A sketch of modern molecular spectroscopy

The frequency hierarchy

Example of 16\(\mu\)m 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

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Example of CO\(_2\) rotational (\(\nu=0\)\(\Leftrightarrow\)\(\nu=1\)) bands

Quantum dynamics of \(\infty\)-Square well and Bohr rotor: What makes that “dipole” spectra?

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The frequency hierarchy

<table>
<thead>
<tr>
<th>Radio-frequency</th>
<th>Microwave to far-infrared</th>
<th>Infrared</th>
<th>Near-infrared to visible to ultraviolet to X-ray</th>
</tr>
</thead>
<tbody>
<tr>
<td>fine structure</td>
<td>rotational spectra</td>
<td>vibrational spectra</td>
<td>electronic spectra</td>
</tr>
<tr>
<td>CF₄ and SF₆</td>
<td>(n=0, ν = 0) rotational levels</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>J=8</td>
<td>v=9</td>
<td>Typical VISIBLE</td>
</tr>
<tr>
<td></td>
<td>J=7</td>
<td>v=8</td>
<td>ν=600 THz</td>
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<tr>
<td></td>
<td>J=6</td>
<td>v=7</td>
<td>1/λ=2.10⁻⁶ m⁻¹</td>
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<tr>
<td></td>
<td>J=5</td>
<td>v=6</td>
<td>=2.10⁻⁶ cm⁻¹</td>
</tr>
<tr>
<td></td>
<td>J=4</td>
<td>v=5</td>
<td>λ=0.5 μm</td>
</tr>
<tr>
<td></td>
<td>J=3</td>
<td>v=4</td>
<td>=500 nm</td>
</tr>
<tr>
<td></td>
<td>J=2</td>
<td>v=3</td>
<td>Eᵥ=2.48 eV</td>
</tr>
<tr>
<td></td>
<td>J=1</td>
<td>v=2</td>
<td>or</td>
</tr>
<tr>
<td></td>
<td>J=0</td>
<td>v=1</td>
<td>H-Lyman α</td>
</tr>
<tr>
<td></td>
<td></td>
<td>v=0</td>
<td>ULTRAVIOLET</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>ν=2.4PHz</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Eᵥ=10.2 eV</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>λ=125 nm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other types of spectral splitting</td>
<td></td>
<td>rovibrational spectra</td>
<td>vibronic spectra</td>
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<tr>
<td>Ammonia NH₃</td>
<td>inversion doublet</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(-) (+)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nuclear spin</td>
<td>hyperfine splitting</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

CO₂ laser INFRARED
ν=30 THz
λ=10 μm
1/λ=1000 cm⁻¹
Eᵥ=0.124 eV

From Fig. 6.5.5.
Principles of Symmetry, Dynamics, and Spectroscopy

Spectral Quantities

<table>
<thead>
<tr>
<th>Frequency ν</th>
<th>Hertz (sec⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>THz</td>
<td>10¹² s⁻¹</td>
</tr>
<tr>
<td>GHz</td>
<td>10⁹ s⁻¹</td>
</tr>
<tr>
<td>MHz</td>
<td>10⁶ s⁻¹</td>
</tr>
<tr>
<td>kHz</td>
<td>10³ s⁻¹</td>
</tr>
</tbody>
</table>

Wavelength λ

<table>
<thead>
<tr>
<th>meters (m)</th>
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</thead>
<tbody>
<tr>
<td>fm</td>
</tr>
<tr>
<td>pm</td>
</tr>
<tr>
<td>nm</td>
</tr>
<tr>
<td>μm</td>
</tr>
<tr>
<td>mm</td>
</tr>
<tr>
<td>cm</td>
</tr>
<tr>
<td>km</td>
</tr>
</tbody>
</table>

Wavenumber per meter (m⁻¹)

<table>
<thead>
<tr>
<th>cm⁻¹</th>
<th>10² m⁻¹</th>
</tr>
</thead>
</table>

Energy eν

electronVolts (eV)
Example of frequency hierarchy for 16μm spectra of CF₄ (Freon-14)
W.G. Harter
Ch. 31
Atomic, Molecular, & Optical Physics Handbook
Am. Int. of Physics
Gordon Drake Editor
(1996)
Example of frequency hierarchy for 16µm spectra of CF₄ (Freon-14)
W.G.Harter
Fig. 32.7
Springer Handbook of Atomic, Molecular, & Optical Physics
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*Units of frequency (Hz), wavelength (m), and energy (eV)*

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- Farey-Sums and Ford-products
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### Units of frequency (Hz), wavelength (m), and energy (eV)

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

**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:** $10^{-18}$

---

**From:** Electromagnetic Spectrum  
**Wikipedia Commons (2013)**

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

\[
\nu \cdot \lambda = c = 2.997 \cdot 10^8 \text{m/s}
\]

---

**From:** Electromagnetic Spectrum  
**Wikipedia Commons (2013)**

---

Monday, March 25, 2013
Units of frequency (Hz), wavelength (m), and energy (eV)

Penetrates Earth’s Atmosphere?

Radiation Type

<table>
<thead>
<tr>
<th></th>
<th>Radio</th>
<th>Microwave</th>
<th>Infrared</th>
<th>Visible</th>
<th>Ultraviolet</th>
<th>X-ray</th>
<th>Gamma ray</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength (m)</td>
<td>$10^3$</td>
<td>$10^{-2}$</td>
<td>$10^{-5}$</td>
<td>$0.5 \times 10^{-6}$</td>
<td>$10^{-8}$</td>
<td>$10^{-10}$</td>
<td>$10^{-12}$</td>
</tr>
<tr>
<td>Approximate Scale of Wavelength</td>
<td>Buildings</td>
<td>Humans</td>
<td>butterflies</td>
<td>Needle Point</td>
<td>Protozoans</td>
<td>Molecules</td>
<td>Atoms</td>
</tr>
<tr>
<td>Frequency (Hz)</td>
<td>$10^4$</td>
<td>$10^8$</td>
<td>$10^{12}$</td>
<td>$10^{15}$</td>
<td>$10^{16}$</td>
<td>$10^{18}$</td>
<td>$10^{20}$</td>
</tr>
<tr>
<td>Temperature of objects at which this radiation is the most intense wavelength emitted</td>
<td>1 K</td>
<td>-272 °C</td>
<td>100 K</td>
<td>-173 °C</td>
<td>10,000 K</td>
<td>9,727 °C</td>
<td>10,000,000 K</td>
</tr>
</tbody>
</table>

From: Electromagnetic Spectrum
Wikipedia Commons (2013)
A sketch of modern molecular spectroscopy

*The frequency hierarchy*  
*Example of 16µm spectra of CF₄*

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

*Spectral windows in atmosphere due to molecules*

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*Wavepacket explodes! (Then revives)*

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*Farey-Sums and Ford-products*
*Ford Circles and Farey-Trees*
The electromagnetic spectrum includes various types of radiation, each with different wavelengths and frequencies. The spectrum is divided into regions such as radio waves, microwaves, infrared, visible light, ultraviolet, X-rays, and gamma rays. The wavelengths of these regions range from $10^{-12}$ m to $10^3$ m, with corresponding frequencies ranging from $10^4$ Hz to $10^{20}$ Hz.

The approximate scale of wavelength includes visual representations of various objects and phenomena, such as buildings, humans, butterflies, needle points, protozoans, molecules, atoms, and atomic nuclei. The temperature of objects at which this radiation is the most intense is also indicated, ranging from 1 K to $10^8$ K.

Spectral windows in Earth's atmosphere are highlighted, showing which wavelengths are absorbed by atmospheric gases and which are blocked by the upper atmosphere. This diagram provides a visual representation of the electromagnetic spectrum and its interaction with the Earth's atmosphere.
Penetrates Earth’s Atmosphere?

<table>
<thead>
<tr>
<th>Radiation Type</th>
<th>Wavelength (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radio</td>
<td>$10^3 m$</td>
</tr>
<tr>
<td>Microwave</td>
<td>$10^{-2} m$</td>
</tr>
<tr>
<td>Infrared</td>
<td>$10^{-1} m$</td>
</tr>
<tr>
<td>Visible</td>
<td>$0.5 \times 10^{-6} m$</td>
</tr>
<tr>
<td>Ultraviolet</td>
<td>$10^{-8} m$</td>
</tr>
<tr>
<td>X-ray</td>
<td>$10^{-10} m$</td>
</tr>
<tr>
<td>Gamma ray</td>
<td>$10^{-12} m$</td>
</tr>
</tbody>
</table>

Approximate Scale of Wavelength

- Buildings
- Humans
- Butterflies
- Needle Point
- Protozoans
- Molecules
- Atoms
- Atomic Nuclei

Frequency (Hz)

- $10^4 Hz$
- $10^8 Hz$
- $10^{12} Hz$
- $10^{15} Hz$
- $10^{16} Hz$
- $10^{18} Hz$
- $10^{20} Hz$

Temperature of objects at which this radiation is the most intense wavelength emitted

- 1 K ($-272 ^\circ C$)
- 100 K ($-173 ^\circ C$)
- 10,000 K (9,727 ^\circ C)
- 10,000,000 K ($\sim 10,000,000 ^\circ C$)

Gamma rays, X-rays and ultraviolet light blocked by the upper atmosphere (best observed from space).

Visible light observable from Earth, with some atmospheric distortion.

Most of the infrared spectrum absorbed by atmospheric gasses (best observed from space).

Radio waves observable from Earth.

Long-wavelength radio waves blocked.

Note peak of human visual acuity is $\sim 548 Hz = 548 nm$ which is also peak of terrestrial solar spectrum.

From: Electromagnetic Spectrum

Wikipedia Commons (2013)
Temperature of objects at which this radiation is the most intense wavelength emitted:

- 1 K (~272 °C)
- 100 K (~173 °C)
- 10,000 K (9,727 °C)
- 10,000,000 K (~10,000,000 °C)

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

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

- **Penetrates Earth’s Atmosphere?**
  - Y: Yes, N: No

**Radiation Type**
- **Radio:** $10^2$ m
- **Microwave:** $10^{-2}$ m
- **Infrared:** $10^{-8}$ m
- **Visible:** $5\times10^{-10}$ m
- **Ultraviolet:** $10^{-3}$ m
- **X-ray:** $10^{-10}$ m
- **Gamma ray:** $10^{-12}$ m

**Approximate Scale of Wavelength**
- **Buildings:** $10^{-2}$ m
- **Humans:** $10^{-9}$ m
- **Butterflies:** $10^{-10}$ m
- **Needle Point:** $10^{-12}$ m
- **Protozoans:** $10^{-13}$ m
- **Molecules:** $10^{-14}$ m
- **Atoms:** $10^{-15}$ m
- **Atomic Nuclei:** $10^{-16}$ m

**Frequency (Hz)**
- **$10^4$ Hz**: $10^3$ m
- **$10^8$ Hz**: $10^2$ m
- **$10^{12}$ Hz**: $10^{-1}$ m
- **$10^{15}$ Hz**: $10^{-2}$ m
- **$10^{16}$ Hz**: $10^{-3}$ m
- **$10^{18}$ Hz**: $10^{-4}$ m
- **$10^{20}$ Hz**: $10^{-5}$ m

**Temperature of objects at which this radiation is the most intense wavelength emitted**
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- **$100\text{ K}$**: $173 \degree$C
- **$10,000\text{ K}$**: $9,727 \degree$C
- **$10,000,000\text{ K}$**: $10,000,000 \degree$C

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*From: Electromagnetic Spectrum, Wikipedia Commons (2013)*
Spectral windows in Earth atmosphere

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

Also HUGE radio astronomy window

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(Use symmetry group theory)

- Ammonia NH₃ inversion doublet
- Nuclear spin hyperfine splitting
- CF₄ and SF₆ J-tunneling superfine splitting

2-state U(2)-spin and quasi-spin tunneling models
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U(m)*Sₙ analysis of multi-electron states

Rotational Energy Surface (RES) analysis of rovibronic tensor spectra
More Advanced Molecular Spectra Models

(Involves symmetry algebraic analysis)

2-well tunneling

Bohr mass-on-a-ring

1D harmonic oscillator

Coulomb PE models

2-state U(2)-spin and quasi-spin tunneling models

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

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Nuclear spin hyperfine splitting

Electronic spectra

Rotational spectra

Vibrational spectra

Potential
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$\infty$-Square Well has same levels but half as many states as Bohr Mass-On-a-Ring

Circumference Length = $L = 2\pi r = 2W$

Width = $W = L/2$

$n = 1$

$\pm 1$

$\pm 2$

$\pm 3$

$\pm 4$

$\pm 5$

$\pm 6$
Bohr Mass-On-a-Ring (model of rotation) and related ∞-Square Well (model of quantum dots)

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

Circumference Length = L = 2πr = 2W

Width = W = L/2

n = 1

n = 2

n = 3

Infinite Square Well

Bohr Rotor

L = 2W

m = ±1

m = ±2

m = ±3

m = 0

∅ = π

∅ = 0

∅ = -π

∞-well zero point energy

sin1∅

sin2∅

sin3∅

cos1∅

cos2∅

cos3∅

sin/∅

cos/∅

Monday, March 25, 2013
Bohr Mass-On-a-Ring (model of rotation) and related $\infty$-Square Well (model of quantum dots)

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

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

Width = $W = L/2$

Circumference Length = $L = 2\pi r = 2W$

n=1

n=2

n=3

$\phi = -\pi$

$\phi = 0$

$\phi = \pi$

Bohr Rotor

$m = \pm 3$

$m = \pm 2$

$m = \pm 1$

$m = 0$

Width = $W = L/2$

Circumference Length = $L = 2\pi r = 2W$

Infinite Square Well

$\psi_n = A \sin n\phi$
**Bohr Mass-On-a-Ring** (model of rotation) and related **∞-Square Well** (model of quantum dots)

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

**Bohr Ring** has sine and cosine standing and **\( e^{\pm im \phi} \) moving waves**:

\[
\psi_{\pm m} = A (\cos m \phi \pm i \sin m \phi) = A e^{\pm im \phi}
\]

**Circumference Length** = \( L = 2 \pi r = 2W \)

**Width** = \( W = L/2 \)

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

**Bohr Ring**

\[
\begin{align*}
\phi &=-\pi & &0 & &\pi \\
\phi &=-\pi & &0 & &\pi \\
\phi &=-\pi & &0 & &\pi
\end{align*}
\]
A sketch of modern molecular spectroscopy

*The frequency hierarchy*  
*Example of $16\mu m$ 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

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*Quantum levels of $\infty$-Square well and Bohr rotor*

*Example of CO$_2$ rotational $(\nu=0) \leftrightarrow (\nu=1)$ bands*

*Quantum dynamics of $\infty$-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 $\infty$-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
Quantum levels of $\infty$-Square well and Bohr rotor

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

$$\Rightarrow A \sin\left(\frac{n\pi x}{W}\right) \quad (n=1,2,3,\ldots,\infty)$$
Quantum levels of $\infty$-Square well and Bohr rotor

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

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

Gives energy levels:

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

$n=1 \ 1^2 \varepsilon_1$

$n=2 \ 2^2 \varepsilon_1$

$n=3 \ 3^2 \varepsilon_1$
Quantum levels of $\infty$-Square well and Bohr rotor

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

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Gives energy levels:

- $n=1 \quad 1^2 \varepsilon_1$
- $n=2 \quad 2^2 \varepsilon_1$
- $n=3 \quad 3^2 \varepsilon_1$

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

2nd transition energy $5\varepsilon_1$
Quantum levels of $\infty$-Square well and Bohr rotor

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

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

Gives energy levels:

- $n=1 \quad \varepsilon_1$
- $n=2 \quad 2^2 \varepsilon_1$
- $n=3 \quad 3^2 \varepsilon_1$

Zero-point energy $\varepsilon_1 = \frac{\hbar^2}{8MW^2} (For \infty$-$\text{-Square well}$)

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

2nd transition energy $5\varepsilon_1$

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

For $\infty$-Square well
Quantum levels of ∞-Square well and Bohr rotor

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

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

\[
= \frac{\hbar^2}{8M\pi^2 r^2} n^2 = \frac{\hbar^2}{2Mr^2} n^2 = \frac{\hbar^2}{2I} n^2 \quad \text{rotor energy}
\]

\( \varepsilon_1 = \frac{\hbar^2}{8MW^2} \quad \text{(For ∞-Square well)} \)

rotor energy \( B \)-constant:

\[
B = \frac{\hbar^2}{2I} = B
\]

- n=1 \( 1^2 \varepsilon_1 \)
- n=2 \( 2^2 \varepsilon_1 \)
- n=3 \( 3^2 \varepsilon_1 \)

2nd transition energy \( 5\varepsilon_1 \)

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

Zero-point energy \( \varepsilon_1 = \frac{\hbar^2}{8MW^2} \)
Quantum levels of $\infty$-Square well and Bohr rotor

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Gives energy levels:

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

rotor energy $B$-constant: $B = \frac{\hbar^2}{2 I} = B$ for $W = \pi r$
A sketch of modern molecular spectroscopy

The frequency hierarchy  
Example of 16 µm spectra of CF₄

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

Spectral windows in atmosphere due to molecules

Simple molecular-spectra models

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

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Example of CO$_2$ rotational ($\nu=0) \leftrightarrow (\nu=1)$ bands

Dipole transitions $J \rightarrow (J \pm 1)$ only

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

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Example of CO$_2$ rotational ($\nu=0) \leftrightarrow (\nu=1)$ bands

Dipole transitions $J \rightarrow (J \pm 1)$ only

$R(J_{\text{init}})$: Raise $J_{\text{init}}$
$Q$: status-Quo
$P$: Plummet

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

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

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

$\nu=60$MHz
$\lambda=5$cm
$B_0(1/\lambda)=0.2$cm$^{-1}$
A sketch of modern molecular spectroscopy

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Example of 16 μm spectra of CF₄

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Quantum dynamics of $\infty$-Square well and Bohr rotor
How what makes that “dipole” spectra?

“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

How what makes that “dipole” spectra?

ψ₂(\(x\))

ψ₁(\(x\))

ψ₁(\(x\))

ψ₂(\(x\))

"Slosh!"

"Slosh!"

\[ \Psi(x, 0) = \psi_1(x) + \psi_2(x) \]

\[ \Psi(x, t) = \psi_1(x) - \psi_2(x) \]

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

Rotating charge broadcasts* circularly polarized radiation

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

*Or receives (Depending on relative phase)
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- Farey-Sums and Ford-products
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Quantum dynamics of Double-well tunneling
Cheap models of NH$_3$ inversion doublet and general 2-state quantum systems

Other types of spectral splitting

Ammonia NH$_3$ inversion doublet

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...

Ammonia NH$_3$ inversion doublet

2-well tunneling

Other types of spectral splitting

fine structure rotational spectra

$n=0 \nu=0$ rotational levels

$\nu=0 \ J=0$

$\nu=1 \ J=1$

$\nu=2 \ J=2$

$\nu=3 \ J=3$

$\nu=4 \ J=4$

$\nu=5 \ J=5$

$\nu=6 \ J=6$

$\nu=7 \ J=7$

$\nu=8 \ J=8$

$\nu=9 \ J=9$

$\nu=10 \ J=10$

$\nu=11 \ J=11$

$\nu=12 \ J=12$

$\nu=13 \ J=13$

$\nu=14 \ J=14$

$\nu=15 \ J=15$

$\nu=16 \ J=16$

$\nu=17 \ J=17$

$\nu=18 \ J=18$

$\nu=19 \ J=19$

$\nu=20 \ J=20$

$\nu=21 \ J=21$

$\nu=22 \ J=22$

$\nu=23 \ J=23$

$\nu=24 \ J=24$

$\nu=25 \ J=25$

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$\nu=36 \ J=36$

$\nu=37 \ J=37$

$\nu=38 \ J=38$

$\nu=39 \ J=39$

$\nu=40 \ J=40$

$\nu=41 \ J=41$

$\nu=42 \ J=42$

$\nu=43 \ J=43$

$\nu=44 \ J=44$

$\nu=45 \ J=45$

$\nu=46 \ J=46$

$\nu=47 \ J=47$

$\nu=48 \ J=48$

$\nu=49 \ J=49$

$\nu=50 \ J=50$
Quantum dynamics of Double-well tunneling
Cheap models of NH$_3$ inversion doublet and general 2-state quantum systems

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

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

2-well tunneling
Quantum dynamics of Double-well tunneling
Cheap models of NH₃ inversion doublet and general 2-state quantum systems

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

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

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

Other types of spectral splitting

Ammonia NH₃ inversion doublet

(n = 0 or = 1) rotational levels

fine structure

rotational spectra

2-well tunneling

Other types of spectral splitting

Ammonia NH₃ inversion doublet

(n = 0 or = 1) rotational levels

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Cheap models of NH₃ inversion doublet and general 2-state quantum systems

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

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

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

...that tunnels out and “oozes” back & forth
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The frequency hierarchy Example of 16 \mu m spectra of CF₄

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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 \( \infty \)-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)

\[ \Delta t = \tau \]

1 cosine wave

fundamental period = \( \tau \)

\[ \Delta t = \tau / 2 \]

\( \tau / 2 \)

\[ \Delta t = \tau / 5 \]

\( \tau / 5 \)

\[ \Delta t = \tau / 10 \]

\( \tau / 10 \)

\[ \Delta t = \tau / 50 \]

this dimension is time

**Spectral width** (harmonic frequency range)

1 CW term

\[ \Delta \nu = \nu = 1/\tau \]

\[ \Delta \nu = 2\nu \]

(1 CW term, 4 times fundamental frequency)

\[ \Delta \nu = 5\nu \]

(1 CW term, 5 times fundamental frequency)

\[ \Delta \nu = 10\nu \]

(1 CW term, 10 times fundamental frequency)

\[ \Delta \nu = 50\nu \]

(1 CW term, 50 times fundamental frequency)

2 CW terms

\[ \Delta \nu = 2\nu \]

(2 CW terms, up to 2nd octave)

5 CW terms

\[ \Delta \nu = 5\nu \]

(5 CW terms, up to 5th octave)

10 CW terms

\[ \Delta \nu = 10\nu \]

(10 CW terms, up to 10th octave)

50 CW terms

\[ \Delta \nu = 50\nu \]

(50 CW terms, up to 50th octave)
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)

- \( \Delta t = \tau \)
- \( \Delta t = \tau / 2 \)
- \( \Delta t = \tau / 5 \)
- \( \Delta t = \tau / 10 \)
- \( \Delta t = \tau / 50 \)

**Spectral width** (harmonic frequency range)

- 1 CW term
  \[ \Delta \nu = \nu = 1/\tau \]
- 2 CW terms
  \[ \Delta \nu = 2\nu \]
- 5 CW terms
  \[ \Delta \nu = 5\nu \]
- 10 CW terms
  \[ \Delta \nu = 10\nu \]
- 50 CW terms
  \[ \Delta \nu = 50\nu \]

**Fourier-Heisenberg product:** \( \Delta t \cdot \Delta \nu = 1 \) (time-frequency uncertainty relation)
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

A lesson in quantum interference

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

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

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

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

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$$a_n = \langle \varepsilon_n | a \rangle = \left( \frac{2}{W} \right) \sin k_n a \quad (k_n = n\pi/W)$$

$$\Psi (x) = \frac{2}{W} \sum_{n=1}^{\infty} \sin k_n a \sin k_n x$$

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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
\]

\[a_n = \langle \varepsilon_n|a \rangle = \left(\frac{2}{W}\right) \sin k_n a \quad (k_n = n\pi/W)\]

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

\[
\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} \frac{\Delta n}{\Delta k} \sin ka \sin kx
\]

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

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

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

$\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$

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

Fig. 12.2.2 Ultra-thin prisoner $M$.

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

$$\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

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

$$\Psi(x) \cong \frac{2}{\pi} \frac{K_{\text{max}}}{K_{\text{max}}} \int_{0}^{K_{\text{max}}} dk \sin ka \sin kx = \frac{1}{\pi} \frac{K_{\text{max}}}{K_{\text{max}}} \int_{0}^{K_{\text{max}}} dk \left( \cos k(x - a) - \cos k(x + a) \right)$$

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\[
\delta(x - a) = \langle x | a \rangle = \sum_{n=1}^{\infty} \langle x | \mathcal{E}_n \rangle \langle \mathcal{E}_n | a \rangle = \sum_{n=1}^{\infty} a_n \sin k_n x
\]

\[a_n = \langle \mathcal{E}_n | a \rangle = \frac{2}{W} \sin k_n a \quad (k_n = n\pi/W)\]

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

\[\rightarrow \frac{2}{W} K_{\text{max}} \int_{0}^{K_{\text{max}}} \frac{dk}{\Delta k} \frac{\Delta n}{\Delta k} \sin ka \sin kx\]

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

\[\Psi(x) \equiv \frac{2}{\pi} K_{\text{max}} \int_{0}^{K_{\text{max}}} dk \sin ka \sin kx = \frac{1}{\pi} K_{\text{max}} \int_{0}^{K_{\text{max}}} dk \left( \cos k(x - a) - \cos k(x + a) \right)\]

\[\equiv \frac{\sin K_{\text{max}}(x - a)}{\pi(x - a)} - \frac{\sin K_{\text{max}}(x + a)}{\pi(x + a)} \equiv \frac{\sin K_{\text{max}}(x - a)}{\pi(x - a)} \quad \text{for: } x \approx a\]
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$$\delta(x - a) = \langle x | a \rangle = \sum_{n=1}^{\infty} \langle x | \varepsilon_n \rangle \langle \varepsilon_n | a \rangle = \sum_{n=1}^{\infty} a_n \sin k_n x$$

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

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

$$\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

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

$$\Psi(x) \equiv \frac{2}{\pi} \int_{0}^{K_{\text{max}}} dk \sin ka \sin kx = \frac{1}{\pi} \int_{0}^{K_{\text{max}}} dk \left( \cos k(x - a) - \cos k(x + a) \right)$$

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

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and “inside” $K$ get "smothered" by interference with neighbors.
A sketch of modern molecular spectroscopy

The frequency hierarchy
Example of 16 µm spectra of CF₄
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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
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level). The fundamental zero-point period $\tau_1 = 1/\nu_1$.

- $t = 0.0004\tau_1$
- $t = 0.0008\tau_1$
- $t = 0.0012\tau_1$
- $t = 0.0016\tau_1$
- $t = 0.0020\tau_1$
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level).

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

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

$\text{Re}\Psi(x,t)$  $\text{Im}\Psi(x,t)$

Envelope $|\Psi(x,t)|$
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level).

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

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

**$\varepsilon_n$-level classical velocity:**

$$v_n = \frac{d\omega_n}{dk} = \frac{1}{h}\frac{d\varepsilon_n}{dk}$$

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

$$= \frac{h2k_n}{2M} = \frac{hn\pi}{MW} = \frac{hn}{2MW}$$
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level).

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

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

**$\varepsilon_n$-level classical velocity:**

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

**$\varepsilon_n$-level classical round trip time $T_n(2W)$**

$$T_n(2W) = \frac{2W}{V_n} = 2W \frac{2MW}{\hbar n} = \frac{4MW^2}{\hbar n} = \frac{1}{2n} \frac{8MW^2}{h} = \frac{\tau_1}{2n}$$
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level). The fundamental zero-point period $\tau_1 = 1/\nu_1$ is given by

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

**$\varepsilon_n$-level classical velocity:**

$$V_n = \frac{d\omega_n}{dk} = \frac{d\varepsilon_n}{dk} = \frac{h^2}{2hM} \frac{dk}{dk} = \frac{h2k_n}{2M} = \frac{hn\pi}{MW} = \frac{hn}{2MW}$$

**$\varepsilon_n$-level classical round trip time $T_n(2W)$**

$$T_n(2W) = \frac{2W}{V_n} = 2W \frac{2MW}{hn} = \frac{4MW^2}{hn} = \frac{1}{2n} \frac{8MW^2}{h} = \frac{\tau_1}{2n}$$

**$\varepsilon_n$-level 1-way time $T_n(W)$**

$$T_n(W) = T_n(2W) / 2 = \frac{\tau_1}{4n} \left(= 0.0025 \tau_1 \text{ for } n=100\right)$$
Wavepacket explodes!

Time given in units of period $\tau_1$ (slowest phasor of ground level).

fundamental zero-point period $\tau_1 = \frac{1}{\nu_1}$ is

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

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

$\varepsilon_n$-level classical velocity:

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

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

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

$\varepsilon_n$-level classical round trip time $T_n(2W)$

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

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

$\varepsilon_n$-level 1-way time $T_n(W)$

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

($= 0.0025 \tau_1$ for: $n=100$)

"Last-in-first-out" effect
A sketch of modern molecular spectroscopy

The frequency hierarchy
Example of 16µm spectra of CF₄
Units of frequency (Hz), wavelength (m), and energy (eV)
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Wavepacket explodes! (Then revives)

Zero-point period $\tau_1$ is just enough time for "particle" in $\epsilon_n$-level to make $2n$ round trips.

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

In time $\tau_1$ ground $\epsilon_1$-level particle does 2 round trips,
- $\epsilon_2$-level particle makes 4 round trips,
- $\epsilon_3$-level particle makes 6 round trips,..

At time $\tau_1$, $M$ undergoes a full revival and "unexplodes" into his original spike at $x=0.2W$, $t = 1.0000\tau_1 = 3.0\tau_{\text{beat}}$
Wavepacket explodes! (Then revives)

Zero-point period $\tau_1$ is just enough time for "particle" in $\varepsilon_n$-level to make $2n$ round trips.

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

In time $\tau_1$ ground $\varepsilon_1$-level particle does 2 round trips,
- $\varepsilon_2$-level particle makes 4 round trips,
- $\varepsilon_3$-level particle makes 6 round trips,..

At time $\tau_1$, $M$ undergoes a full revival and "unexplodes" into his original spike at $x=0.2W$.

\[ t = 0.5000\tau_1 = 1.5\tau_{\text{beat}} \]

\[ t = 1.0000\tau_1 = 3.0\tau_{\text{beat}} \]

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 $\tau_{1/n} M$ 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.*
A sketch of modern molecular spectroscopy

The frequency hierarchy  Example of $16\mu m$ spectra of $CF_4$
Units of frequency (Hz), wavelength (m), and energy (eV)
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Quantum “revivals” of gently*localized rotor waves
A lesson in quantum number theory

*gently means gently-truncated Gaussian distributions
\[ \Delta m = 9 \]

\[ 2\Delta x = 4\% \]

Time \( t \) (units of fundamental period \( \tau_1 \))

Coordinate \( \phi \) (units of \( 2\pi \))

(Imagine "wrap-around" \( \phi \)-coordinate)

[Harter, J. Mol. Spec. 210, 166-182 (2001)]
$N$-level-rotor pulse wave and revival-beat wave dynamics

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

Zeros (clearly) and “particle-packets” (faintly) have paths labeled by fraction sequences like:

$\frac{0}{1} \frac{1}{1} \frac{2}{1} \frac{3}{1} \frac{4}{1} \frac{5}{1} \frac{6}{1}$

$\frac{0}{7} \frac{1}{7} \frac{2}{7} \frac{3}{7} \frac{4}{7} \frac{5}{7} \frac{6}{7}$

Time $t$

(units of $\tau_1$)

$\Delta m = 9$

$2\Delta x = 4\%$

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

Coordinate $\phi$

(units of $2\pi$)
Note, for example series:

0 1 2 3 4 5 6 1
7 7 7 7 7 7 7 1

Zeros start here
Wave packet starts here
Zeros start here
A sketch of modern molecular spectroscopy

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Farey-Sums and Ford-products
Ford Circles and Farey-Trees
Farey Sum algebra of revival-beat wave dynamics

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

Time $t$
(units of $\tau_1$)

$(n_1 + 1)/d_1$

$(n_2 - 1)/d_2$

$1/d_1$

$1/2$

$0/1$

$1/2$

$1/4$

$0$

$-1/4$

$-1/2$

Coordinate $\phi$
(units of $2\pi$)

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

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

$n_1/d_1$ and $n_2/d_2$ path fractions numerator/denominator
Farey Sum algebra of revival-beat wave dynamics
Label by numerators $N$ and denominators $D$ of rational fractions $N/D$

Time $t$
(units of $\tau_1$)

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

($\phi$ intersection point
(Binary-Cross)

$14/d_1$

$13/d_1$

$12/d_1$

$1/2 - \phi \otimes = 1/d_2$

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

$n_1 d_1 - t \otimes = -1/d_1$

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

Coordinate $\phi$
(units of $2\pi$)

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

$0/1$

$1/2$

$0$

$1/4$

$1/4$

$-1/2$

$-1/4$

$-1/4$

$-1/2$


[John Farey, Phil. Mag. (1816)]
A sketch of modern molecular spectroscopy

*The frequency hierarchy*  Example of 16µm spectra of CF₄

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

*Spectral windows in atmosphere due to molecules*

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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

(a)

Denominator Axis D

Numerator Axis N

Unit Real Interval

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

$\mathbf{v}_f = (1,1)$
Farey Sum related to vector sum and Ford Circles

1/1-circle has diameter $I$

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 $1/d^2$

\[
\begin{align*}
\text{Numerator Axis N} & \\
\text{Denominator Axis D} & \\
\text{v}_0 &= (0, 1) \\
\text{v}_{1/2} &= (1, 2) \\
\text{v}_{1/3} &= (1, 3) \\
\text{v}_{2/5} &= (2, 5) \\
\end{align*}
\]
**Farey Tree up to \( D=8 \) spectral half-width**

| \( D \leq 1 \) | \( \frac{0}{1} \) | \( 1 \) | \( \frac{1}{1} \)  
| \( D \leq 2 \) | \( \frac{0}{1} \) | \( \frac{1}{2} \) | \( \frac{1}{1} \)  
| \( D \leq 3 \) | \( \frac{0}{1} \) | \( \frac{1}{3} \) | \( \frac{2}{3} \) | \( \frac{1}{1} \)  
| \( D \leq 4 \) | \( \frac{0}{1} \) | \( \frac{1}{4} \) | \( \frac{2}{3} \) | \( \frac{3}{4} \) | \( \frac{1}{1} \)  
| \( D \leq 5 \) | \( \frac{0}{1} \) | \( \frac{1}{5} \) | \( \frac{2}{3} \) | \( \frac{3}{4} \) | \( \frac{4}{5} \) | \( \frac{1}{1} \)  
| \( D \leq 6 \) | \( \frac{0}{1} \) | \( \frac{1}{6} \) | \( \frac{2}{3} \) | \( \frac{3}{4} \) | \( \frac{4}{5} \) | \( \frac{5}{6} \) | \( \frac{1}{1} \)  
| \( D \leq 7 \) | \( \frac{0}{1} \) | \( \frac{1}{7} \) | \( \frac{2}{3} \) | \( \frac{3}{4} \) | \( \frac{4}{5} \) | \( \frac{5}{6} \) | \( \frac{6}{7} \) | \( \frac{1}{1} \)  
| \( D \leq 8 \) | \( \frac{0}{1} \) | \( \frac{1}{8} \) | \( \frac{2}{3} \) | \( \frac{3}{4} \) | \( \frac{4}{5} \) | \( \frac{5}{6} \) | \( \frac{6}{7} \) | \( \frac{7}{8} \) | \( \frac{1}{1} \)  

Monday, March 25, 2013
(Quantum computer simulation)

That makes an ∞-ly deep “3D-Magic-Eye” picture
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

A lesson in quantum uncertainty

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

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

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

$$\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

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

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and “inside” K get "smothered" by interference with neighbors.
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

*A lesson in quantum uncertainty*

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

\[
a_n = \langle \varepsilon_n \mid a \rangle = \frac{2}{W} \sin k_n a \quad (k_n = n\pi/W)
\]

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

\[
\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx
\]

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

\[\Psi(x) \text{ peaks at } (x=a) \text{ and goes to zero on either side at } (x=a\pm\Delta x) \text{ with half-width } \Delta x\]

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and "inside" $K$ get "smothered" by interference with neighbors.
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$$a_n = \langle \varepsilon_n | a \rangle = (2/W) \sin k_n a \quad (k_n = n\pi/W)$$

$$\Psi(x) = \frac{2}{W} \sin k_n a \sin k_n x$$

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

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

$$\Psi(x) \text{ peaks at } (x=a) \text{ and goes to zero on either side at } (x=a \pm \Delta x) \text{ with } \text{half-width } \Delta x$$

$$\sin K_{\text{max}} (\Delta x) = 0 \text{, which implies: } (\Delta x)K_{\text{max}} = \pm \pi$$

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and "inside" $K$ get "smothered" by interference with neighbors.
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

A lesson in quantum uncertainty

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

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

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

$$
\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx
$$

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

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

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

$\Psi(x)$ peaks at $(x=a)$ and goes to zero on either side at $(x=a\pm \Delta x)$ with half-width $\Delta x$

$\sin K_{\text{max}}(\Delta x) = 0$, which implies: $(\Delta x)K_{\text{max}} = \pm \pi$, or: $\Delta x = \pm \pi / K_{\text{max}}$

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and “inside” $K$ get "smothered" by interference with neighbors.
Quantum “blasts” of strongly localized $\infty$-well or rotor waves

A lesson in quantum uncertainty

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

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

$$\rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx$$

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

$$\Psi(x) \approx \sum_{n}^{N_{\text{max}}} a_n (x-a)$$

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

$$\Psi(x) \text{ peaks at } (x=a) \text{ and goes to zero on either side at } (x=a \pm \Delta x) \text{ with half-width } \Delta x$$

$$\sin K_{\text{max}} (\Delta x)=0, \text{ which implies: } (\Delta x)K_{\text{max}} = \pm \pi, \text{ or: } \Delta x = \pm \pi / K_{\text{max}}$$

$$\Delta x \cdot |K_{\text{max}}| = \Delta x \cdot \Delta k = \pi$$

"Last-in-first-out" effect. Last $K_{\text{max}}$-value dominates and “inside” K get "smothered" by interference with neighbors.
Quantum “blasts” of strongly localized ∞-well or rotor waves

A lesson in quantum uncertainty

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

\[ a_n = \langle \xi_n | a \rangle = (2/W) \sin k_n a \quad (k_n = n\pi/W) \]

\[ \Psi(x) = \frac{2}{W} \sum_{n=1}^{N_{\text{max}}} \sin k_n a \sin k_n x \]

\[ \rightarrow \frac{2}{W} \int_{0}^{K_{\text{max}}} dk \frac{\Delta n}{\Delta k} \sin ka \sin kx \]

\[ = \frac{2}{W} \frac{K_{\text{max}}}{\pi} \int_{0}^{\infty} dk \sin ka \sin kx \]

Fig. 12.2.2 Ultra-thin prisoner M.

Initial wavepacket combination of 100 energy states.

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

\[ \Psi(x) \text{ peaks at } (x=a) \text{ and goes to zero on either side at } (x=a\pm\Delta x) \text{ with half-width } \Delta x \]

\[ \sin K_{\text{max}}(\Delta x) = 0, \text{ which implies: } (\Delta x)K_{\text{max}} = \pm \pi, \text{ or: } \Delta x = \pm \pi / K_{\text{max}} \]

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

"Last-in-first-out" effect. Last \( K_{\text{max}} \)-value dominates and “inside” \( K \) get "smothered" by interference with neighbors.
Polygonal geometry of $U(2) \supseteq C_N$ 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
$\infty$-Square well PE versus Bohr rotor
$\sin \frac{Nx}{x}$ wavepackets bandwidth and uncertainty
$\sin \frac{Nx}{x}$ 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

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

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

**Complete the square in exponent to simplify \(\phi\)-angle wavefunction.**
Gaussian wave-packet bandwidth and uncertainty

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

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

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

Complete the square in exponent to simplify $\phi$-angle wavefunction.
Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

Complete the square in exponent to simplify $\phi$-angle wavefunction.
Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

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

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

Complete the square in exponent to simplify $\phi$-angle wavefunction.
Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

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

$$A(\Delta m, \phi) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta m} - \frac{\Delta m \phi}{2}\right)^2} \rightarrow \int_{-\infty}^{\infty} dk e^{-\left(\frac{k}{\Delta m} - \frac{\Delta m \phi}{2}\right)^2} \quad (\Delta m >> 1)$$

$m=0, \pm 1, \pm 2, \pm 3, \ldots$ are momentum quanta in wavevector formula: $k_m = 2\pi m / L \quad (k_m = m \quad if: \ L = 2\pi)$
**Gaussian wave-packet bandwidth and uncertainty**

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

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

\[
= \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta m}\right)^2 + i m \phi + \left(\frac{\Delta m \phi}{2}\right)^2 + \left(\frac{\Delta m}{2}\phi\right)^2}
\]

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

\[
= \frac{A(\Delta m, \phi)}{2\pi} e^{\left(\frac{\Delta m}{2}\phi\right)^2}
\]

\[
A(\Delta m, \phi) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta m} - i\frac{\Delta m}{2}\phi\right)^2} \Delta m \rightarrow \int_{-\infty}^{\infty} dk \, e^{-\left(\frac{k}{\Delta m} - i\frac{\Delta m}{2}\phi\right)^2}
\]

[let: \( K = \frac{k}{\Delta m} - i\frac{\Delta m}{2}\phi \) so: \( dk = \Delta m \, dK \)]

\( m = 0, \pm 1, \pm 2, \pm 3, \ldots \) are momentum quanta in wavevector formula: \( k_m = 2\pi m / L \)  \( (k_m = m \text{ if: } L = 2\pi) \)
Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

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

$$A(\Delta m, \phi) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m-i\Delta m \phi}{\Delta m \phi}\right)^2} \stackrel{\Delta m \gg 1}{\longrightarrow} \int_{-\infty}^{\infty} dk \ e^{-\left(\frac{k-i\Delta m \phi}{\Delta m \phi}\right)^2}$$

let: $$K = \frac{k}{\Delta m} - i \frac{\Delta m \phi}{2} \text{ so: } dk = \Delta m \ dK$$

then: $$A(\Delta m, \phi) \approx \Delta m \int_{-\infty}^{\infty} dK \ e^{-\left(K\right)^2} = \Delta m \sqrt{\pi}$$

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

Complete the square in exponent to simplify $\phi$-angle wavefunction.

Gaussian integral:

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

$$= \sqrt{\int_{0}^{2\pi} \int_{0}^{\infty} e^{-r^2} \ r \ dr \ d\theta} = \sqrt{2\pi} \int_{0}^{\infty} e^{-r^2} \frac{dr^2}{2} = \sqrt{\pi}$$
Gaussian wave-packet bandwidth and uncertainty

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

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

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

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

\[ = \frac{A(\Delta m, \phi)}{2\pi} e^{-\left(\frac{\Delta m}{2}\phi\right)^2} \]

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

\[ \qquad \longrightarrow_{\Delta m \gg 1} \int_{-\infty}^{\infty} dk \ e^{-\left(\frac{k}{\Delta m} - i\frac{\Delta m}{2}\phi\right)^2} \]

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

\[ m=0, \pm 1, \pm 2, \pm 3, \ldots \text{ are momentum quanta in wavevector formula: } k_m = \frac{2\pi m}{L} \quad (k_m=m \text{ if: } L=2\pi) \]
Gaussian wave-packet bandwidth and uncertainty

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

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

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

\[
= \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta m} - \frac{\Delta m}{2}\phi\right)^2} - \left(\frac{\Delta m}{2}\phi\right)^2 e^{-\left(\frac{\Delta m}{2}\phi\right)^2}
\]

\[
A(\Delta m,\phi) = \sum_{m=-\infty}^{\infty} e^{-\left(\frac{m}{\Delta m} - \frac{\Delta m}{2}\phi\right)^2} \rightarrow \int_{-\infty}^{\infty} dk e^{-\left(\frac{k}{\Delta m} - \frac{\Delta m}{2}\phi\right)^2}
\]

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

\(m=0, \pm1, \pm2, \pm3,...\) are momentum quanta in wavevector formula: \(k_m = \frac{2\pi m}{L}\) (\(k_m = m\) if \(L = 2\pi\))

Complete the square in exponent to simplify \(\phi\)-angle wavefunction.

\[
\Psi(\phi,t=0) = \frac{A(\Delta m,\phi)}{2\sqrt{\pi}} e^{-\left(\frac{\Delta m}{2}\phi\right)^2}
\]

It is a Gaussian distribution, too

\[
\Psi(\phi,t=0) = \frac{\Delta m}{2\sqrt{\pi}} e^{-\left(\frac{\phi}{\Delta m}\right)^2}
\]

where: \(\Delta = \frac{2}{\Delta m}\) or: \(\Delta \Delta_m = 2\)
Suppose we excite a Gaussian combination of Bohr momentum-\(m\) plane waves:

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

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

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

where: \(\Delta_m = \frac{2}{\Delta_m}\) or: \(\Delta_m\Delta_m = 2\)

**Gaussian uncertainty relation**

(Compare to \(\Delta x \cdot \Delta k = \pi\) for \(\infty\)-Well)

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

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

\[
E_m = (\hbar k_m)^2/2M = m^2 [\hbar^2/2ML^2] = m^2 \hbar \nu_1 = m^2 \hbar \omega_1
\]

**Fundamental Bohr \(\angle\) -frequency** \(\omega_1 = 2\pi \nu_1\) and lowest transition (beat) frequency \(\nu_1 = (E_1 - E_0)/\hbar\)
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’. 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.

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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).