Molecules and Molecular Spectroscopy: Learning about molecules from Quantum theory

and

Learning about Quantum theory from molecules William G. Harter Research Sketch 11.17.17

A sketch of modern molecular spectroscopy The molecular frequency hierarchy Units of frequency (Hz), wavelength (m), energy (eV), and wavenumber (cm⁻¹) Spectral windows in atmosphere due to molecules Example of~16μm (670cm⁻¹) spectral hierarchy of CO₂ (simple) Example of~16μm (631cm⁻¹) spectral hierarchy of CF₄ (complicated) Example of ~16μm (615cm⁻¹) spectral hierarchy of SF₆ (really complicated) Rotational Energy Surface (RES) analysis, J-vector geometry, and tunneling

Nuclear spin hyperfine effects rule mol-spec.

Quantum "revivals" of gently localized rotor waves: Bohr-rotor wave dynamics gives lessons for quantum number theory Gaussian wave-packet bandwidth and uncertainty Gaussian Bohr-rotor revivals and quantum fractals Understanding fractals using geometry of fractions (Rationalizing rationals) Farey-Sums and Ford-products Ford Circles and Farey-Trees

The molecular frequency hierarchy

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





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*Example of CO*₂ *rotational* $(v=0) \Leftrightarrow (v=1)$ *bands*



*Example of CO*₂ *rotational* $(v=0) \Leftrightarrow (v=1)$ *bands*



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 Gordon Drake Editor (2005)



Example of ~16 μ *m* (615*cm*⁻¹) *spectral hierarchy of* SF₆ (*really* complicated)



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Rotational Energy Surface (RES) analysis, J-vector geometry, and tunneling

<H $> \sim v_{vib}$ +BJ(J+1)+<H^{Scalar Coriolis}>+<H^{Tensor Centrifugal}>+<H^{Tensor Coriolis}>+<H^{Nuclear Spin}>+...















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Some examples of Bose Exclusion

Spherical Top Molecules with Spin-0 Nuclei



Some examples of Fermi (non) Exclusion



Some examples of Fermi (non) Exclusion

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













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

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

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



Farey Sum related to vector sum and *Ford Circles*

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

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

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

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







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Unifying Relativity with Quantum Theory (Why a *Men In Black* candidate shot little Suzy) The simplest molecule: A pair of head-on lasers gives lessons for relativistic quantum theory Light wave zeros draw Minkowski coordinate grid Relawavity geometry of waves defines space-time warp ...and per-space-time quantum mechanics



Men In Black candidate shot little Suzy

Bad Suzy! Relativity and Quantum Theory need to be unified in *one* book *half* the size of those old tomes!

It's called *Relawavity*.







Three scenarios that look the same to Bob





<u>Much</u> cheaper to do the 3rd scenario!\$!





<u>Two Famous-Name Coe</u> Review of Lect. 30 p.106	effici	<u>ents</u>	$\frac{Time}{(unit)}$ $\lambda_A = 1/2$	e ct' s of 2μm)	2		He. Min 180	rman nkowski 54-1909	Λ
Albert Einstein 1859-1955					1.5				
This number is called an: Einstein time-dilation (dilated by 25% here) This number					-0 /group=	v'phase= 0.8	-1.25	Sp (1) λ_A	o <mark>ace x'</mark> units of =1/2μm)
is called a: LOPENTZ length-contraction			-0.5			5		1.5	
(contracted by 20% here)	phase	$b_{\scriptscriptstyle RED}^{\scriptscriptstyle Doppler}$	$\frac{c}{V_{phase}}$	$rac{\kappa_{phase}}{\kappa_{A}}$	$rac{{m au}_{phase}}{{m au}_A}$	$\left(egin{array}{c} v_{phase} \ v_A \end{array} ight)$	$rac{\lambda_{phase}}{\lambda_A}$	V _{phase} C	$b_{\scriptscriptstyle BLUE}^{\scriptscriptstyle Doppler}$
Hendrik A. Lorentz 1853-1928	group	$\frac{1}{b_{\textit{BLUE}}^{Doppler}}$	$rac{V_{group}}{c}$	$rac{oldsymbol{v}_{group}}{oldsymbol{v}_{A}}$	$ \underbrace{ \frac{\lambda_{group}}{\lambda_A} } $	$\frac{\kappa_{group}}{\kappa_A}$	$rac{oldsymbol{ au}_{group}}{oldsymbol{ au}_A}$	$rac{c}{V_{group}}$	$rac{1}{b_{\scriptscriptstyle RED}^{\scriptscriptstyle Doppler}}$
Old Evaluitor A Netwice	rapidity ρ	$e^{- ho}$	anh ho	$\sinh ho$	$\operatorname{sech}\rho$	$\cosh \rho$	$\mathrm{csch} ho$	$\mathrm{coth}\rho$	$e^{+ ho}$
Dia-Fashionea Notation	$\beta = \frac{u}{c}$	$\sqrt{\frac{1-\beta}{1+\beta}}$	$\frac{\beta}{1}$	$\frac{1}{\sqrt{\beta^{-2}-1}}$	$\frac{\sqrt{1-\beta^2}}{1}$	$\frac{1}{\sqrt{1-\beta^2}}$	$\frac{\sqrt{\beta^{-2}-1}}{1}$	$\frac{1}{\beta}$	$\sqrt{\frac{1+eta}{1-eta}}$
<u>(Expanded Table)</u>	value for $\beta = 3/5$	$\frac{1}{2} = 0.5$	$\frac{3}{5} = 0.6$	$\frac{3}{4} = 0.75$	$\frac{4}{5} = 0.80$	$\frac{5}{4} = 1.25$	$\frac{4}{3}$ =1.33	$\frac{5}{3} = 1.67$	$\frac{2}{1} = 2.0$



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Relawavity geometry of waves defines space-time warp

...and per-space-time quantum mechanics

Physics of relativity is mostly simple trigonometry of optical wave interference! And, it derives fundamentals of quantum theory, too!

Trigonometric road maps



Physics of relativity is mostly simple trigonometry of optical wave interference!

RelaWavity Web Simulation Relations between Hypergeometric and Hypergeometric functions



Trigonometric road maps

Need to see how trig road maps match the physical maps on next 2 pages.







group	$b_{\scriptscriptstyle RED}^{\scriptscriptstyle Doppler}$	V _{group} C	$rac{oldsymbol{v}_{group}}{oldsymbol{v}_A}$	$rac{\lambda_{group}}{\lambda_A}$	$rac{\kappa_{group}}{\kappa_A}$	$rac{ au_{group}}{ au_A}$	$\frac{c}{V_{group}}$	$b_{\scriptscriptstyle BLUE}^{\scriptscriptstyle Doppler}$
phase	$rac{1}{b_{BLUE}^{Doppler}}$	$\frac{c}{V_{phase}}$	$rac{\kappa_{phase}}{\kappa_{A}}$	$rac{{m au}_{_{phase}}}{{m au}_{_{A}}}$	$rac{oldsymbol{v}_{phase}}{oldsymbol{v}_A}$	$rac{\lambda_{phase}}{\lambda_A}$	V _{phase} C	$rac{1}{b_{\scriptscriptstyle RED}^{\scriptscriptstyle Doppler}}$
rapidity ρ	$e^{- ho}$	$tanh \rho$	$\sinh ho$	$\operatorname{sech} \rho$	$\cosh ho$	$\mathrm{csch} ho$	$\operatorname{coth} \rho$	$e^{+ ho}$
stellar \forall angle σ	$1/e^{+\rho}$	$\sin \sigma$	$tan \sigma$	$\cos \sigma$	$\sec \sigma$	$\cot \sigma$	csco	1/ <i>e</i> ^{-p}
$\beta \equiv \frac{u}{c}$	$\sqrt{\frac{1-\beta}{1+\beta}}$	$\frac{\beta}{1}$	$\frac{1}{\sqrt{\beta^{-2}-1}}$	$\frac{\sqrt{1-\beta^2}}{1}$	$\frac{1}{\sqrt{1-\beta^2}}$	$\frac{\sqrt{\beta^{-2}-1}}{1}$	$\frac{1}{\beta}$	$\sqrt{\frac{1+eta}{1-eta}}$
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velocity momentum Lagrangian Hamiltonian

