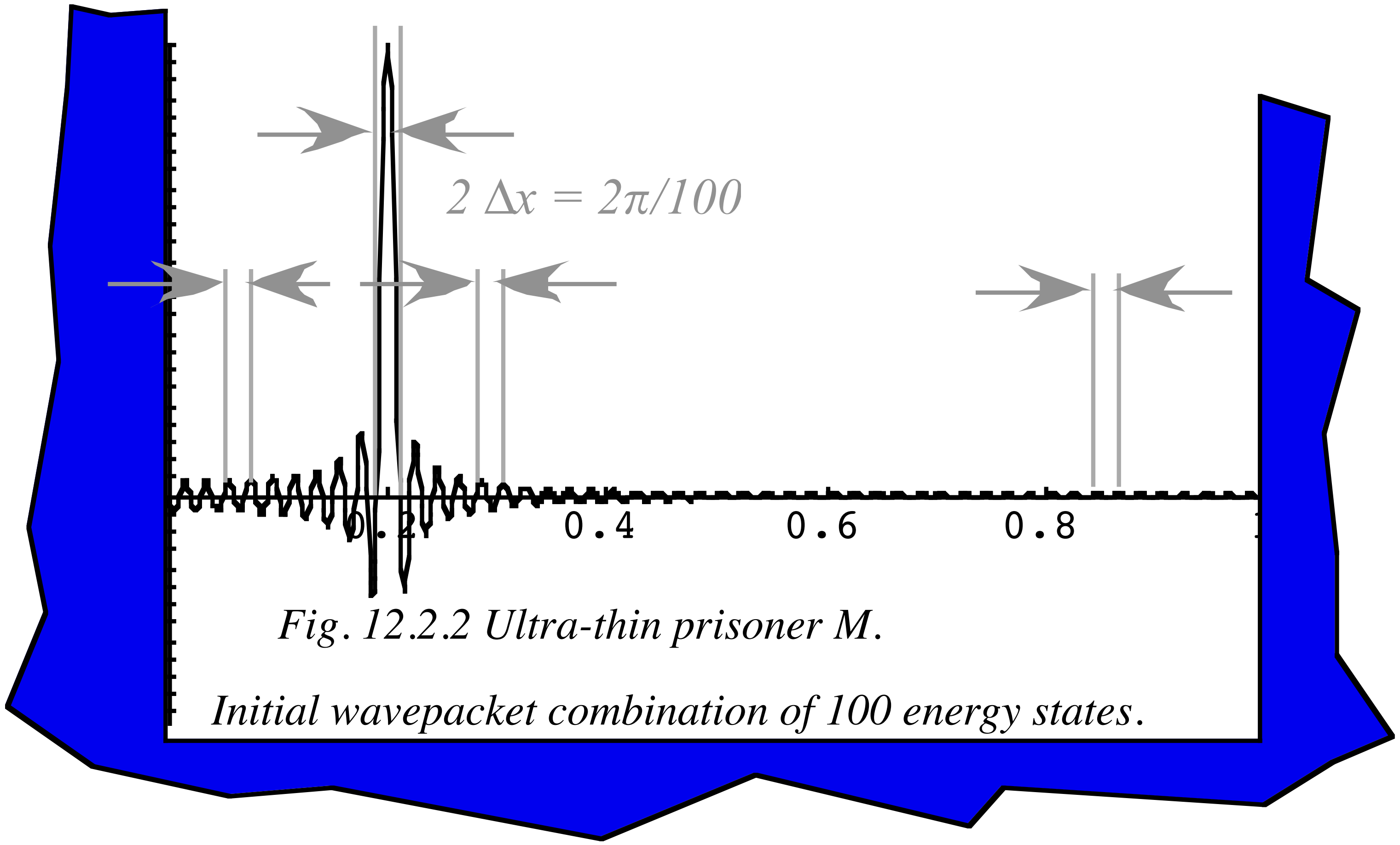


Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

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

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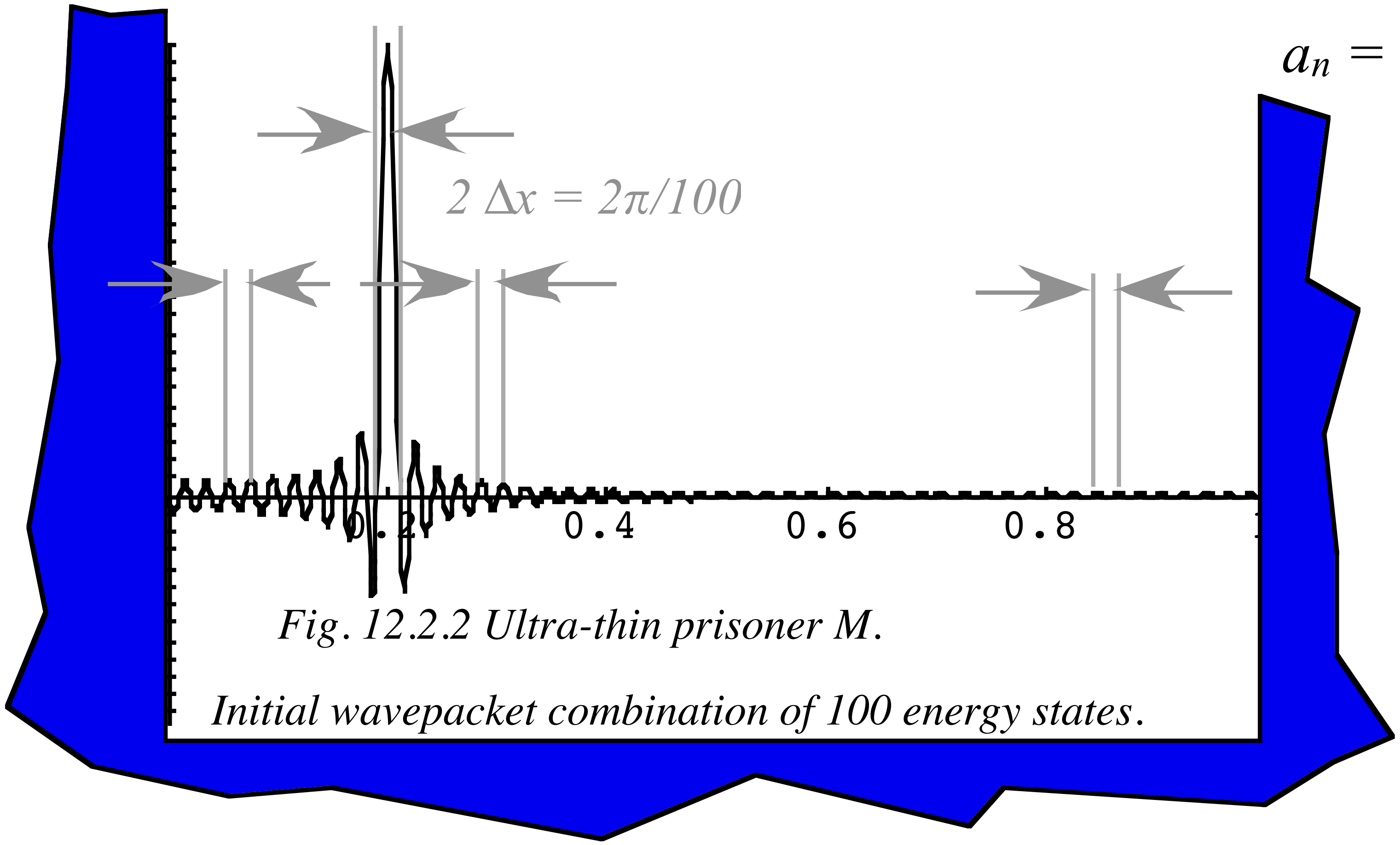

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$a_n = \langle\varepsilon_n|a\rangle = (2/W) \sin k_n a \qquad (k_n = n\pi/W)$

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

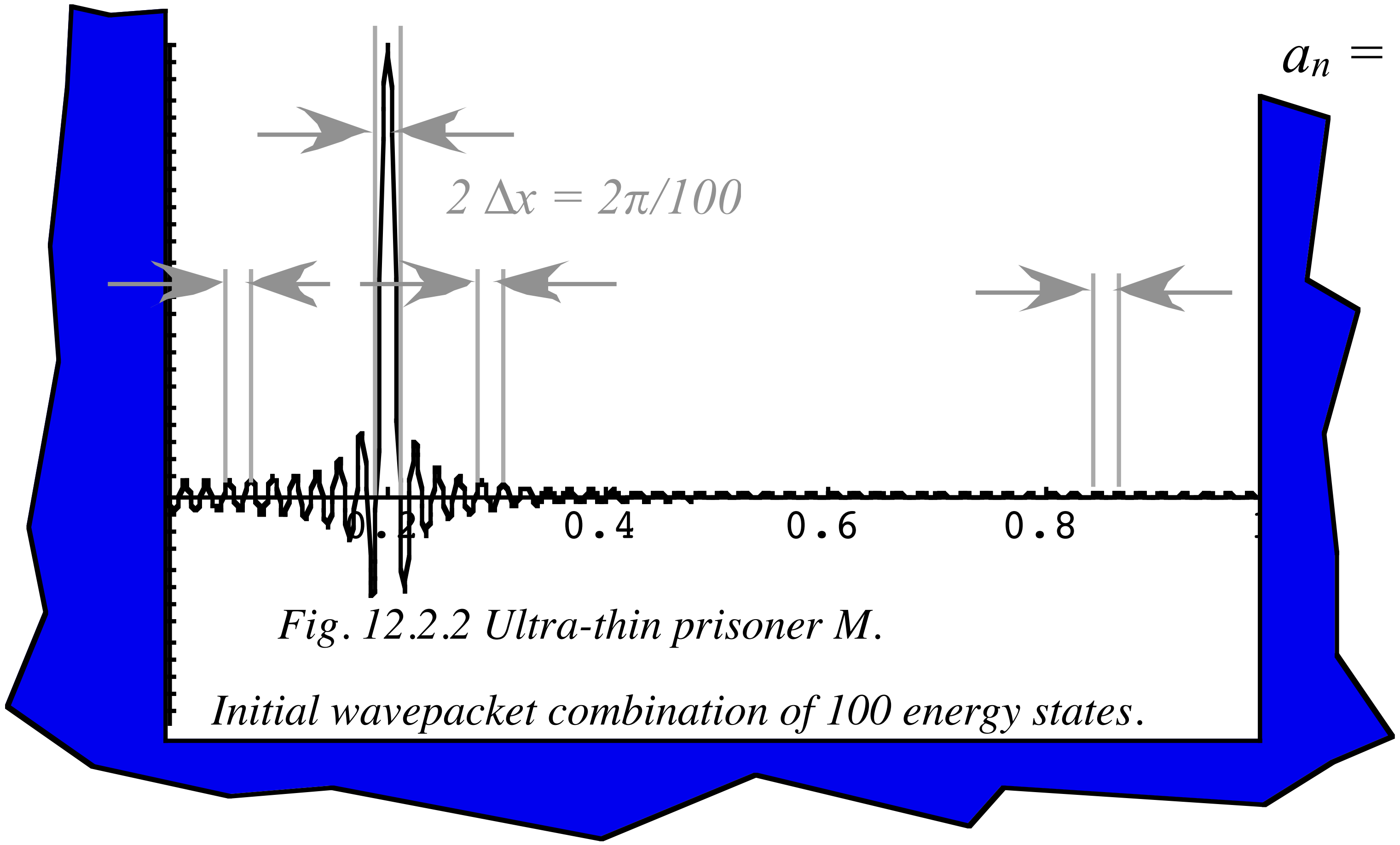

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

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

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

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

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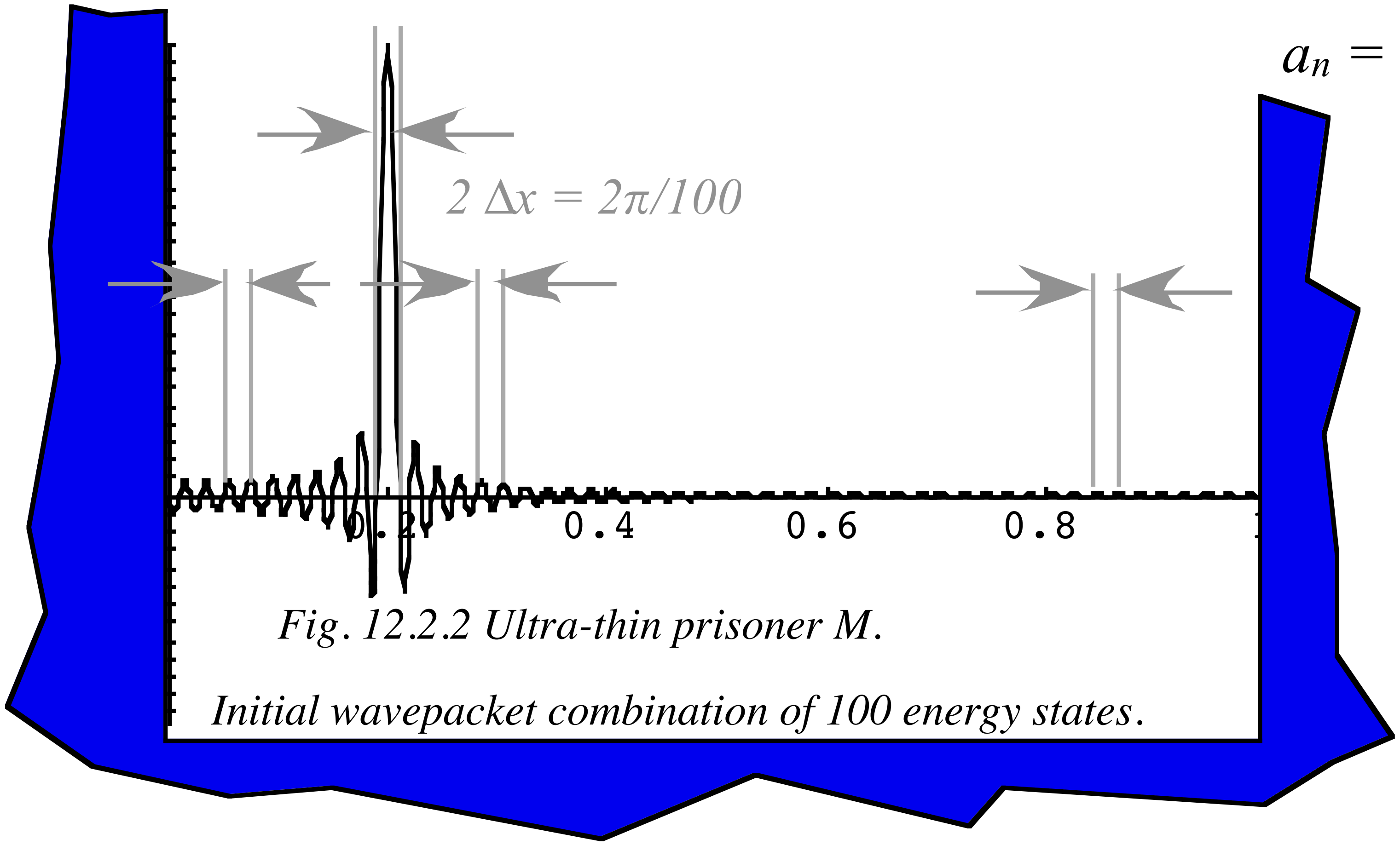
$$\delta(x-a)=\langle x|a\rangle=\sum_{n=1}^{\infty}\langle x|\varepsilon_n\rangle\langle\varepsilon_n|a\rangle=\sum_{n=1}^{\infty}a_n\sin k_n x$$



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

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

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

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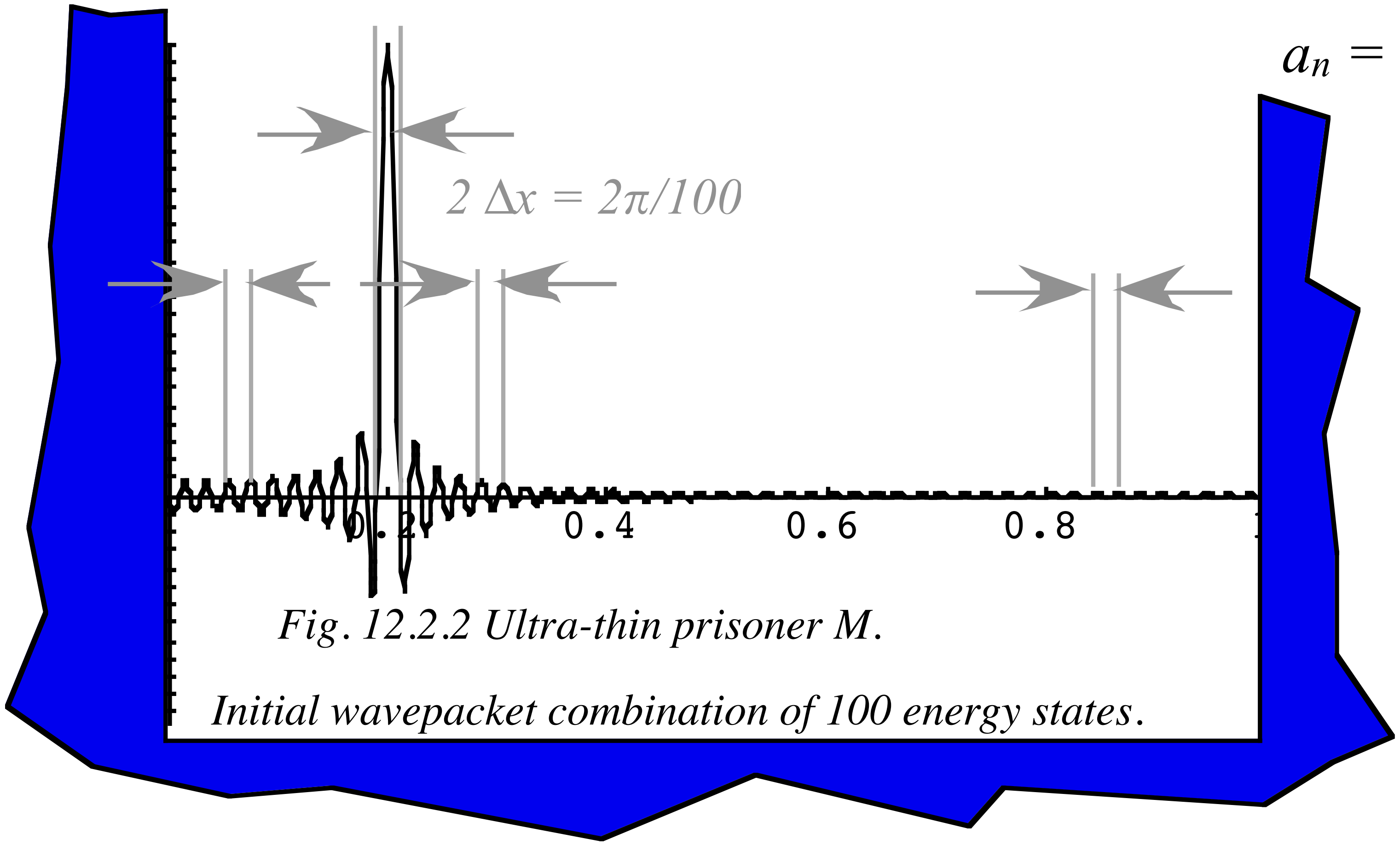

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$$\rightarrow \frac{2}{W}\int_0^{K_{max}} dk\,\frac{\Delta n}{\Delta k}\sin ka \sin kx$$

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

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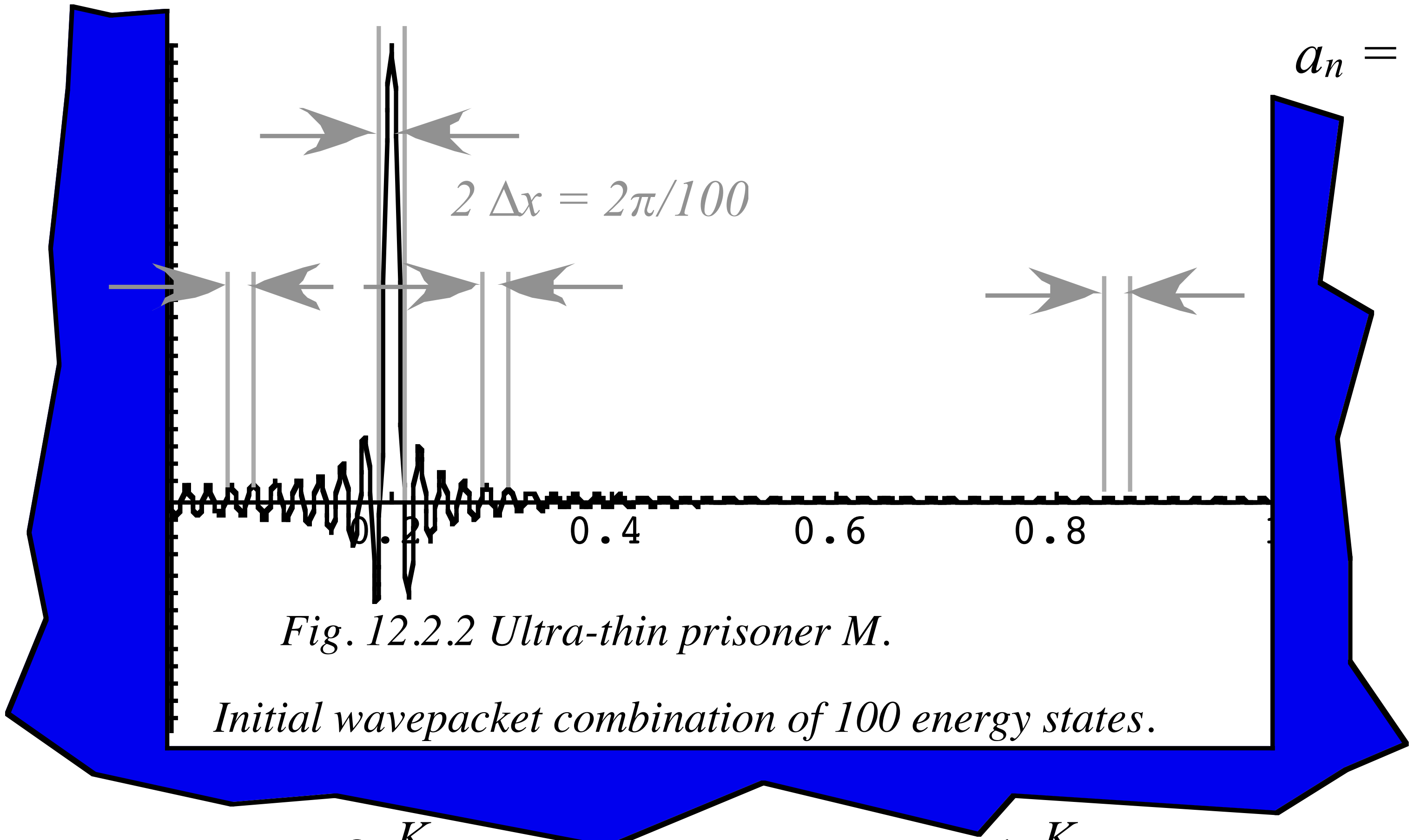

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$$\Psi(x) \cong \frac{2}{\pi}\int_0^{K_{max}} dk \sin ka \sin kx = \frac{1}{\pi}\int_0^{K_{max}} dk\left(\cos k(x-a) - \cos k(x+a)\right)$$

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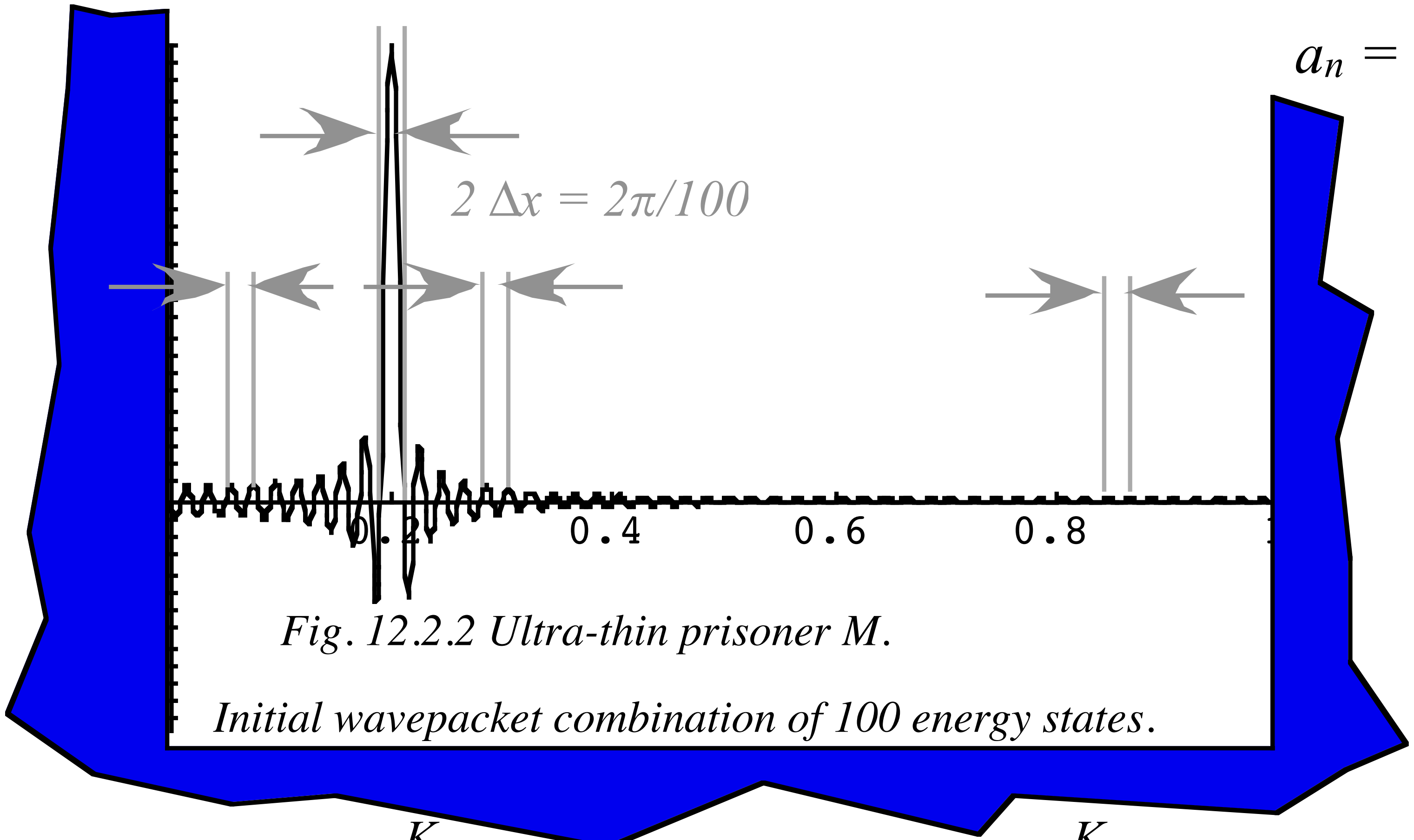

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$$\cong \frac{\sin K_{max}(x\text{-}a)}{\pi(x\text{-}a)} - \frac{\sin K_{max}(x+a)}{\pi(x+a)} \cong \frac{\sin K_{max}(x\text{-}a)}{\pi(x\text{-}a)} \quad \text{for: } x \approx a$$

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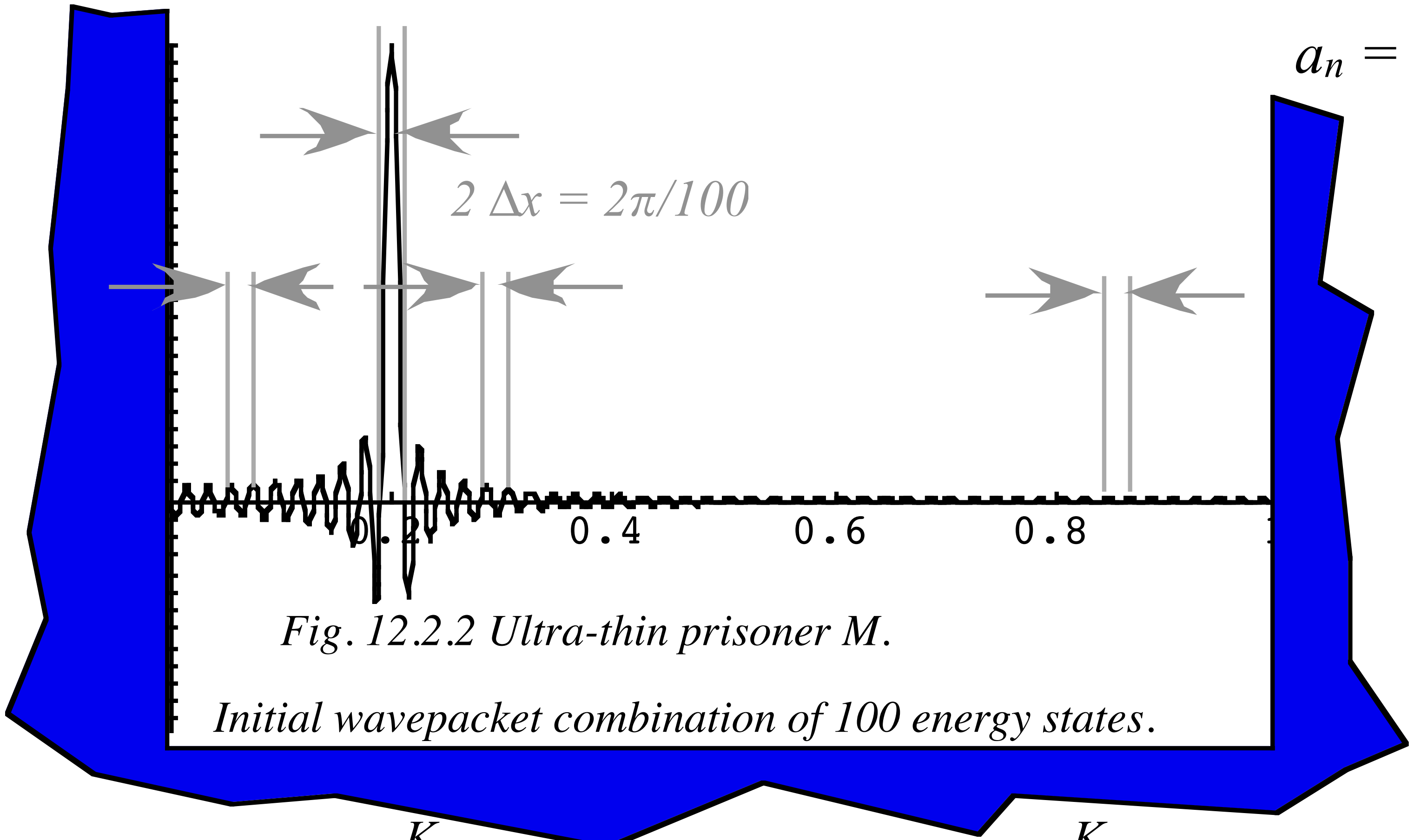

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"Last-in-first-out" effect. Last K_{max}-value dominates and "inside" K get "smothered" by interference with neighbors.

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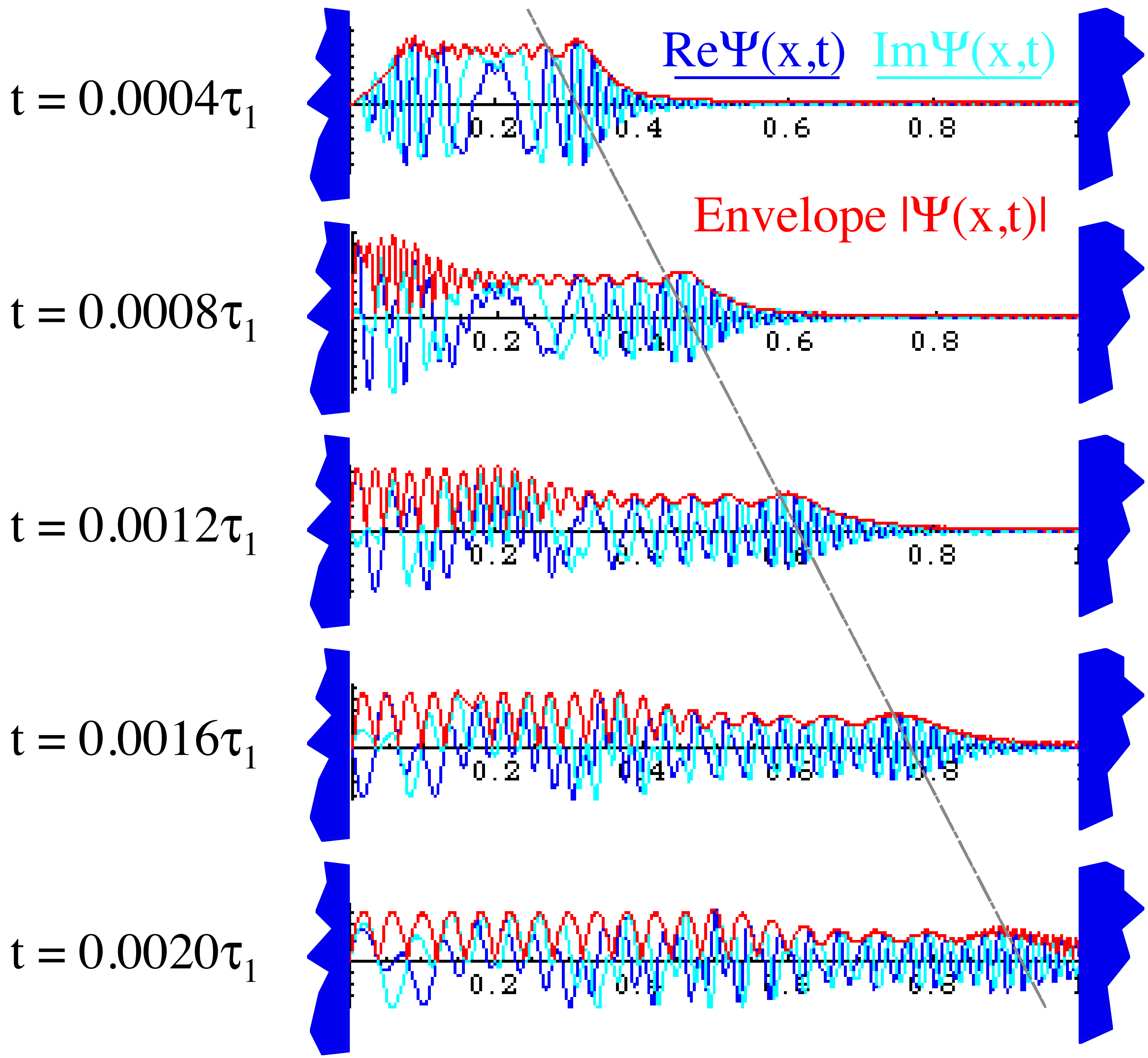
Wavepacket explodes!

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

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



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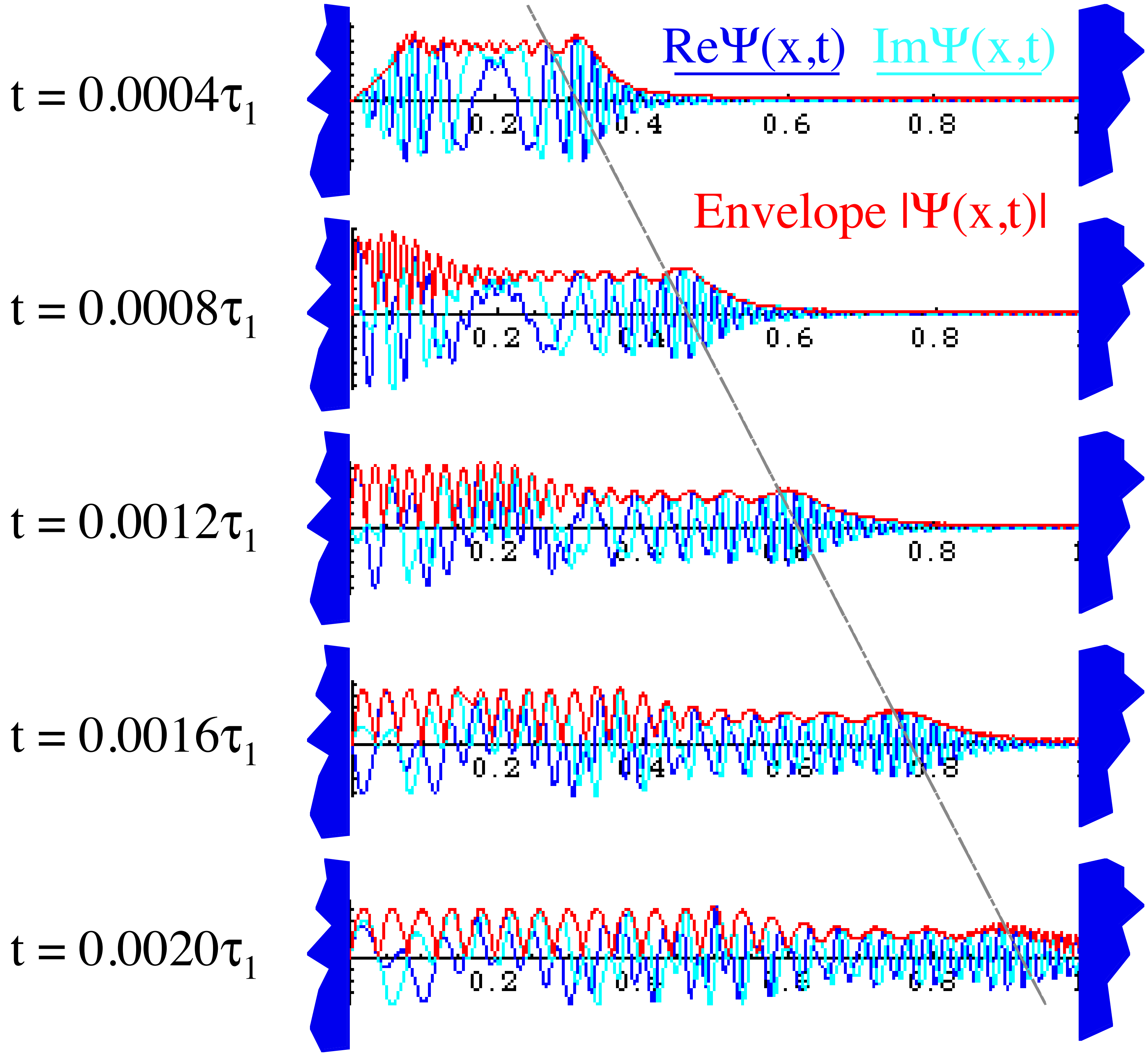
$$= \frac{h}{h^2 / 8MW^2} = \frac{8MW^2}{h}$$



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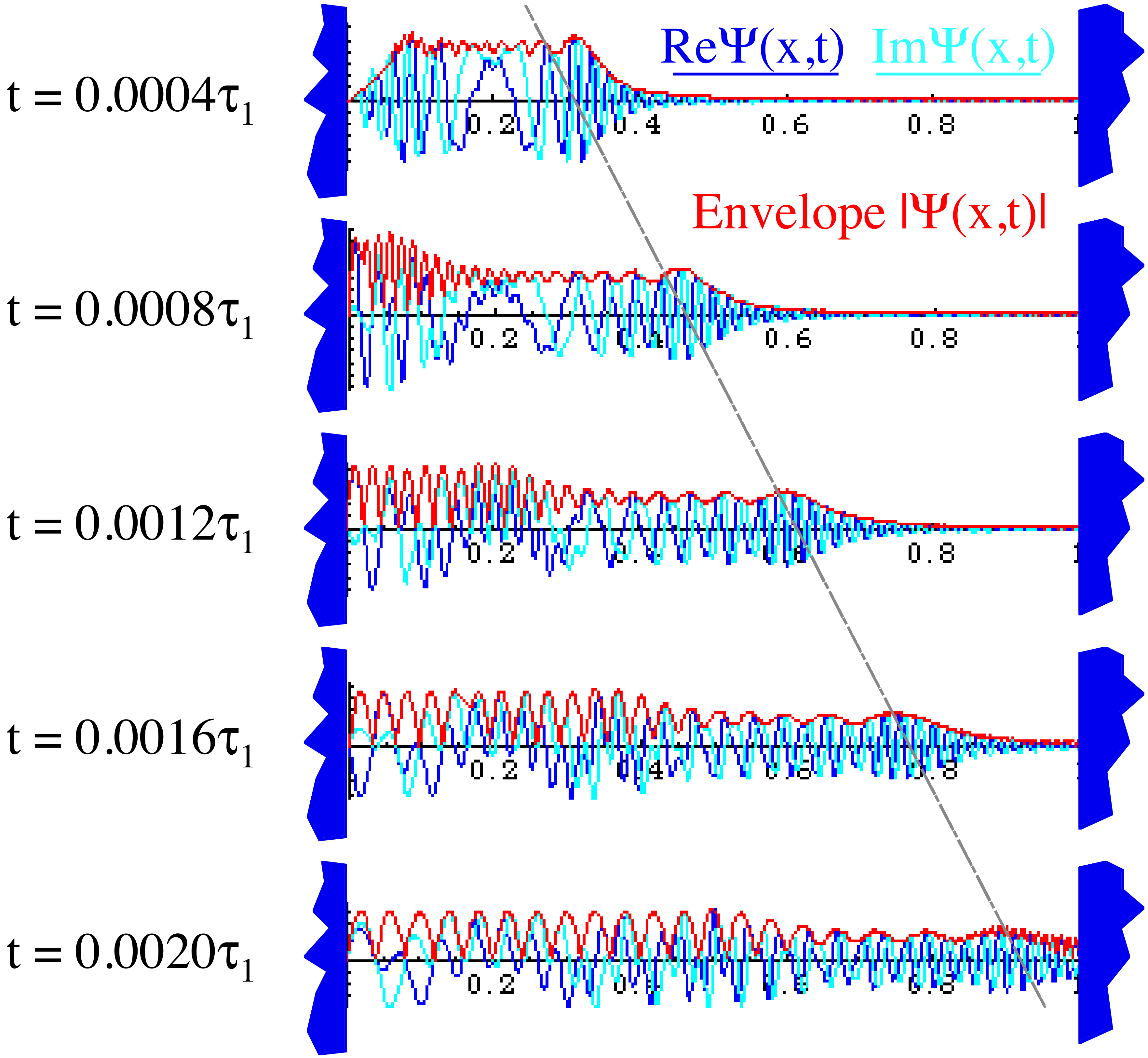

ε_n*-level classical velocity*:

$$V_n = \frac{d\omega_n}{dk} = \frac{1}{\hbar}\frac{d\varepsilon_n}{dk} = \frac{1}{\hbar}\frac{\hbar^2}{2M}\frac{dk^2}{dk} = \frac{\hbar 2k_n}{2M} = \frac{\hbar n\pi}{MW} = \frac{hn}{2MW}$$

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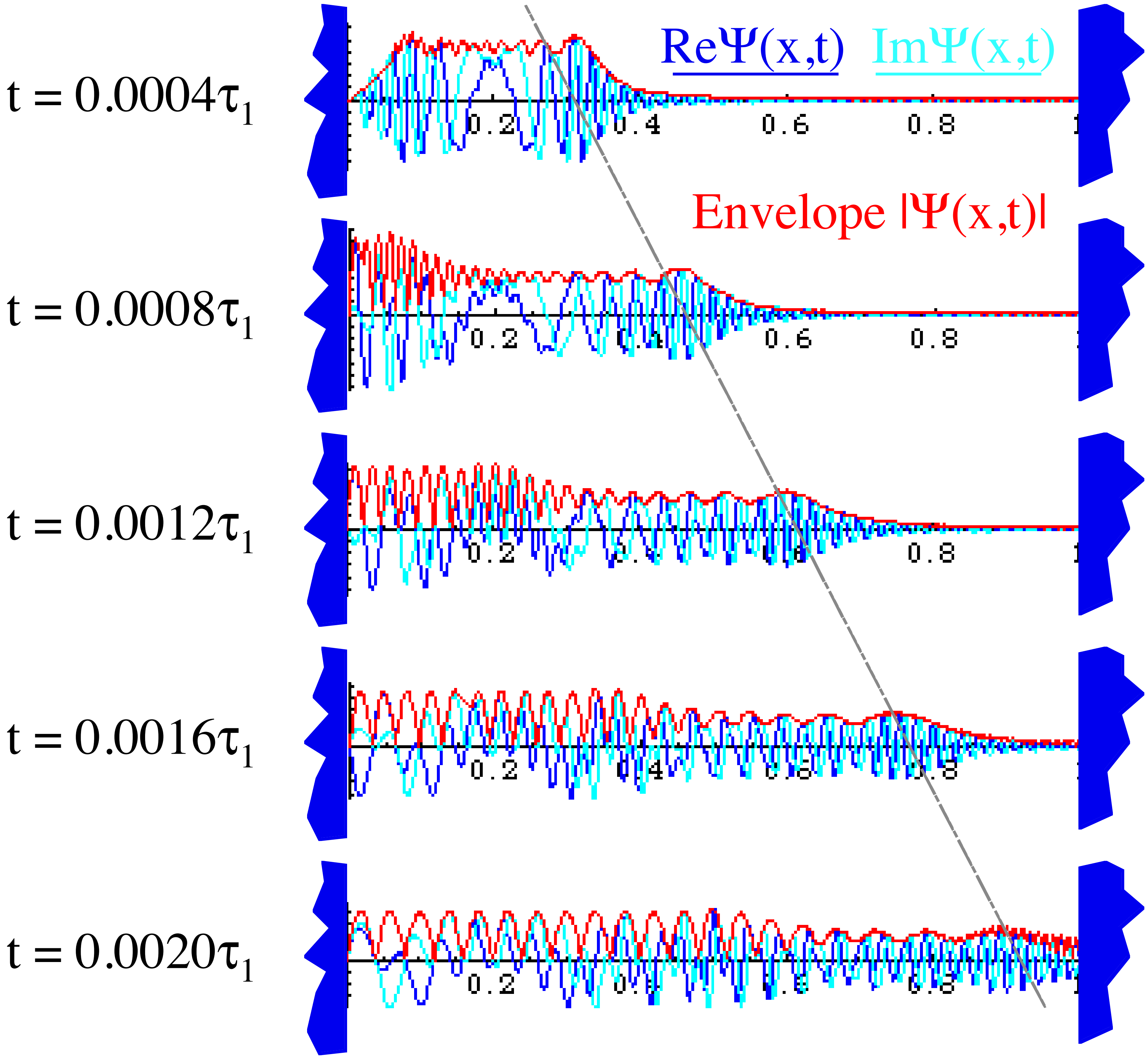

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ε_n*-level classical round trip time* $T_n(2W)$
$$T_n(2W) = \frac{2W}{V_n} = 2W\frac{2MW}{hn} = \frac{4MW^2}{hn}$$
$$= \frac{1}{2n}\frac{8MW^2}{h} = \frac{\tau_1}{2n}$$

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$$\tau_1 = \frac{2\pi}{\omega_1} = \frac{2\pi\hbar}{\varepsilon_1} = \frac{h}{h^2/8MW^2} = \frac{8MW^2}{h}$$

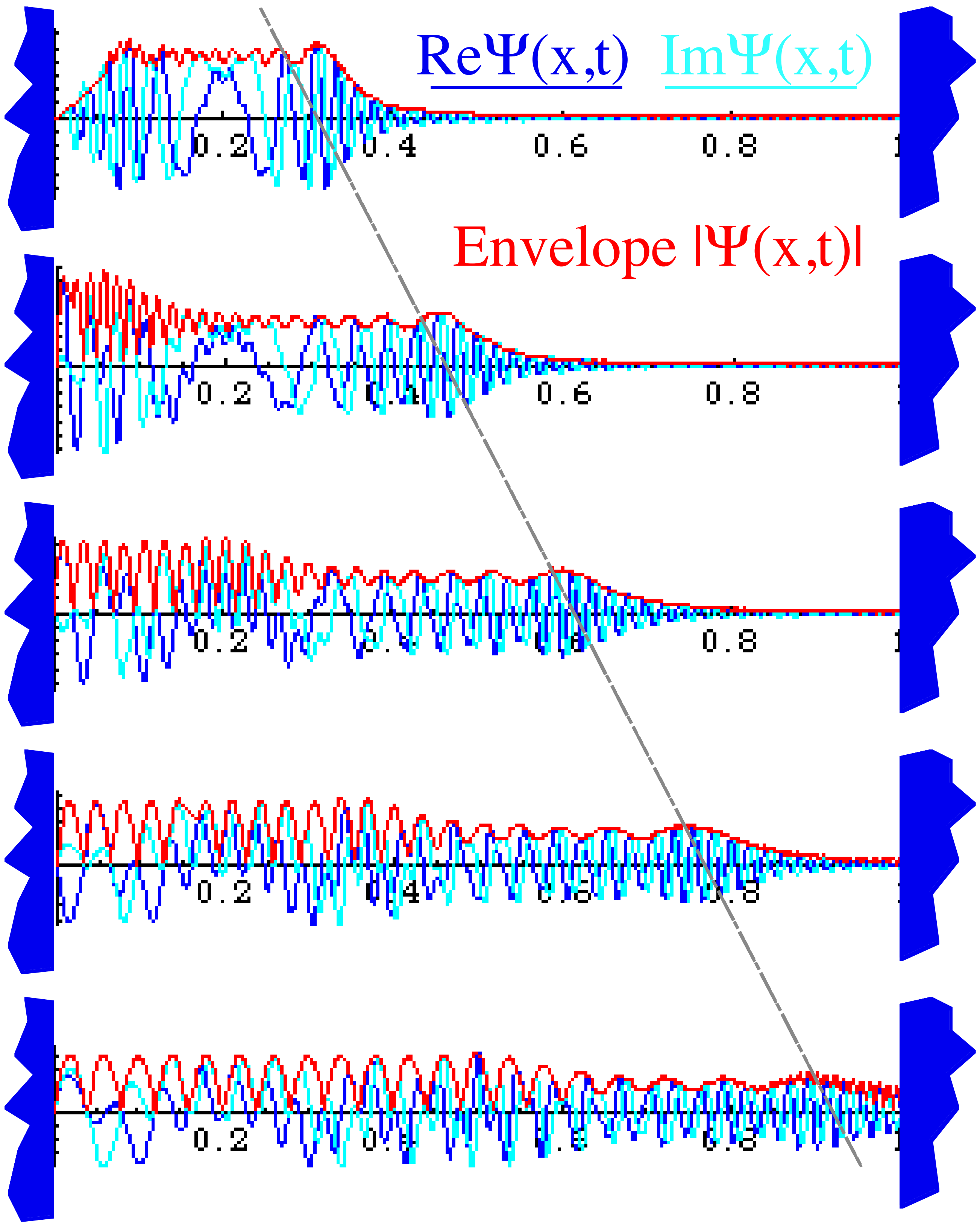
$t = 0.0004\tau_1$

$t = 0.0008\tau_1$

$t = 0.0012\tau_1$

$t = 0.0016\tau_1$

$t = 0.0020\tau_1$



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ε_n-level 1-way time $T_n(W)$

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

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

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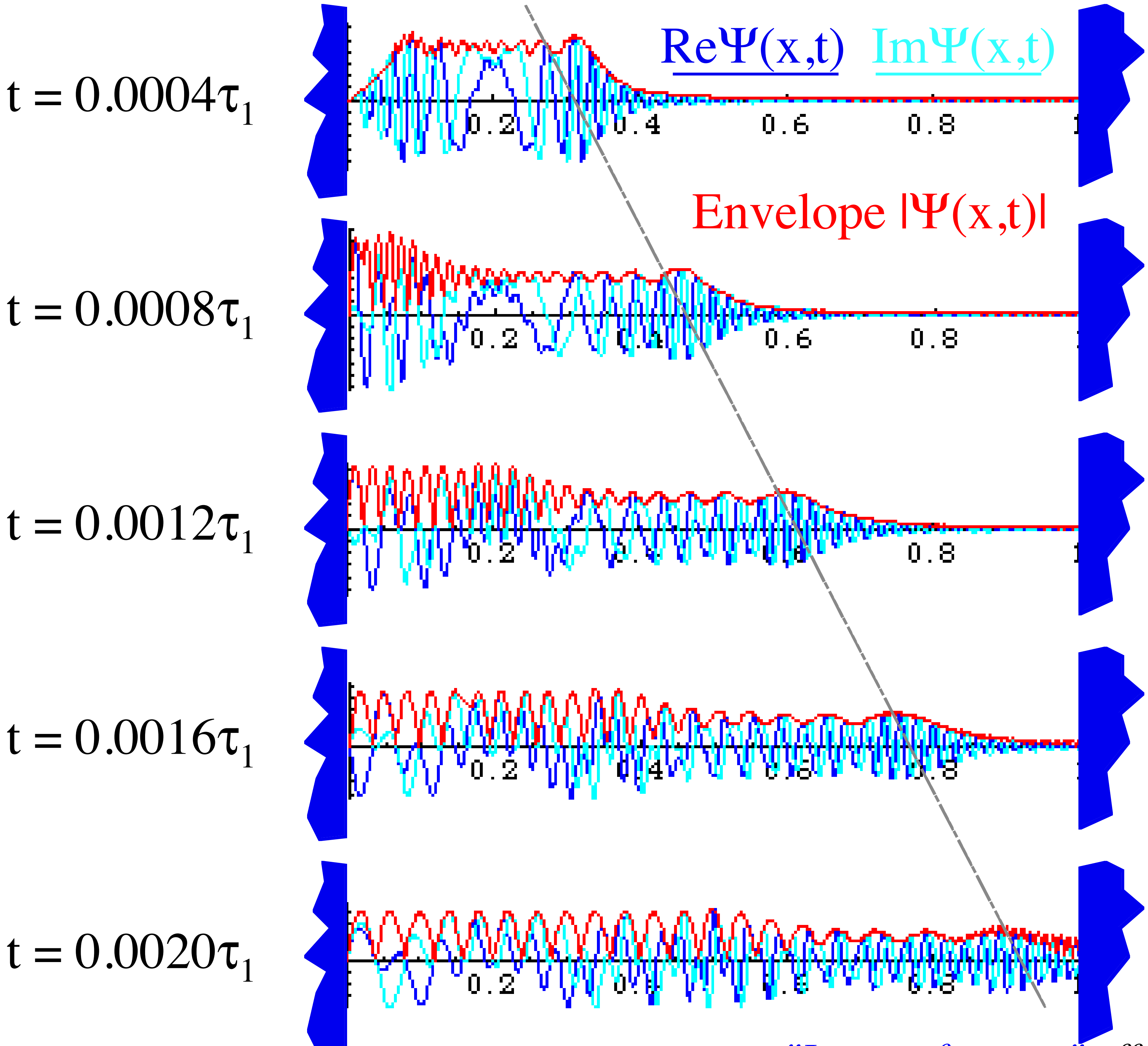

"Last-in-first-out" effect

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Wavepacket explodes! (Then revives)

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,

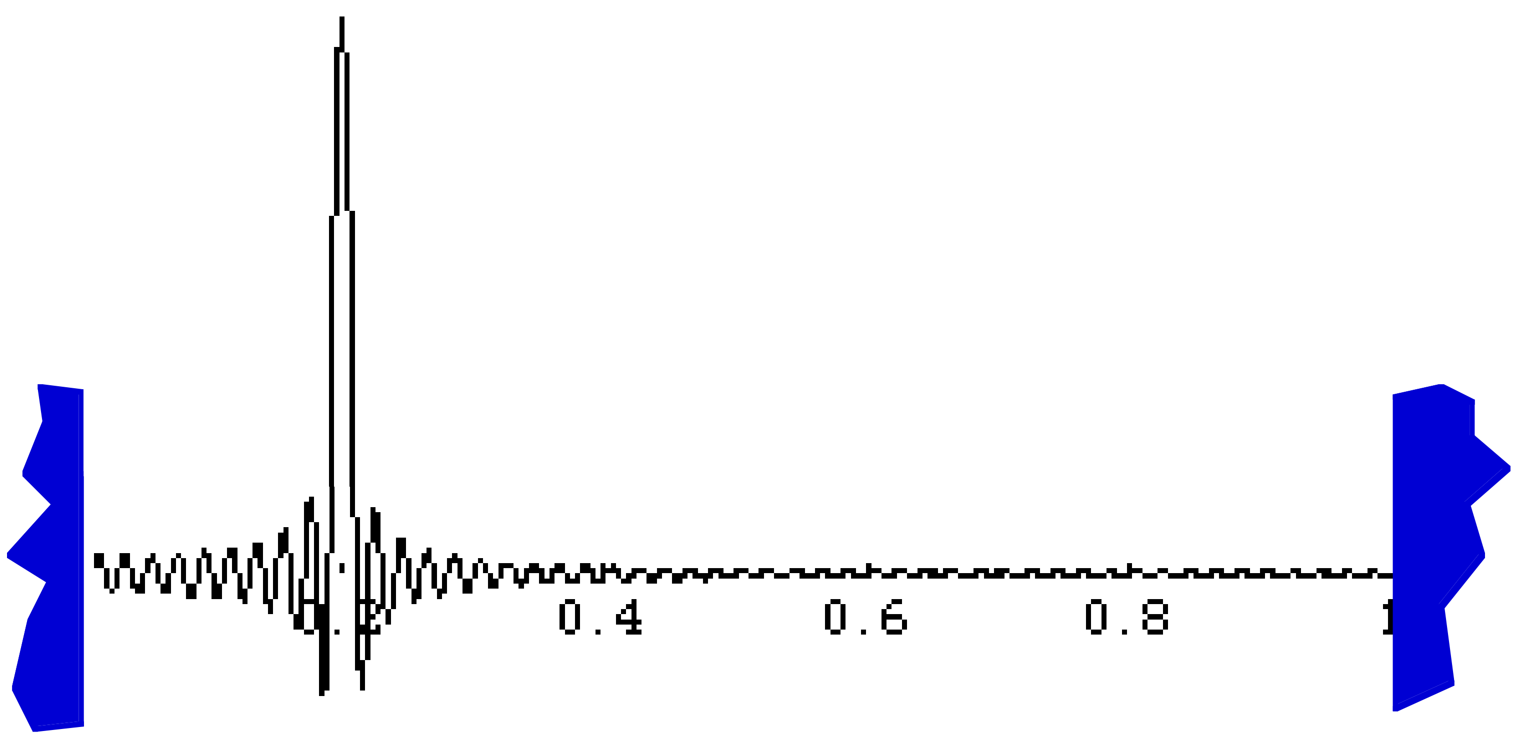
ε_2-level particle makes 4 round trips,

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*,

$t = 1.0000\tau_1$

$= 3.0\tau_{beat}$



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In time τ_1 ground ε_1-level particle does 2 round trips,

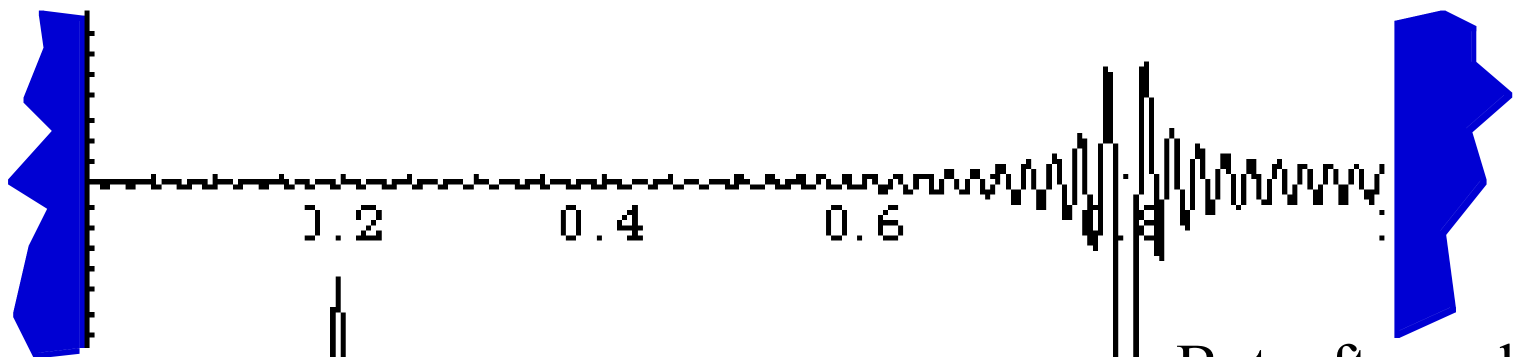
ε_2-level particle makes 4 round trips,

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*,

$t = 0.5000\tau_1$

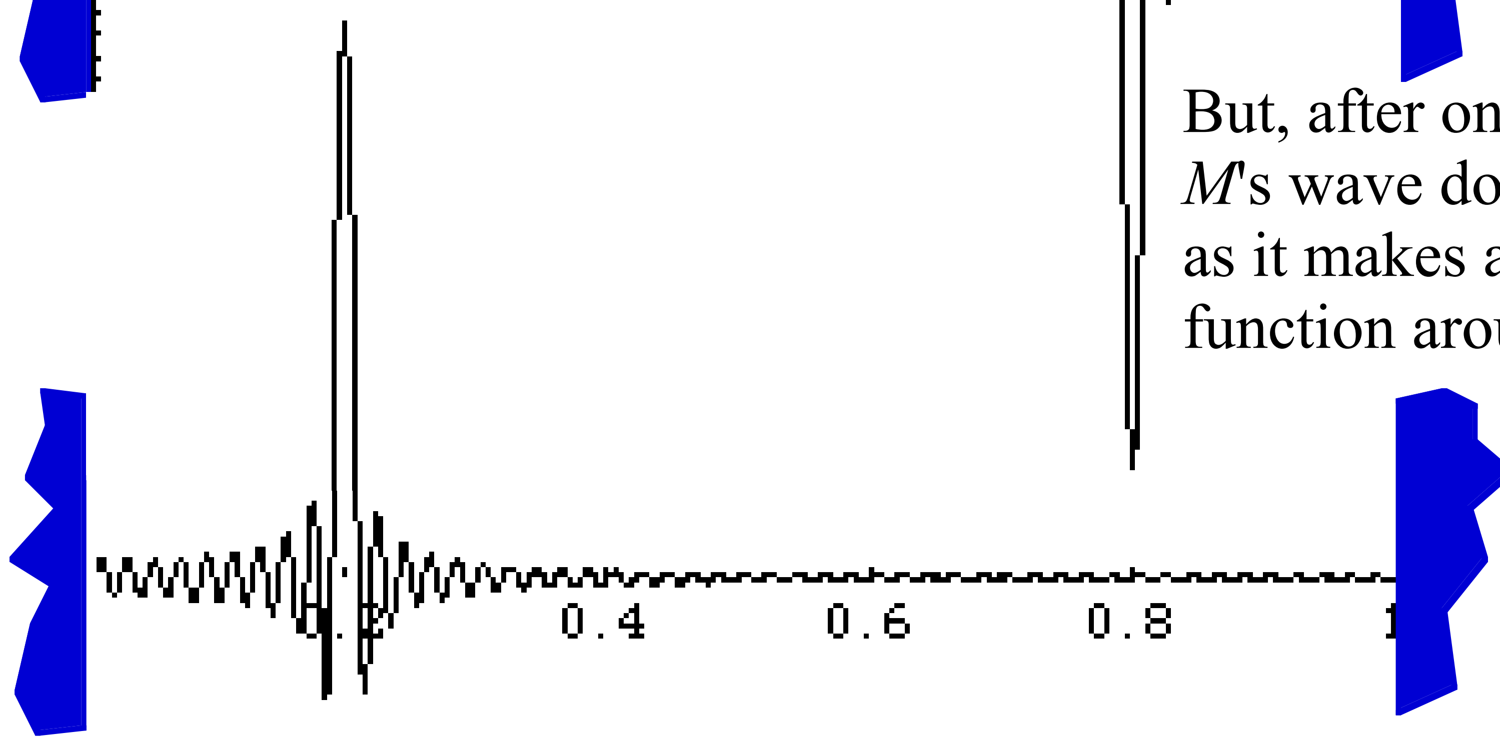
$= 1.5\tau_{beat}$



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*.

$t = 1.0000\tau_1$

$= 3.0\tau_{beat}$



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

$t = \tau_1/3$

$t = \tau_1/5$

$t = \tau_1/7$

$t = \tau_1/9$

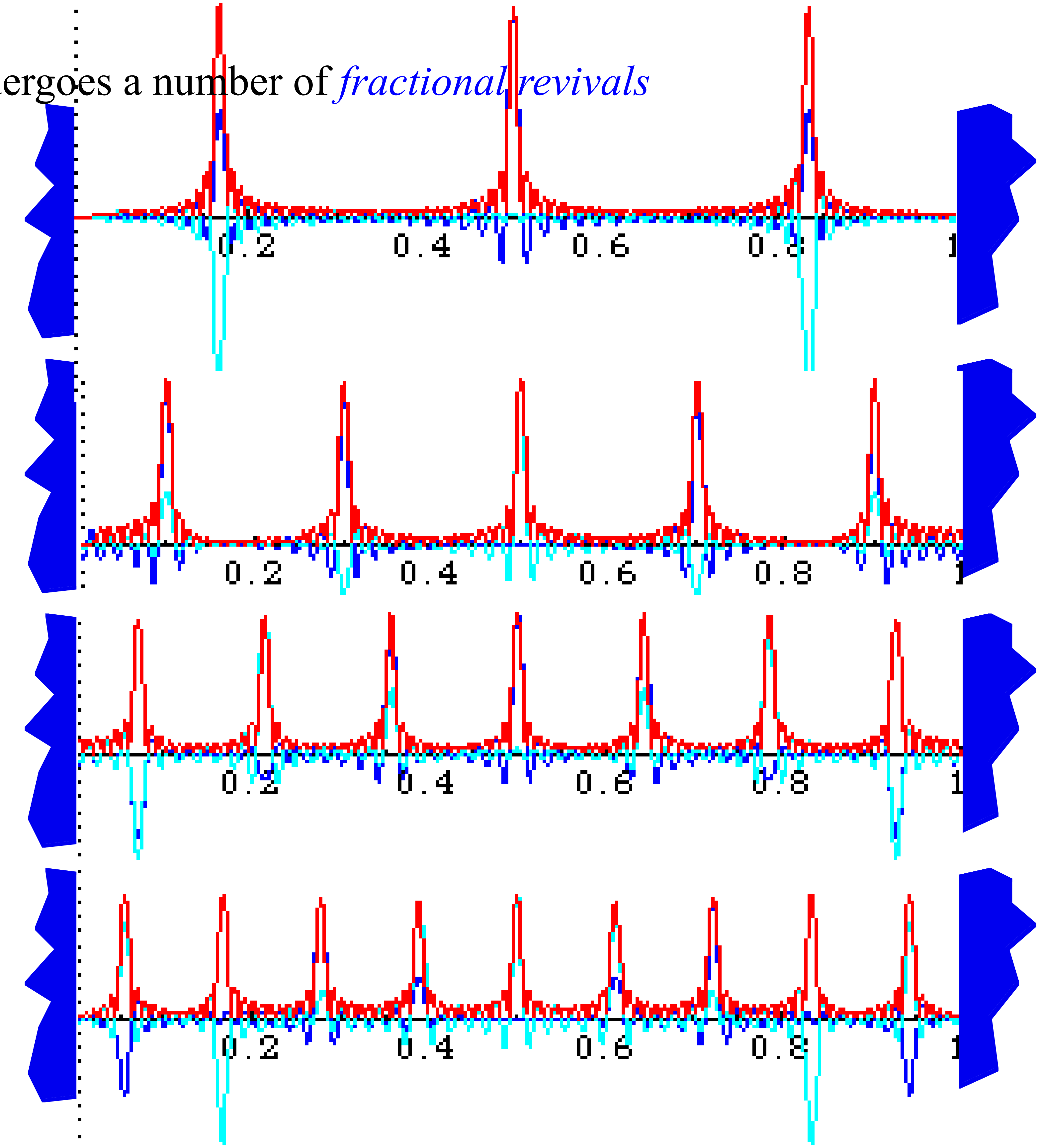


Fig. 12.2.5 The "Dance of the deltas." Mini-Revivals for prisoner M's wavepacket envelope function.

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

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Quantum "revivals" of gently*localized rotor waves

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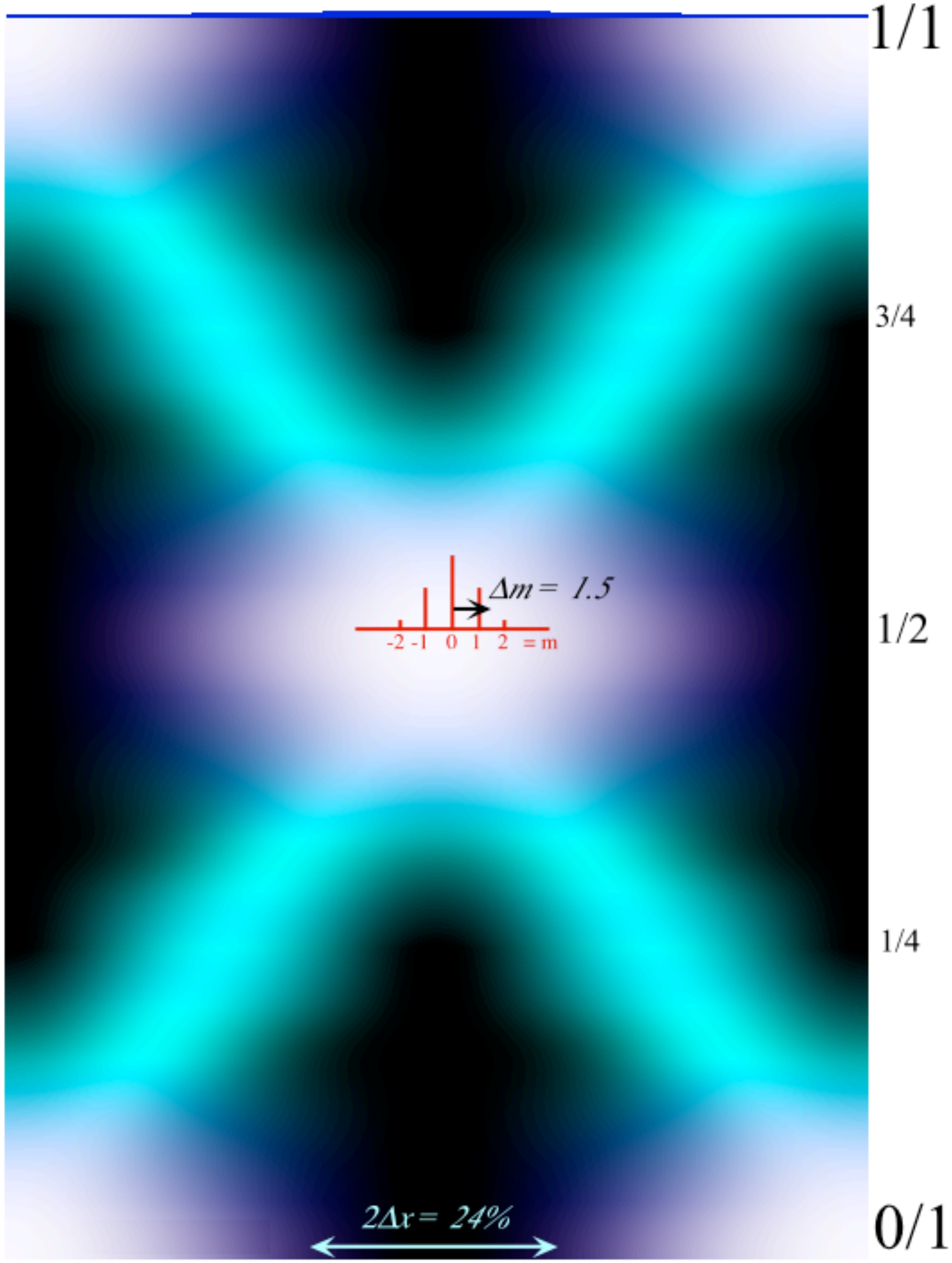
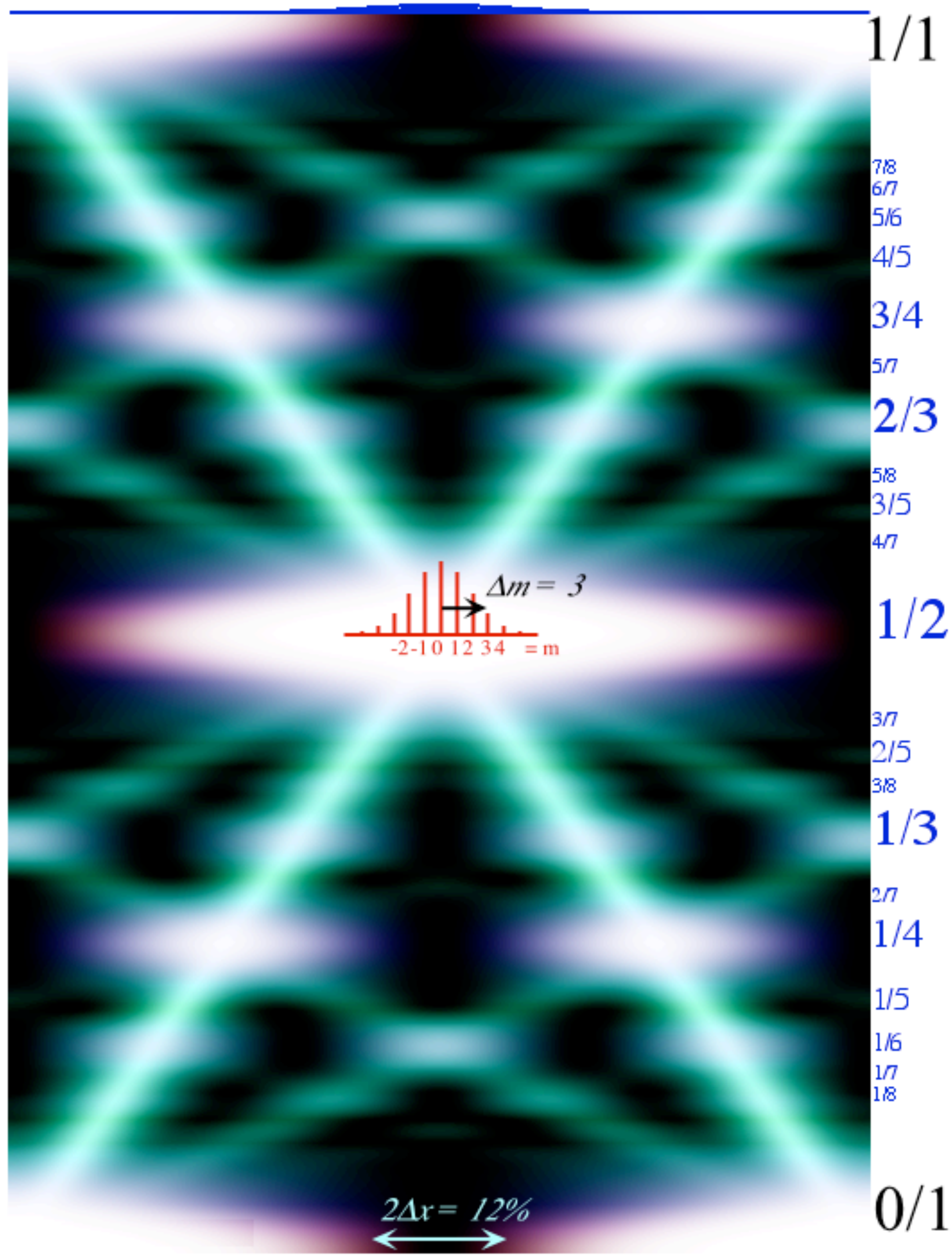
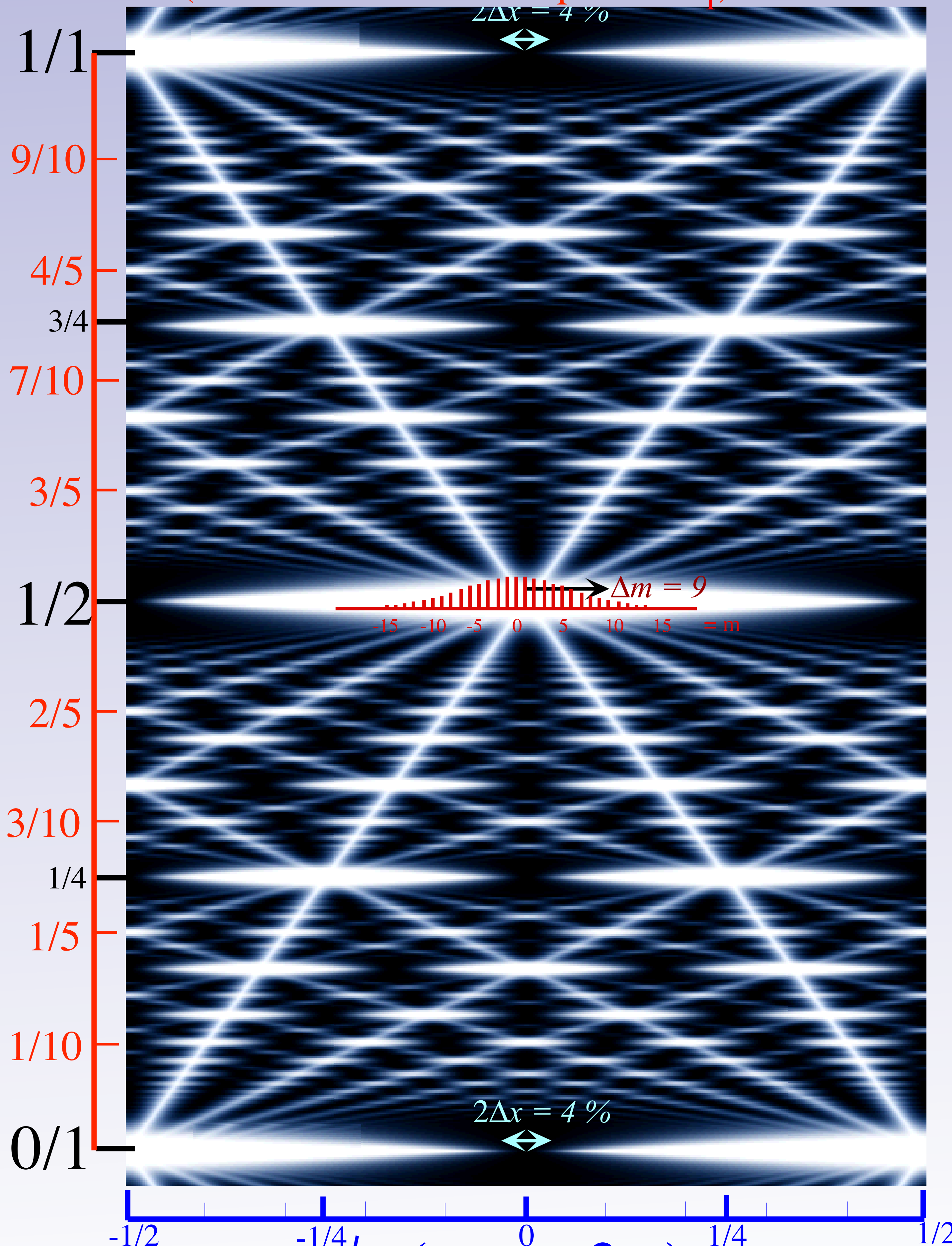
*gently means gently-truncated Gaussian distributions



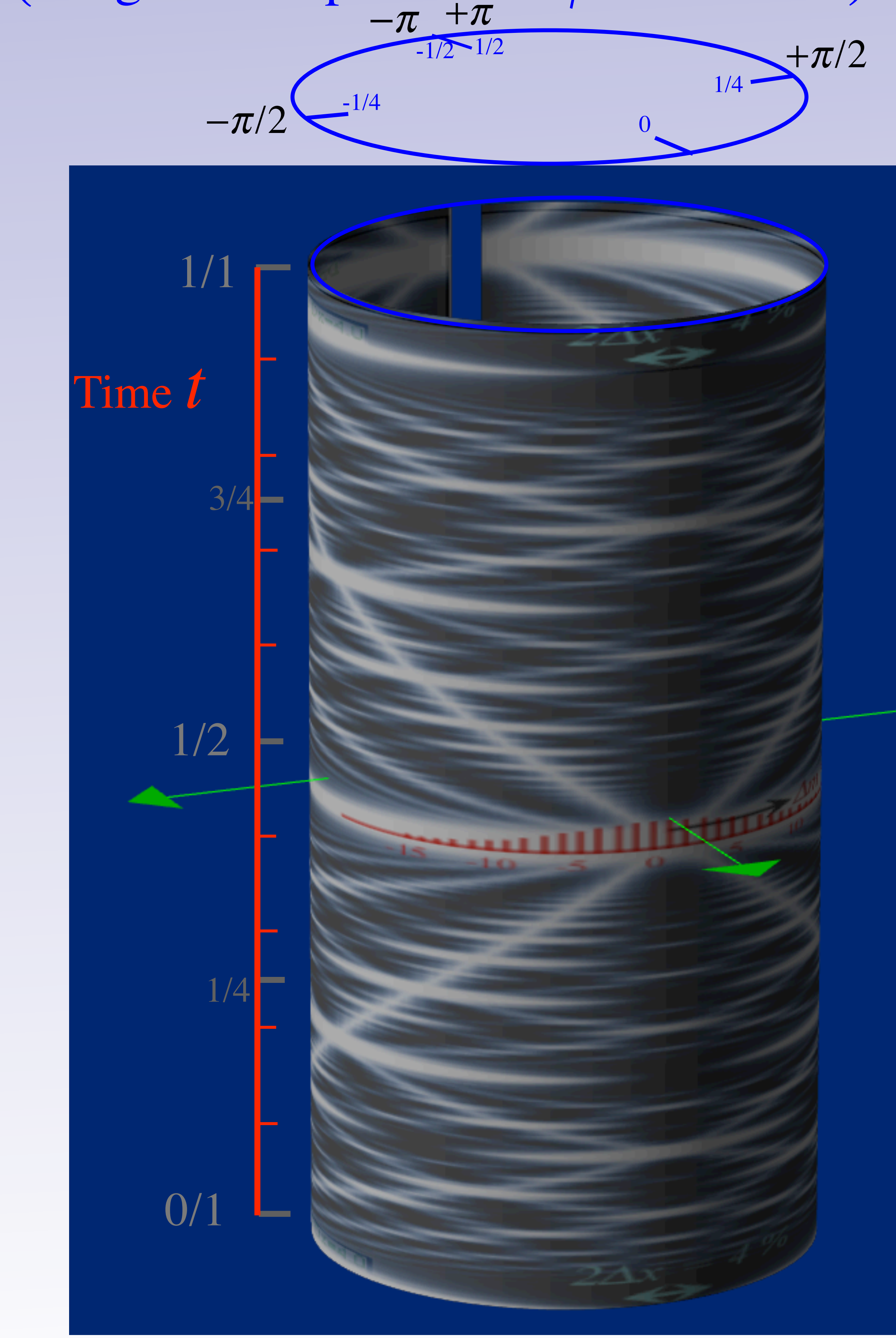


Time t (units of fundamental period τ_1)



Coordinate ϕ (units of 2π)

(Imagine "wrap-around" ϕ-coordinate)

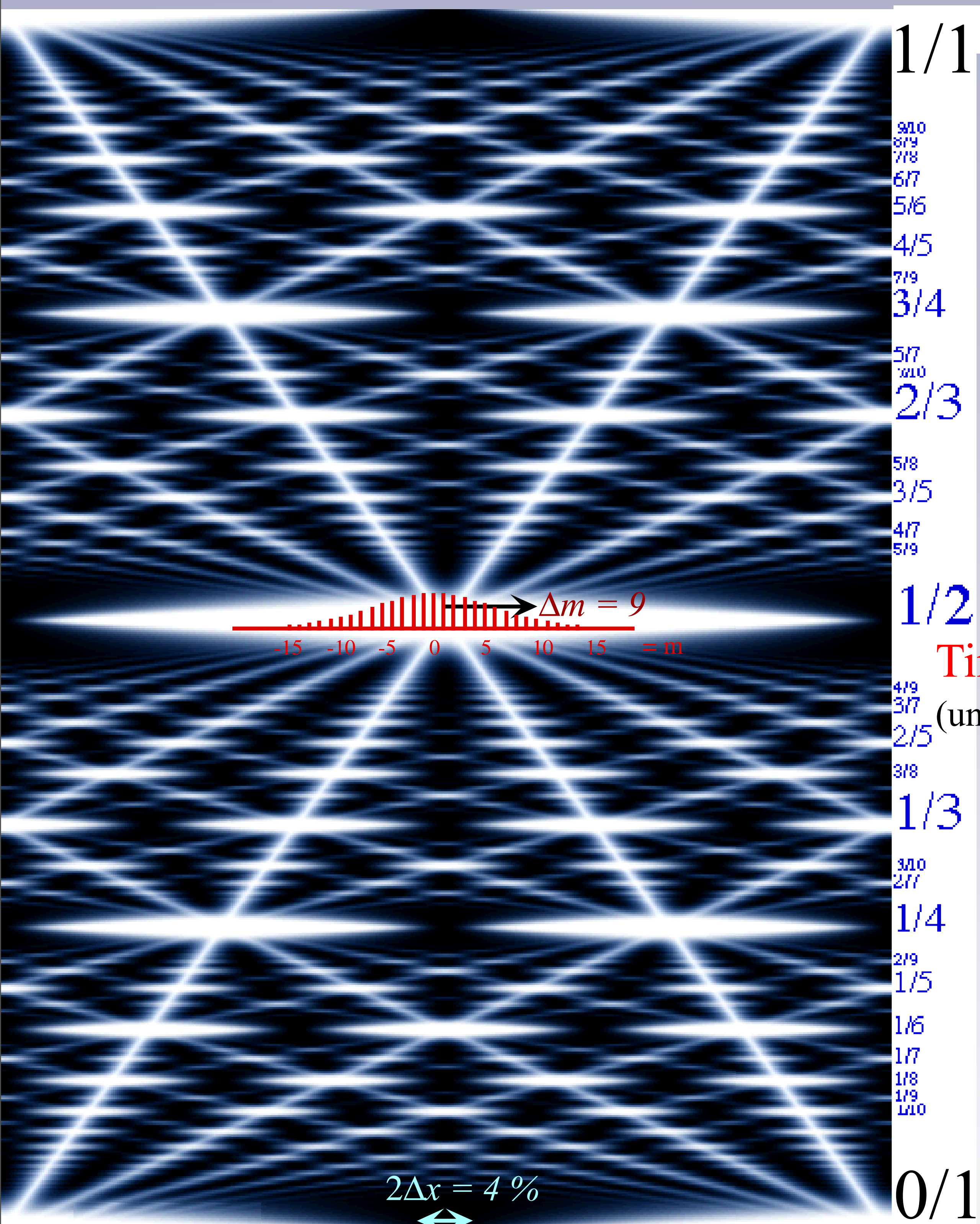


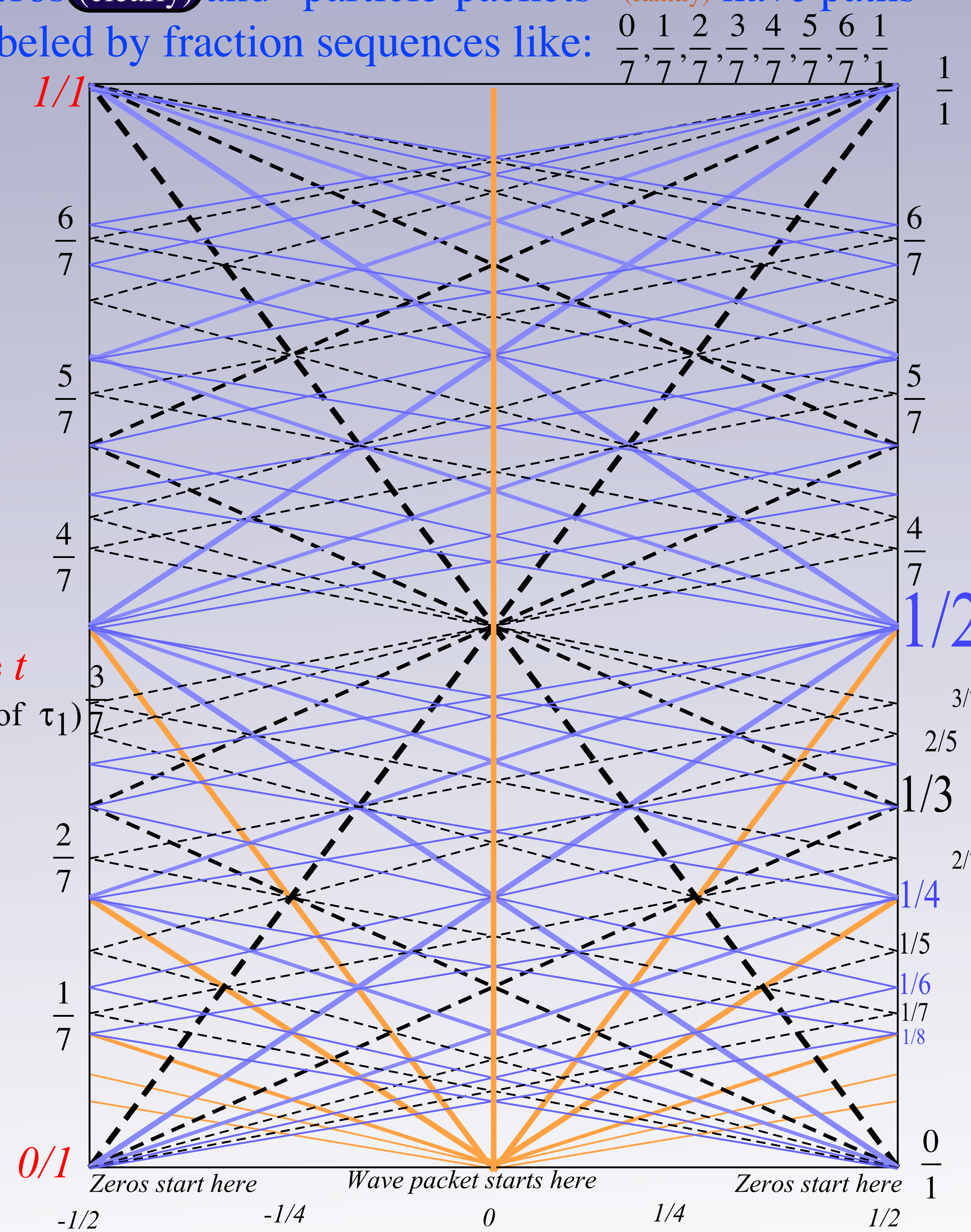
[Harter, J. Mol. Spec. 210, 166-182 (2001)]

N-level-rotor pulse wave and revival-beat wave dynamics

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

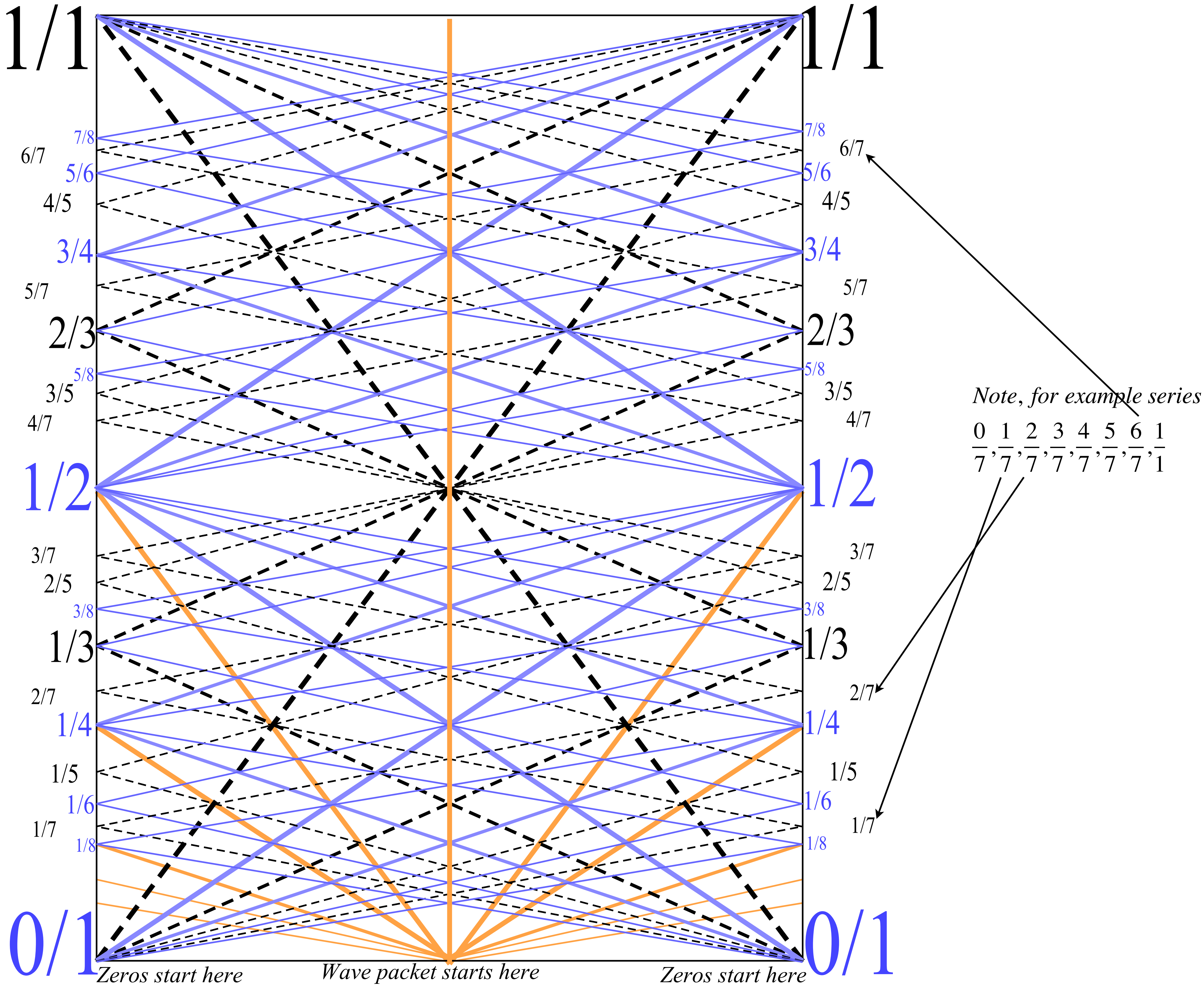
Zeros (clearly) and "particle-packets" (faintly) have paths labeled by fraction sequences like: $\frac{0}{7}, \frac{1}{7}, \frac{2}{7}, \frac{3}{7}, \frac{4}{7}, \frac{5}{7}, \frac{6}{7}, \frac{1}{1}$





Coordinate ϕ
(units of 2π)

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


1/1
7/8
6/7
5/6
4/5
3/4
5/7
2/3
5/8
3/5
4/7
1/2
3/7
2/5
3/8
1/3
2/7
1/4
1/5
1/6
1/7
1/8
0/1
Zeros start here
Wave packet starts here
Zeros start here
Note, for example series:
$\frac{0}{7}, \frac{1}{7}, \frac{2}{7}, \frac{3}{7}, \frac{4}{7}, \frac{5}{7}, \frac{6}{7}, \frac{1}{1}$

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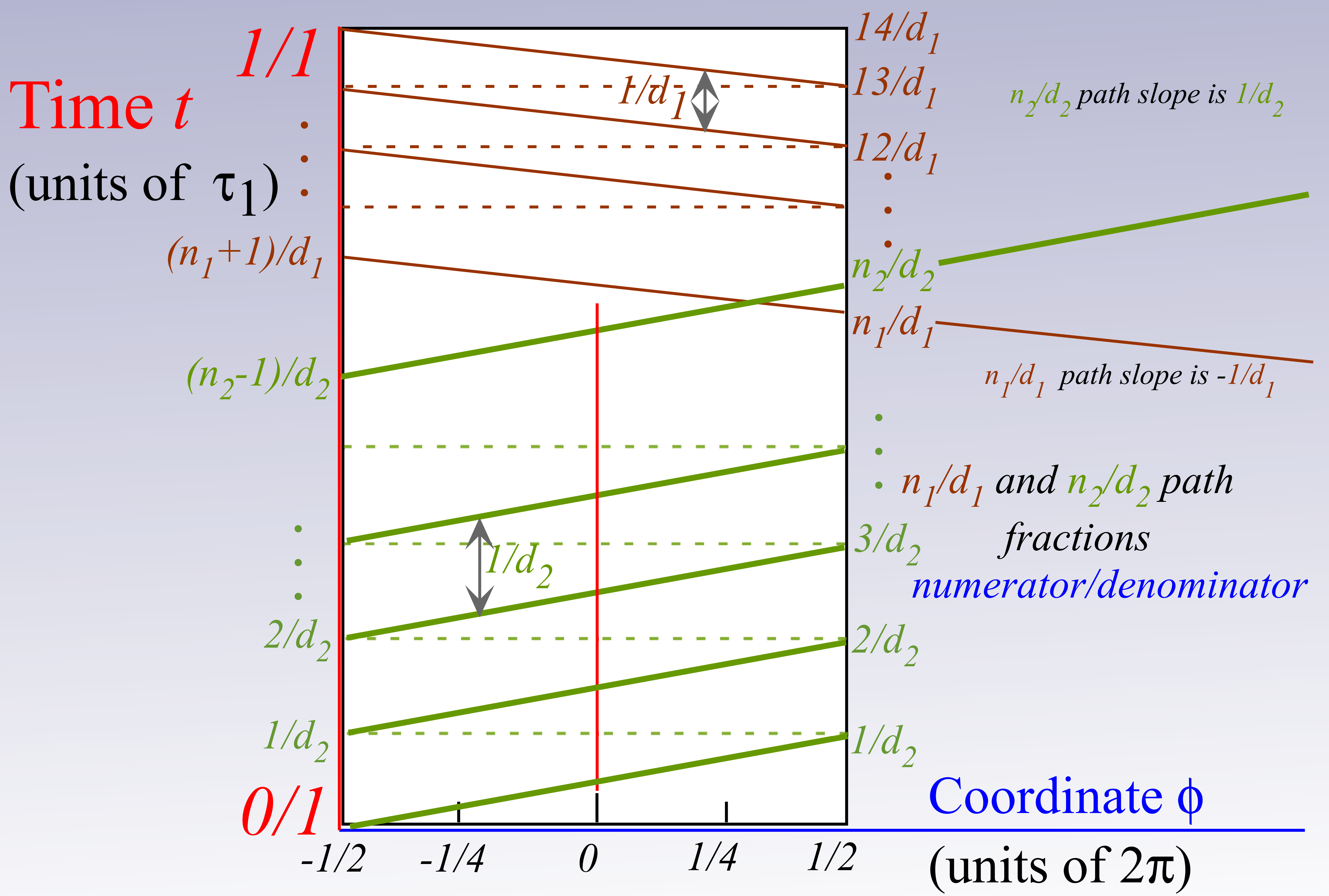
Farey Sum algebra of revival-beat wave dynamics

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



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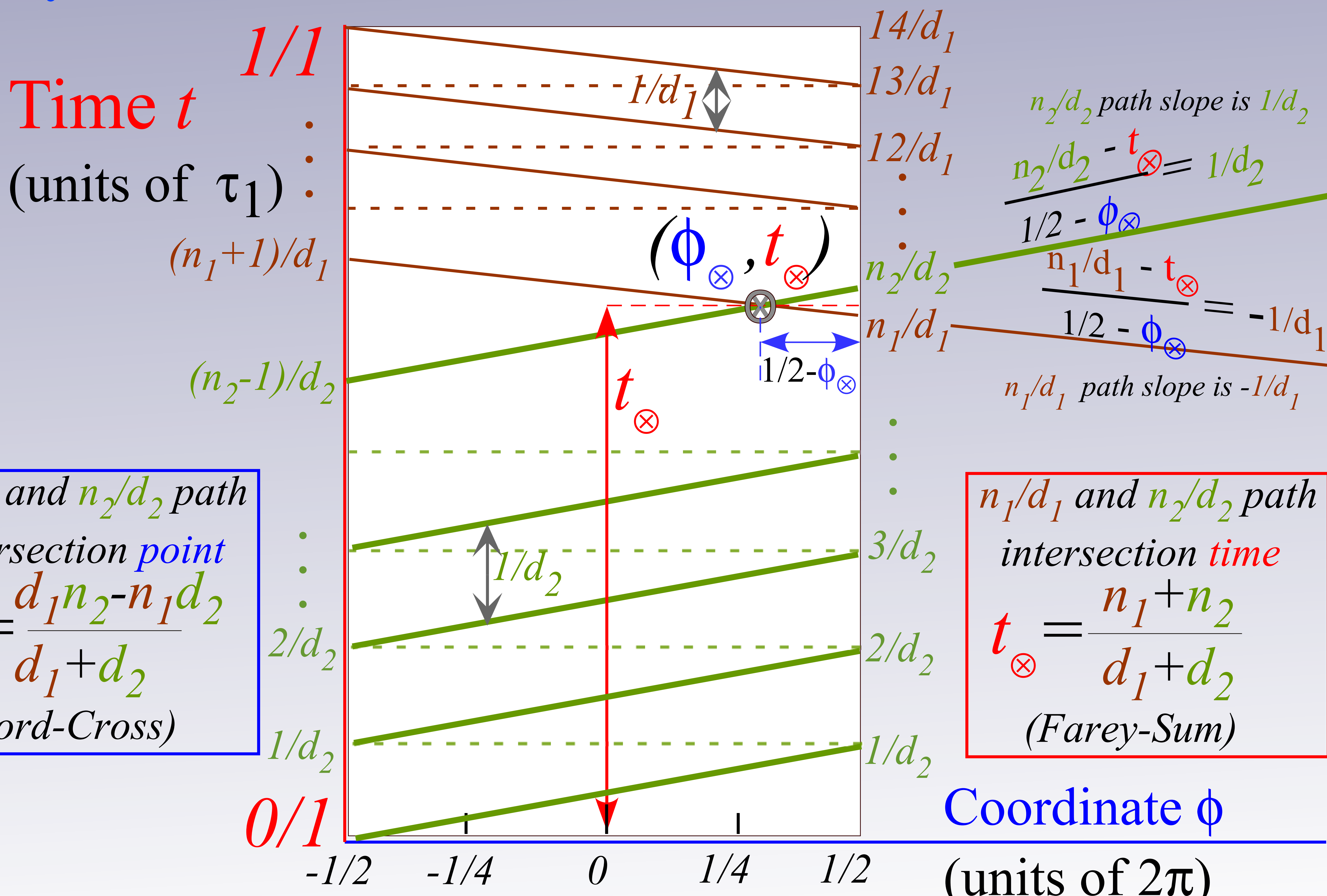


n_1/d_1 and n_2/d_2 path intersection point

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

(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)*]

A sketch of modern molecular spectroscopy

The frequency hierarchy   *Example of16μm spectra of CF_4*

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) 2^{nd} 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

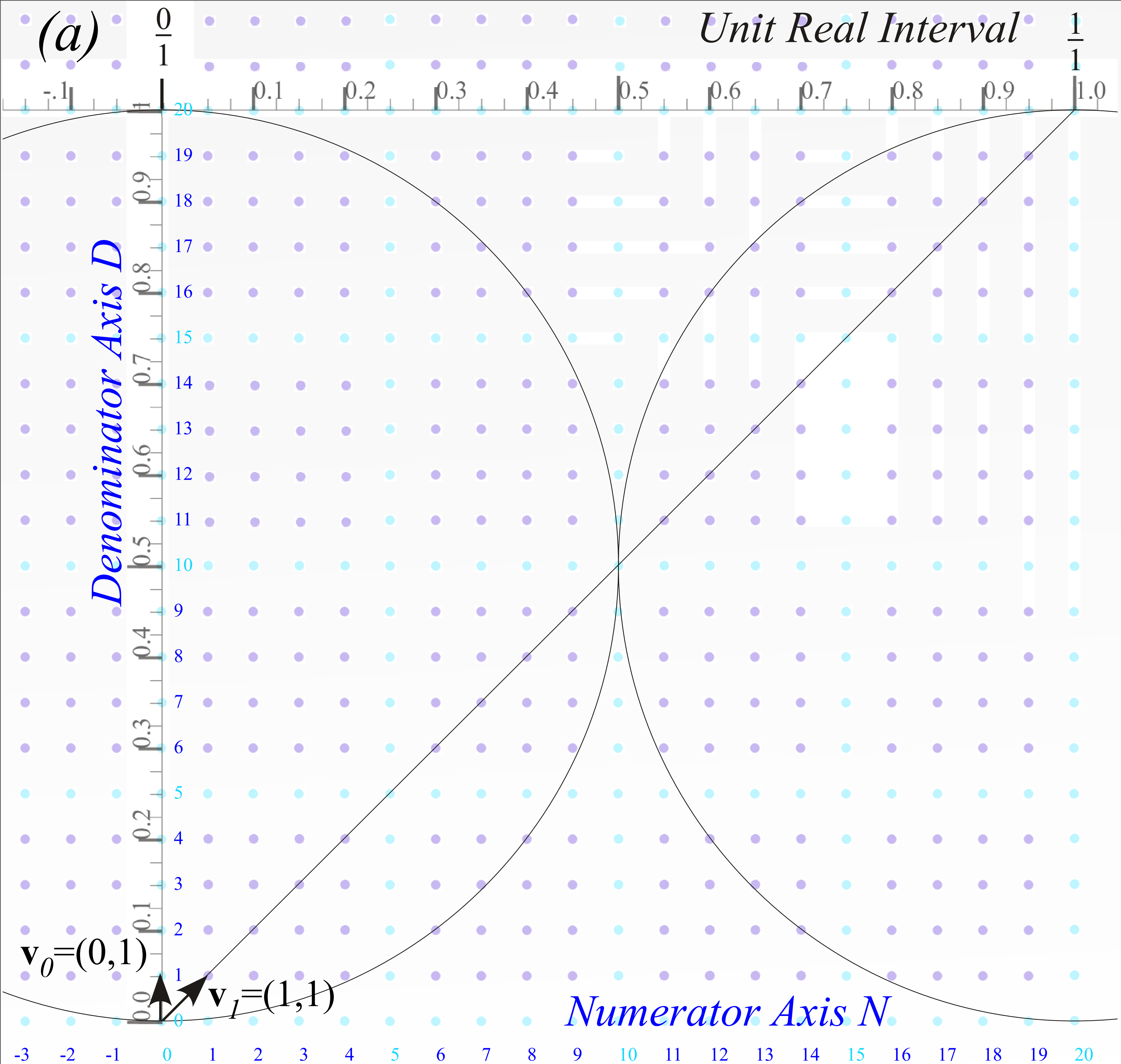
Quantum "blasts" of strongly localized ∞-well or rotor waves: A lesson in quantum interference

Wavepacket explodes! (Then revives)

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

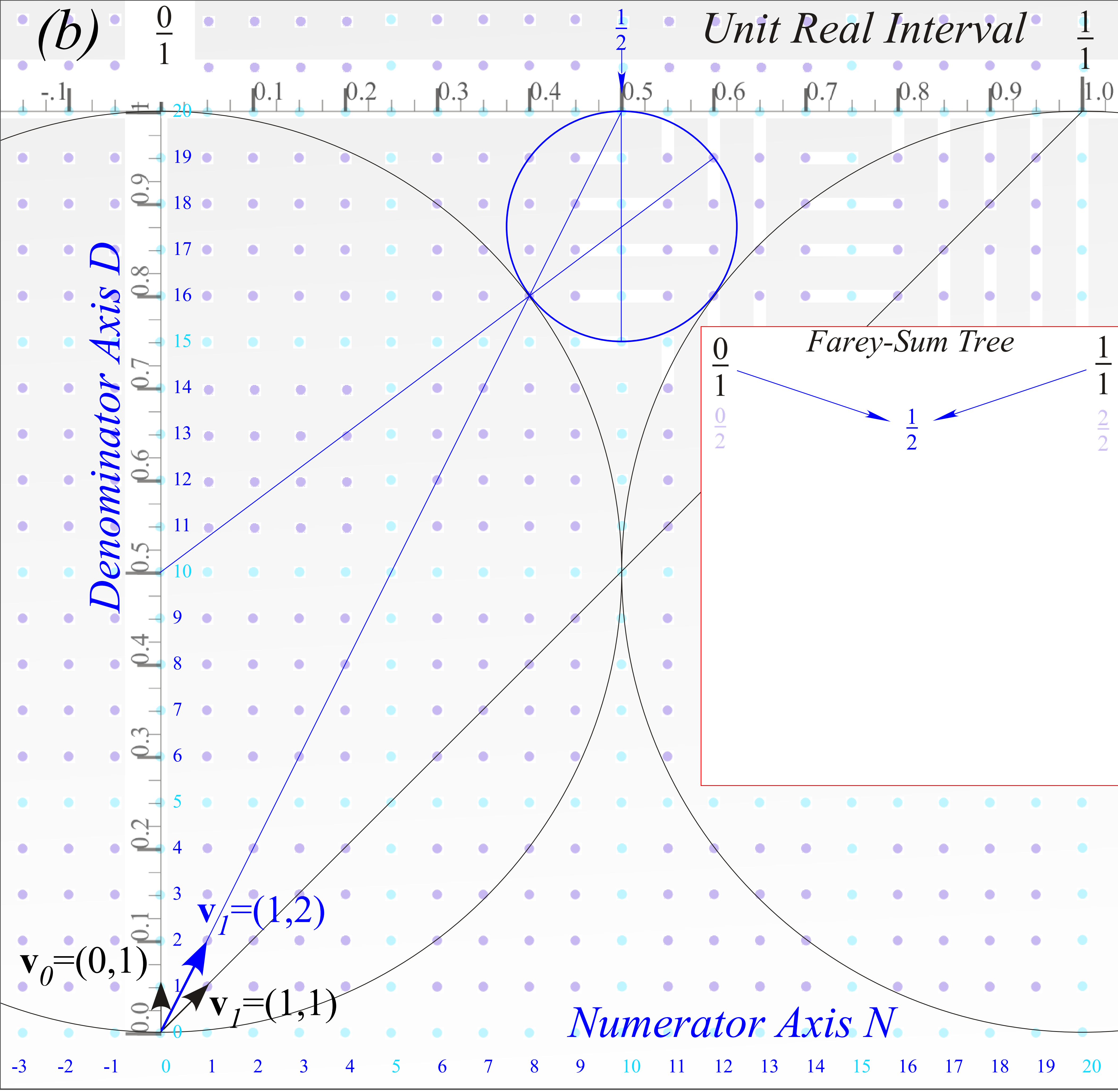
Farey-Sums and Ford-products

→ *Ford Circles and Farey-Trees* ←



Farey Sum related to vector sum and *Ford Circles*

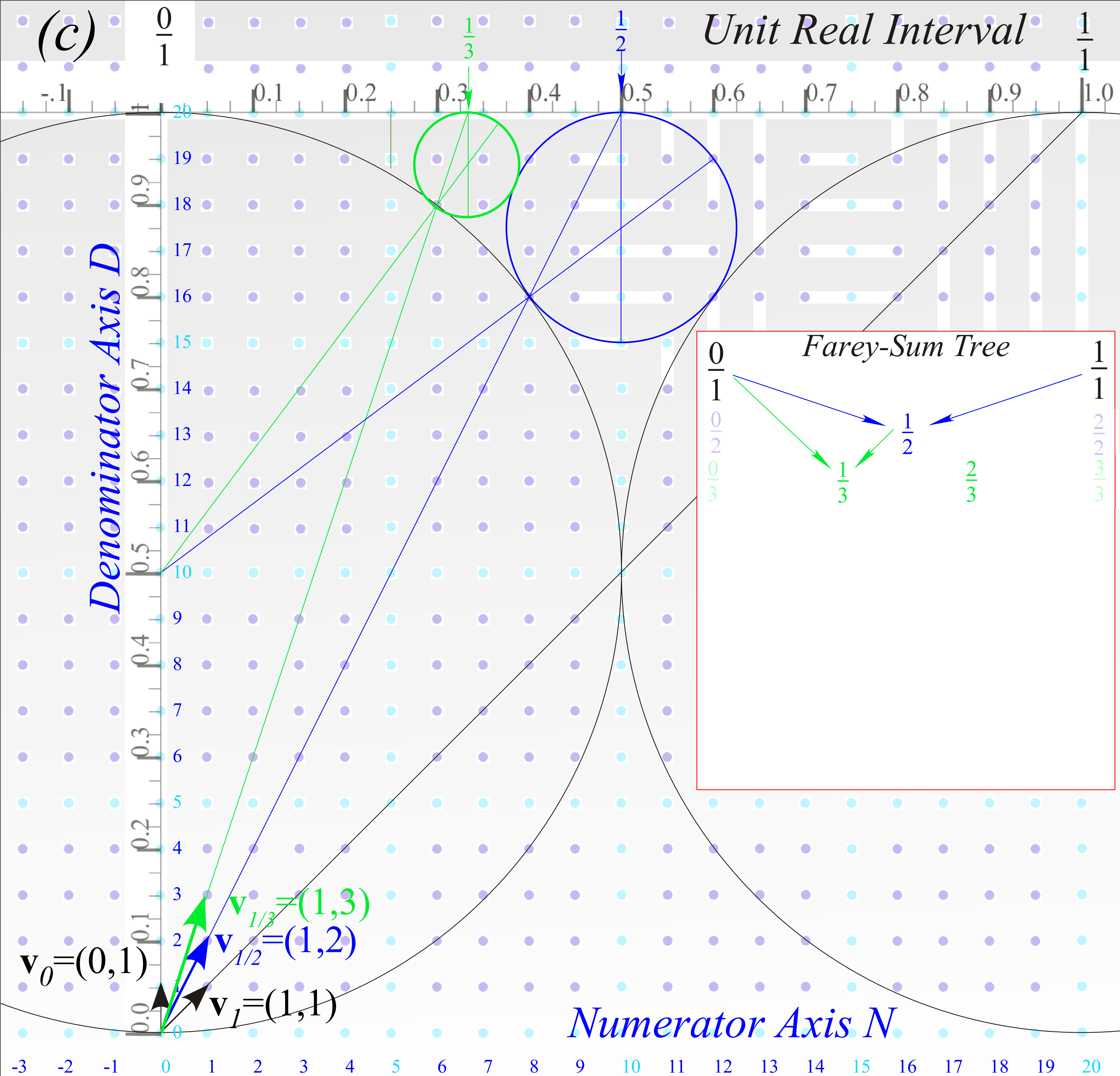
1/1-circle has diameter *1*



Farey Sum related to vector sum and *Ford Circles*

1/1-circle has diameter *1*

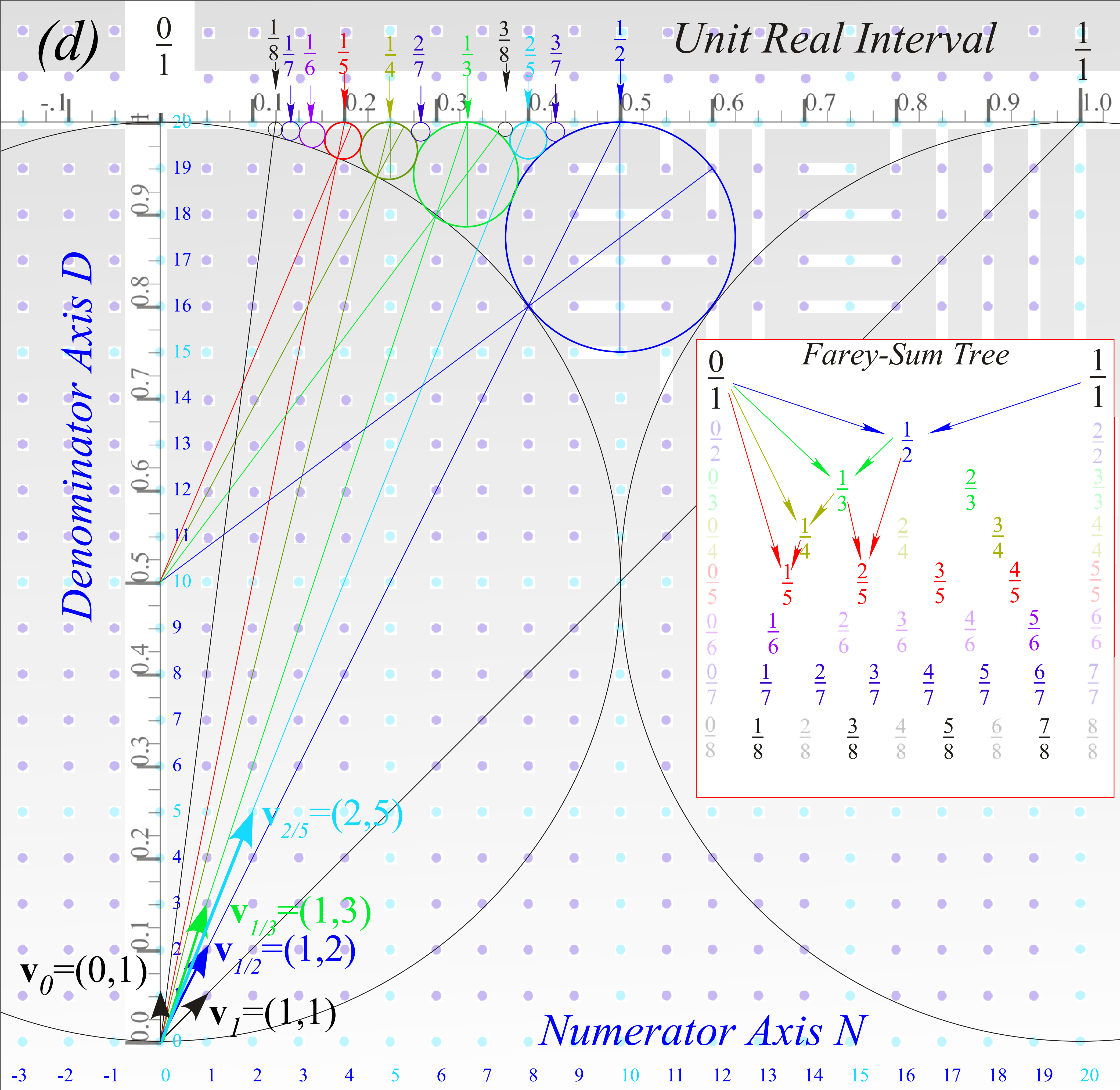
1/2-circle has diameter $1/2^2=1/4$



Farey Sum related to vector sum and *Ford Circles*

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

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



Farey Sum related to vector sum and *Ford Circles*

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

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

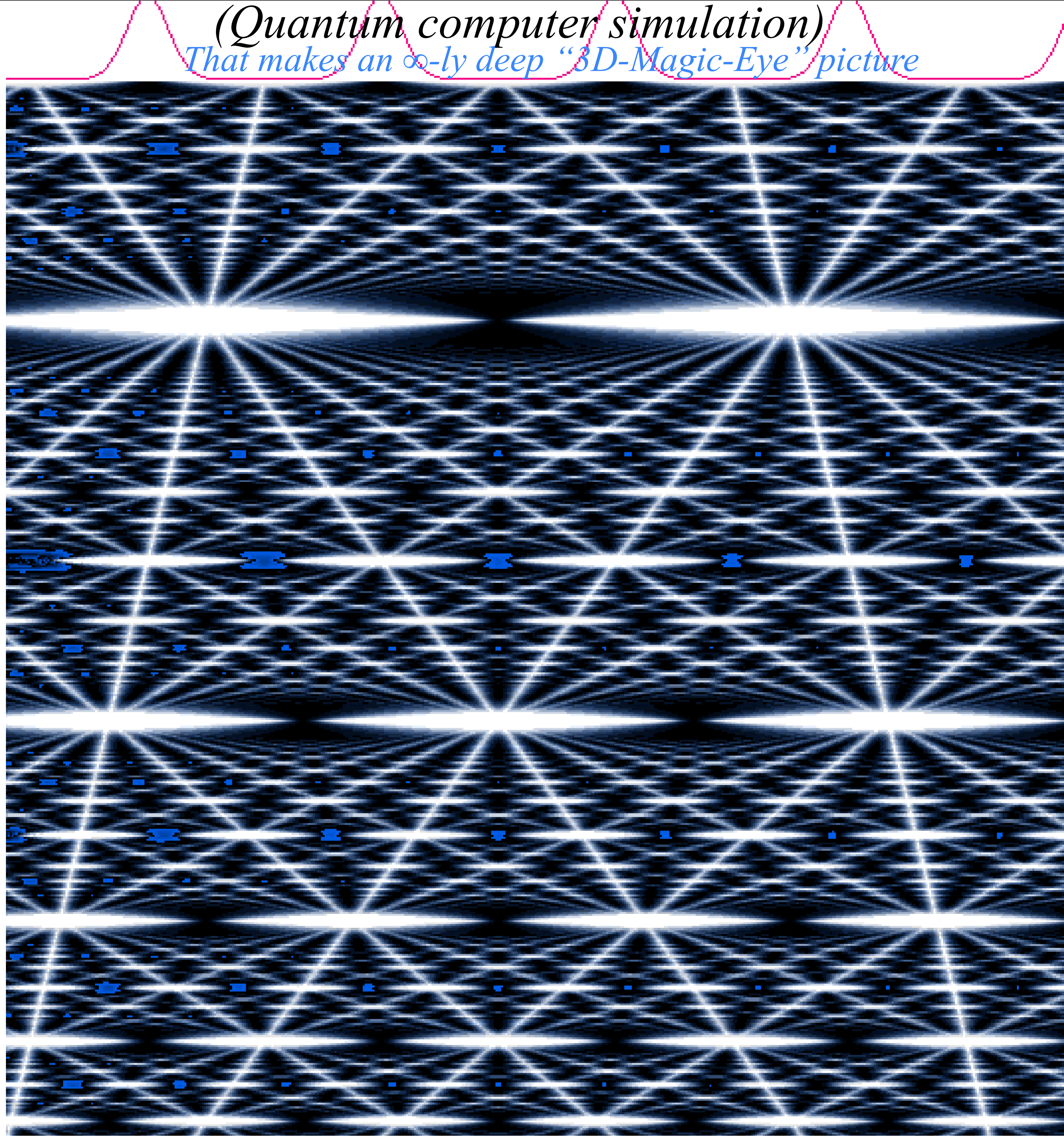
n/d-circles have diameter $1/d^2$

Farey Tree up to D=8 spectral half-width

$D \leq 1$	$\mathbf{\frac{0}{1}}$																						$\mathbf{\frac{1}{1}}$
$D \leq 2$	$\frac{0}{1}$											$\mathbf{\frac{1}{2}}$											$\frac{1}{1}$
$D \leq 3$	$\frac{0}{1}$							$\mathbf{\frac{1}{3}}$				$\frac{1}{2}$				$\mathbf{\frac{2}{3}}$							$\frac{1}{1}$
$D \leq 4$	$\frac{0}{1}$					$\mathbf{\frac{1}{4}}$		$\frac{1}{3}$				$\frac{1}{2}$				$\frac{2}{3}$		$\mathbf{\frac{3}{4}}$					$\frac{1}{1}$
$D \leq 5$	$\frac{0}{1}$				$\mathbf{\frac{1}{5}}$	$\frac{1}{4}$		$\frac{1}{3}$		$\mathbf{\frac{2}{5}}$		$\frac{1}{2}$		$\mathbf{\frac{3}{5}}$		$\frac{2}{3}$		$\frac{3}{4}$	$\mathbf{\frac{4}{5}}$				$\frac{1}{1}$
$D \leq 6$	$\frac{0}{1}$			$\mathbf{\frac{1}{6}}$	$\frac{1}{5}$	$\frac{1}{4}$		$\frac{1}{3}$		$\frac{2}{5}$		$\frac{1}{2}$		$\frac{3}{5}$		$\frac{2}{3}$		$\frac{3}{4}$	$\frac{4}{5}$	$\mathbf{\frac{5}{6}}$			$\frac{1}{1}$
$D \leq 7$	$\frac{0}{1}$		$\mathbf{\frac{1}{7}}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\mathbf{\frac{2}{7}}$	$\frac{1}{3}$		$\frac{2}{5}$	$\mathbf{\frac{3}{7}}$	$\frac{1}{2}$	$\mathbf{\frac{4}{7}}$	$\frac{3}{5}$		$\frac{2}{3}$	$\mathbf{\frac{5}{7}}$	$\frac{3}{4}$	$\frac{4}{5}$	$\frac{5}{6}$	$\mathbf{\frac{6}{7}}$		$\frac{1}{1}$
$D \leq 8$	$\frac{0}{1}$	$\mathbf{\frac{1}{8}}$	$\frac{1}{7}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{2}{7}$	$\frac{1}{3}$	$\mathbf{\frac{3}{8}}$	$\frac{2}{5}$	$\frac{3}{7}$	$\frac{1}{2}$	$\frac{4}{7}$	$\frac{3}{5}$	$\mathbf{\frac{5}{8}}$	$\frac{2}{3}$	$\frac{5}{7}$	$\frac{3}{4}$	$\frac{4}{5}$	$\frac{5}{6}$	$\frac{6}{7}$	$\mathbf{\frac{7}{8}}$	$\frac{1}{1}$

(Quantum computer simulation)

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



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

A lesson in quantum uncertainty

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

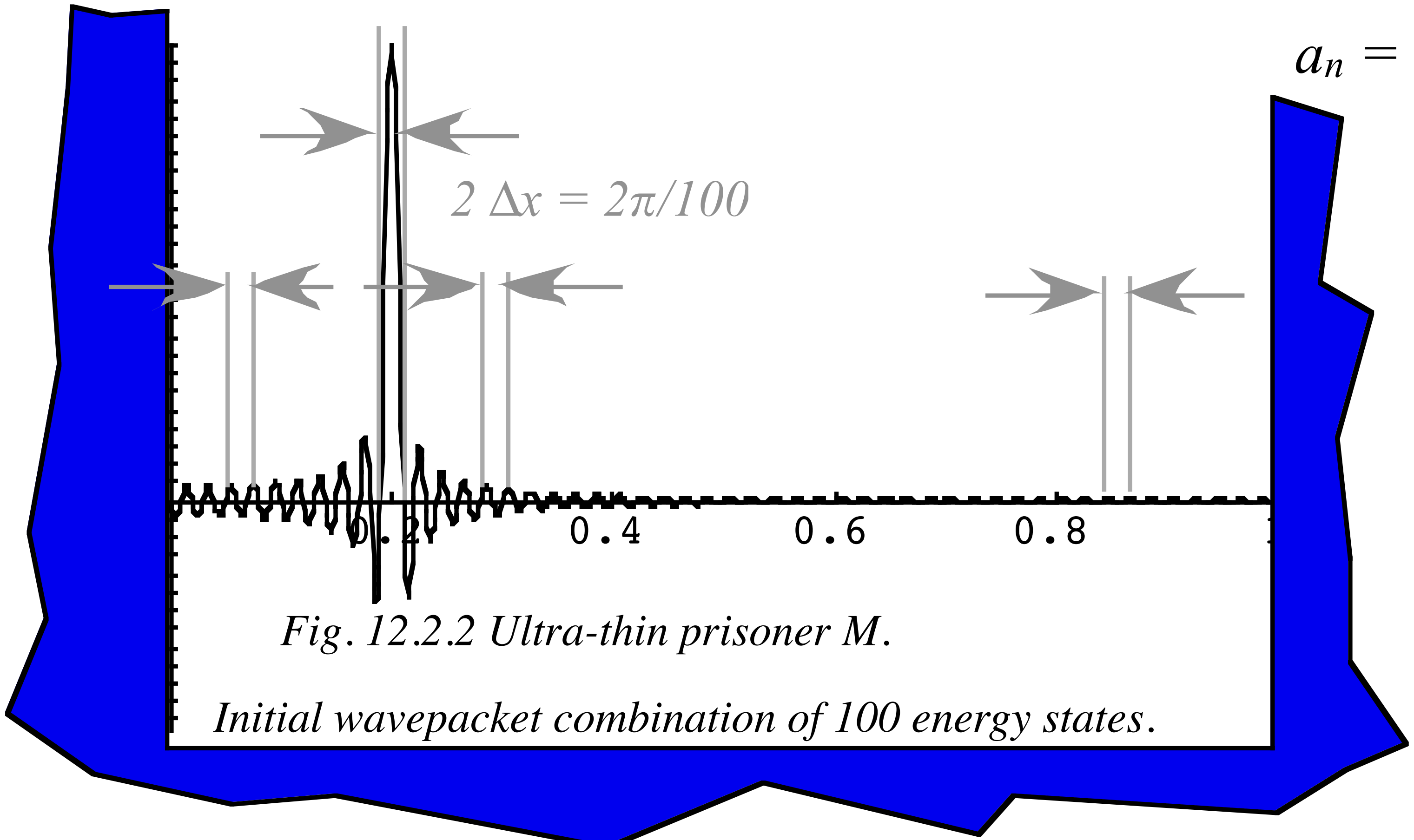


Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

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

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

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

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

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

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

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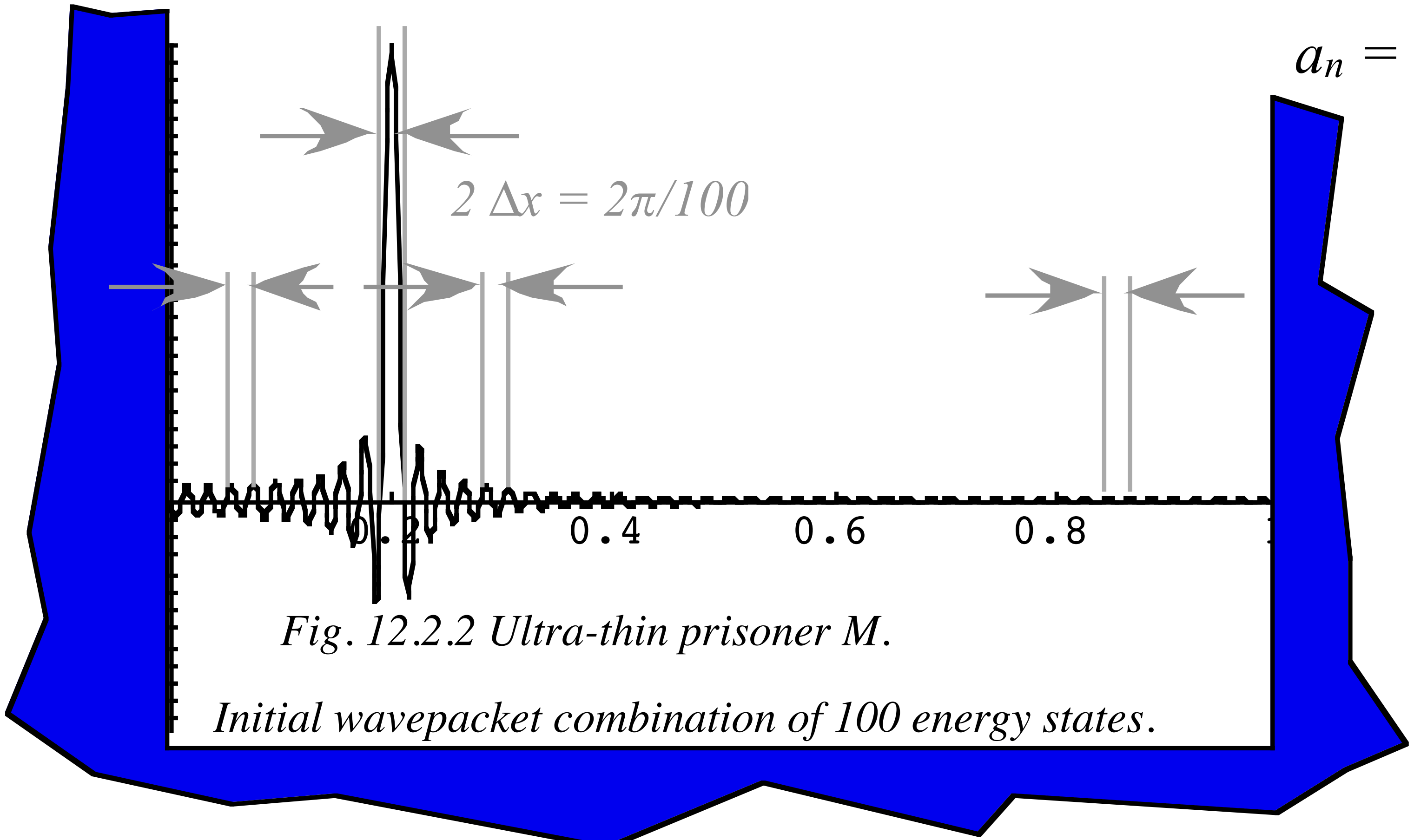

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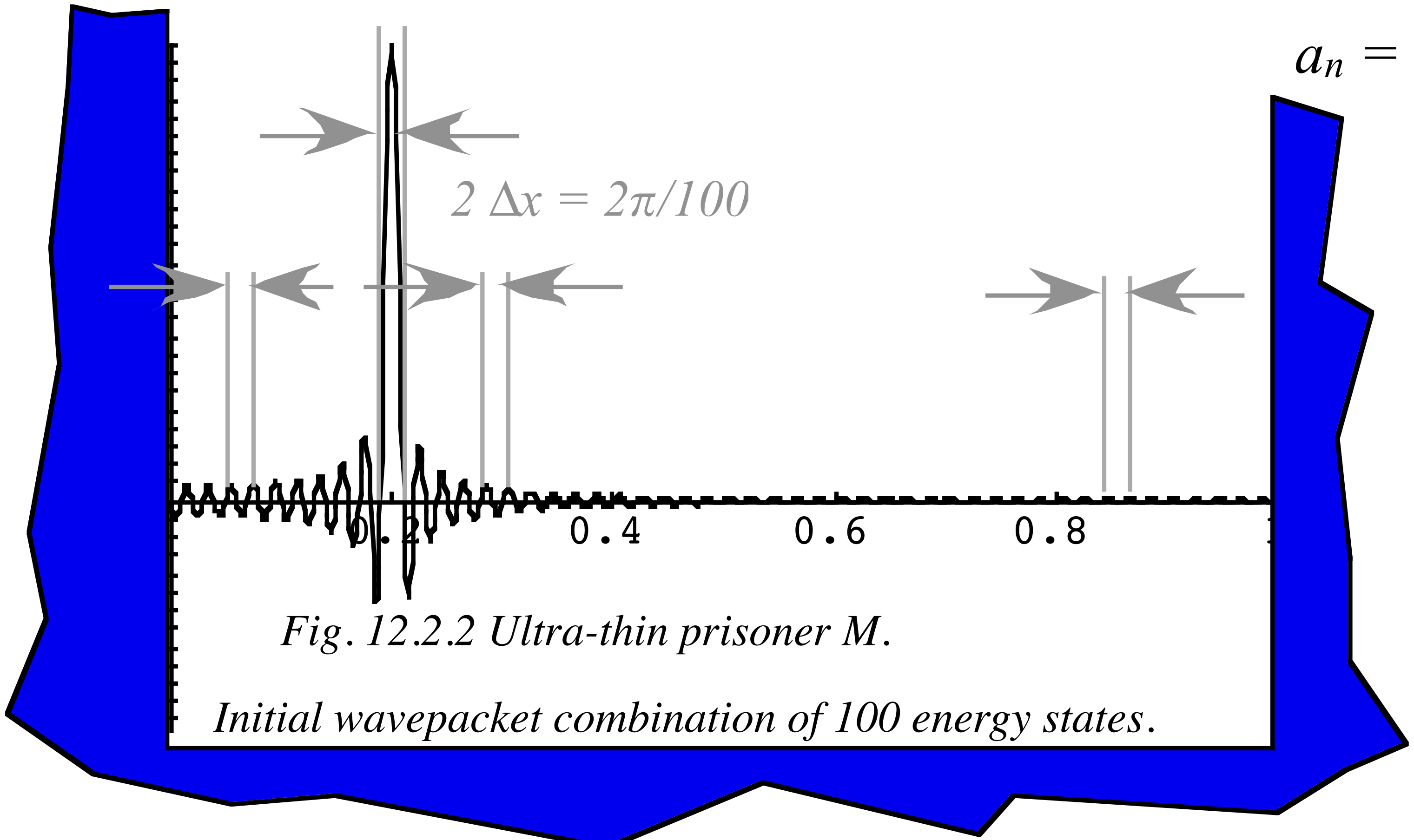

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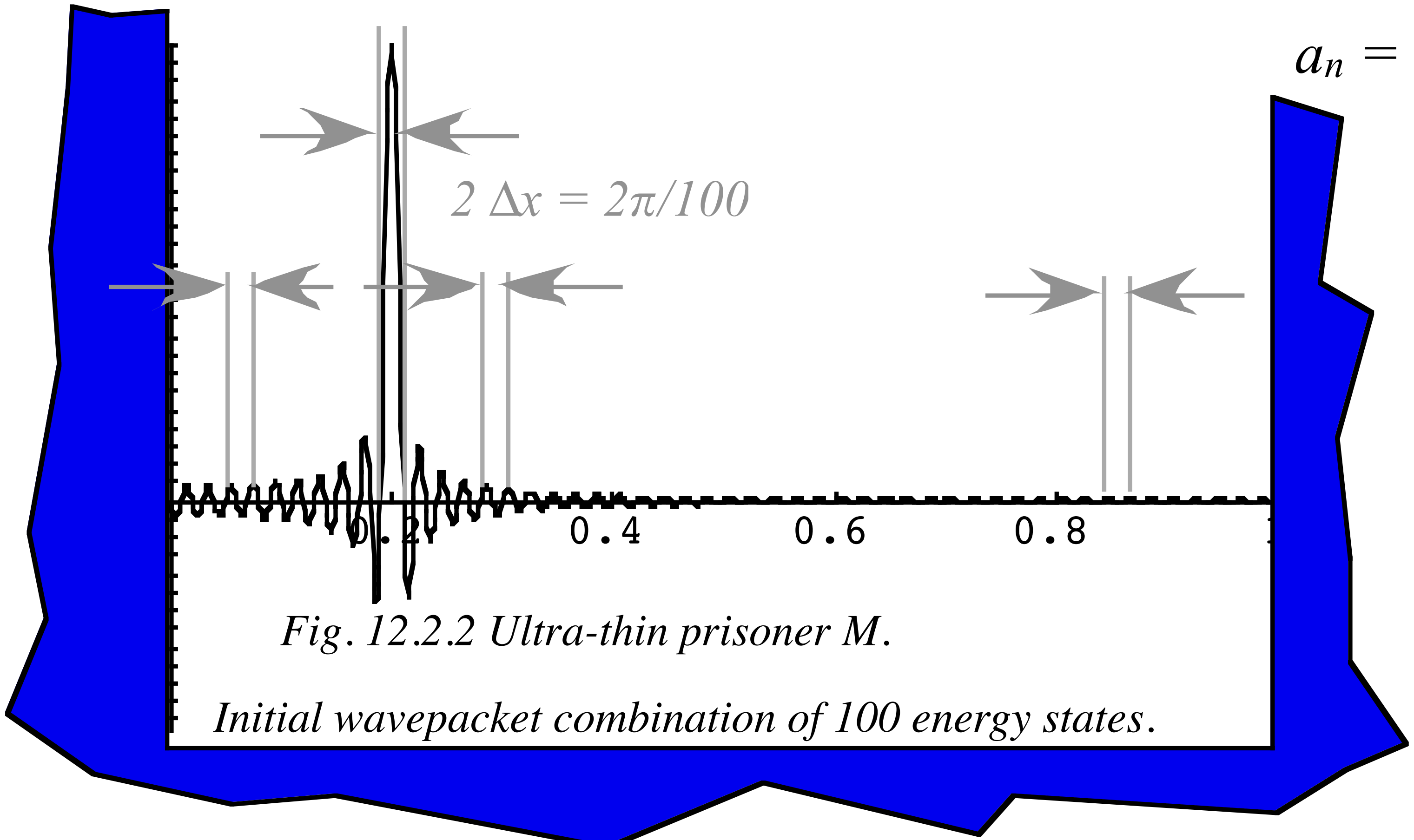

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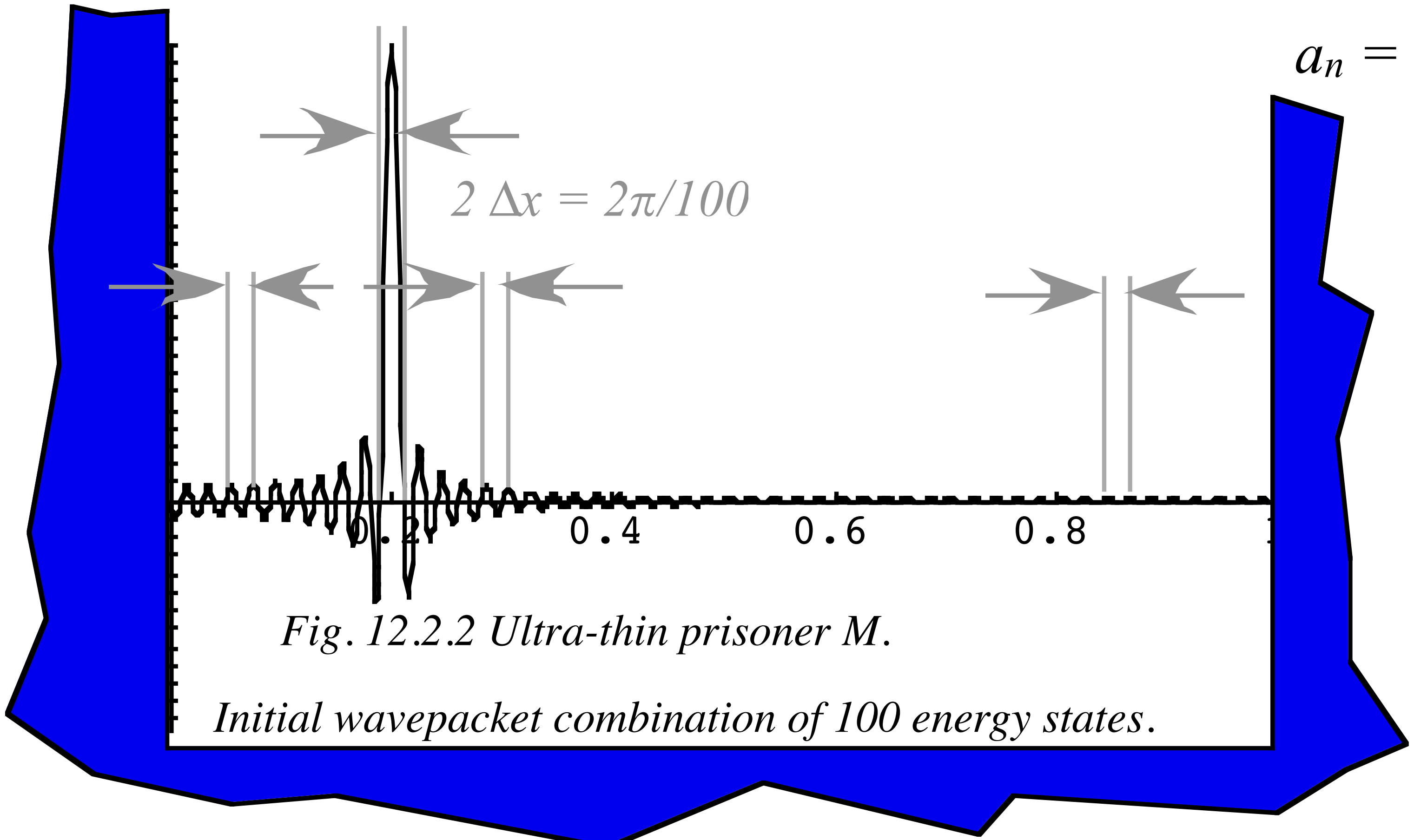

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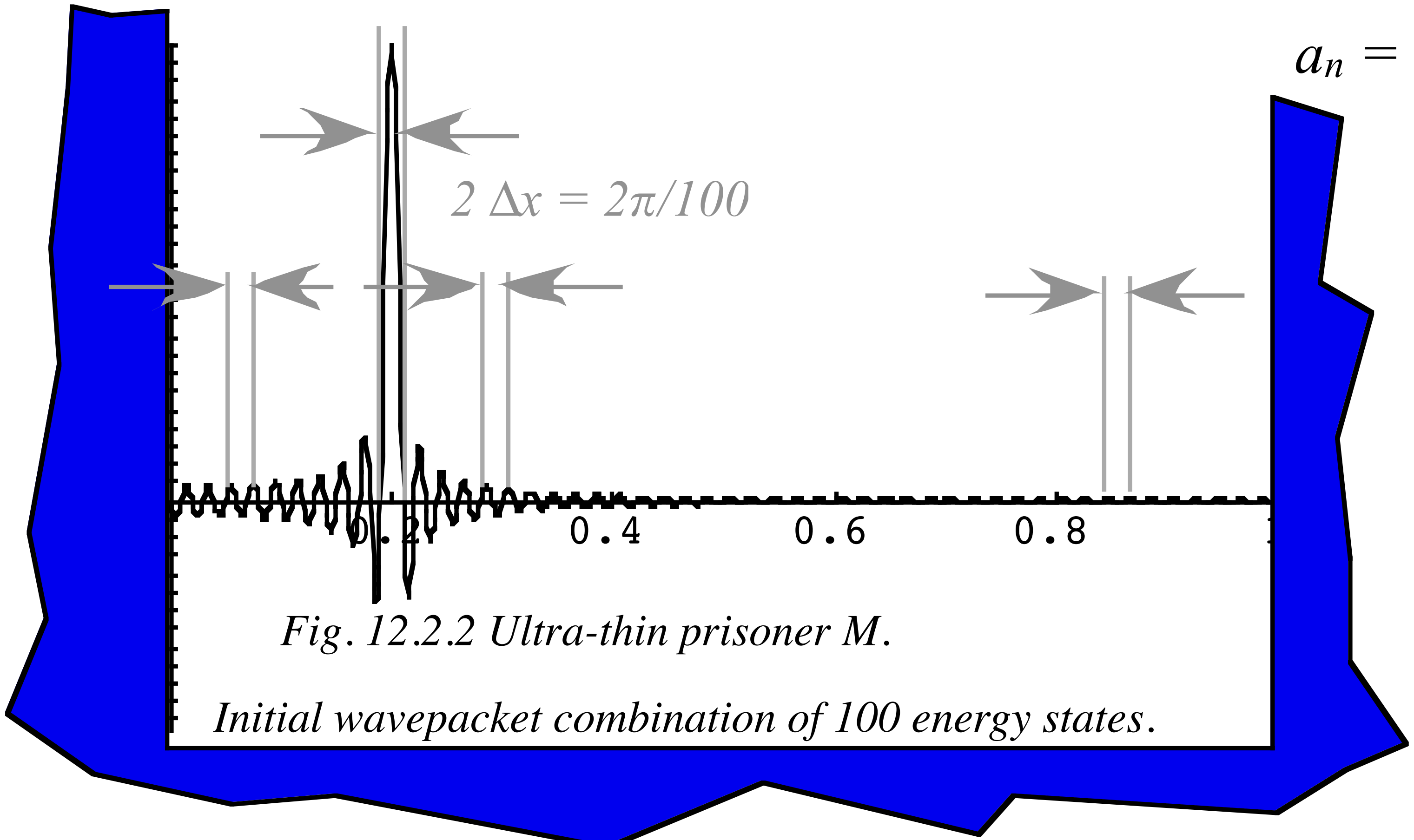

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$\Delta x \cdot |K_{max}| = \Delta x \cdot \Delta k = \pi$ or: $\Delta x \cdot \Delta p = \pi\hbar = h/2$ *∞-Well uncertainty relation*

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

Polygonal geometry of $U(2)\supset C_N$ character spectral function
Algebra
Geometry

Introduction to wave dynamics of phase, mean phase, and group velocity
Expo-Cosine identity
Relating space-time and per-space-time
Wave coordinates
Pulse-waves (PW) vs Continuous -waves (CW)

Introduction to C_N beat dynamics and "Revivals" due to Bohr-dispersion
∞-Square well PE versus Bohr rotor
SinNx/x wavepackets bandwidth and uncertainty
SinNx/x explosion and revivals
Bohr-rotor dynamics
→ *Gaussian wave-packet bandwidth and uncertainty* ←
Gaussian Bohr-rotor revivals
Farey-Sums and Ford-products
Phase dynamics

Gaussian wave-packet bandwidth and uncertainty

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

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

Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

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

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

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Gaussian integral:

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

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

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

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Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

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

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

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

It is a Gaussian distribution, too

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

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

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

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

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

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Gaussian uncertainty relation

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

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

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m=0, ±1, ±2, ±3,...are momentum quanta in wavevector formula: $k_m=2\pi m/L$ $\quad$ ($k_m=m$ *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* $\upsilon_1=(E_1-E_0)/h$

Kershaw's prediction that the year AD 2000 would see the dramatic intervention of God in the world of human affairs was by no means new. Indeed, Kershaw himself refers to the tradition found in both Jewish and Christian circles that 'at the end of 6000 years the Messiah shall come, *and the world shall be renewed*'.[53] In this context, for example, the work of William Whiston, discussed in chapter 3 above, might be further noted. Whiston in his *Essay on the Revelation of Saint John* similarly predicted that the end of all things would come in AD 2000. The reasoning behind this thinking is reasonably plain: the world was created in six days followed by a day of rest; scripture says that 'one day is with the Lord as a thousand years, and a thousand years as one day' (2 Pet. 3.8); therefore there will be 6,000 years of toil followed by a Sabbath-millennium. Kershaw himself appeals to such reasoning.[54]

[53] Kershaw is quoting Thomas Newton at this point. See Thomas Newton, *Dissertation on the Prophecies*, 18th edn, (1834), p. 696. The work was originally published in 1754.

[54] For a discussion of belief in the Sabbath-millennium, see further John Jarick, 'The Fall of the House (of Cards) of Ussher: Why the World as We Know it Did not End at Sunset on 22nd October 1997 (and Will not End at Midnight on 31st December 1999/1st January 2000)', in Stanley E. Porter, Michael A. Hayes and David Tombs (eds.), *Faith in the Millennium* (Roehampton Institute London Papers, 7; Sheffield Academic Press, forthcoming, 2000).

Christopher Rowland; John Barton (2002). Apocalyptic in history and tradition. Sheffield Academic Press. pp. 233–252. ISBN 978-0-8264-6208-4. Retrieved 23 March 2011.