MATHEMATICAL FRONTIERS

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Board on Mathematical Sciences & Analytics

MATHEMATICAL FRONTIERS
2019 Monthly Webinar Series, 2-3pm ET

February 12: *Machine Learning for Materials Science**

March 12: *Mathematics of Privacy**

April 9: *Mathematics of Gravitational Waves**

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** Webinar posted*

Made possible by support for BMSA from the
National Science Foundation
Division of Mathematical Sciences
and the
Department of Energy
Advanced Scientific Computing Research

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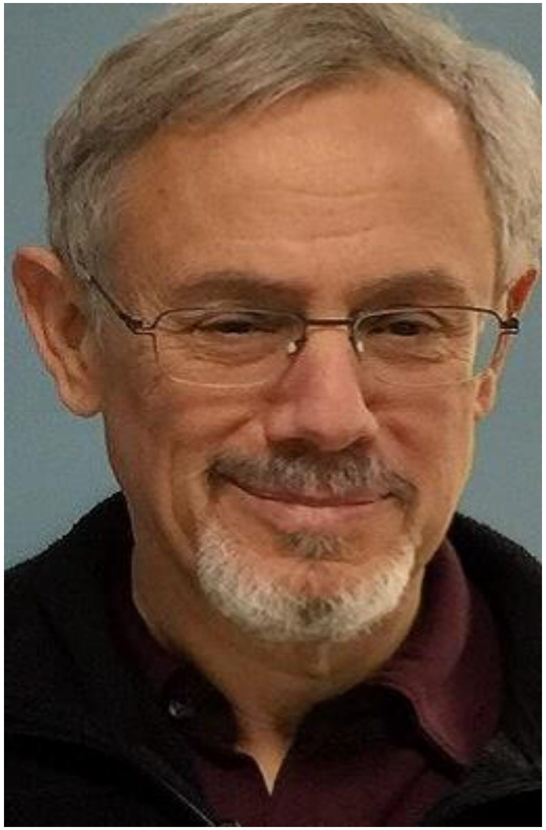
MATHEMATICAL FRONTIERS
Mathematics of Quantum Physics

Rick Heller,
Harvard University

Xiaosong Li,
University of Washington



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MATHEMATICAL FRONTIERS
Mathematics of Quantum Physics

Rick Heller,
Harvard University

Abbott and James Lawrence Professor of Chemistry and Professor of Physics

Quantum Physics and Mathematics

Wave theory

- We should not forget that quantum theory is "just" another wave theory.
- Much of classical wave physics (sound, water, earthquake,…) applies to quantum waves, but the classical waves came much earlier

Quantum Physics in many dimensions has been a wellspring of mathematics

- quantum entanglement, entropy
- decoherence,
- quantum information theory,
- quantum computing,
- quantum chaos theory and semiclassical theory
- string theory

All these aspects and many more are a wellspring of new mathematics

String theory

- String strives to be the ultimate quantum theory.
- Robbert Dijkgraaf writes: “The number of [mathematical] disciplines that it [string theory] touches is dizzying: analysis, geometry, algebra, topology, representation theory, combinatorics, probability — the list goes on and on.”

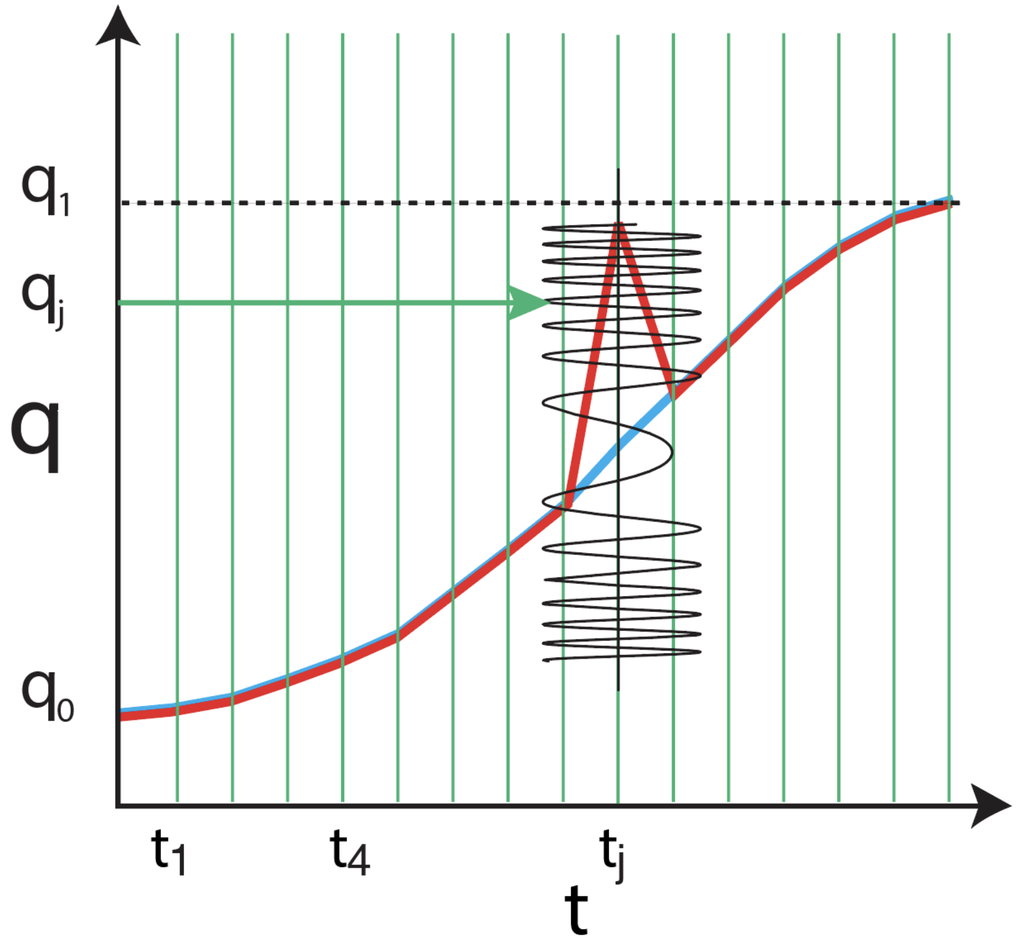
Example-Green function

- The Dirac delta function, with antecedents from the work of Cauchy, Poisson, Kirchhoff, Green, Helmholtz, Kelvin
- Feynman path integral
- Stationary phase evaluation (Stokes, Kelvin) of the path integral leads to the (semi)-classical limit and a window on our reality
- The Feynman path integral is darn close to Huygen's principle and Kirchhoff diffraction theory

Feynman path integral

$$
\begin{aligned}
S_j \equiv S(q_j, q_{j+1}, \tau) &= \frac{m(q_j - q_{j+1})^2}{2\tau} - V(q_{j+1})\tau \\
G(q, q', t) &= \lim_{N\to\infty} \int \cdot \int \prod_j dq_j \; e^{\,i\sum_j S_j/\hbar} \\
&= \sum_{All\ \ Paths} e^{iS_{path}/\hbar}
\end{aligned}
$$

Stationary phase on the Feynman path integral – the classical paths emerge



Quantum Chaos

- Suppose the classical path is (deterministically) chaotic. Does the stationary phase still work?
- This leads to
  - Van Vleck-Morette-Gutzwiller semiclassical propagator
  - Selberg trace formula
  - Gutzwiller trace formula
  - Deep connections between quantum chaos, random matrices, and distribution of prime numbers

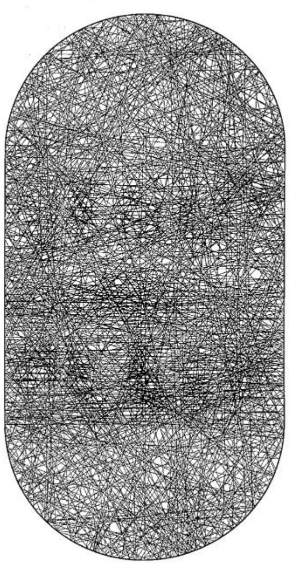
Quantum Chaos

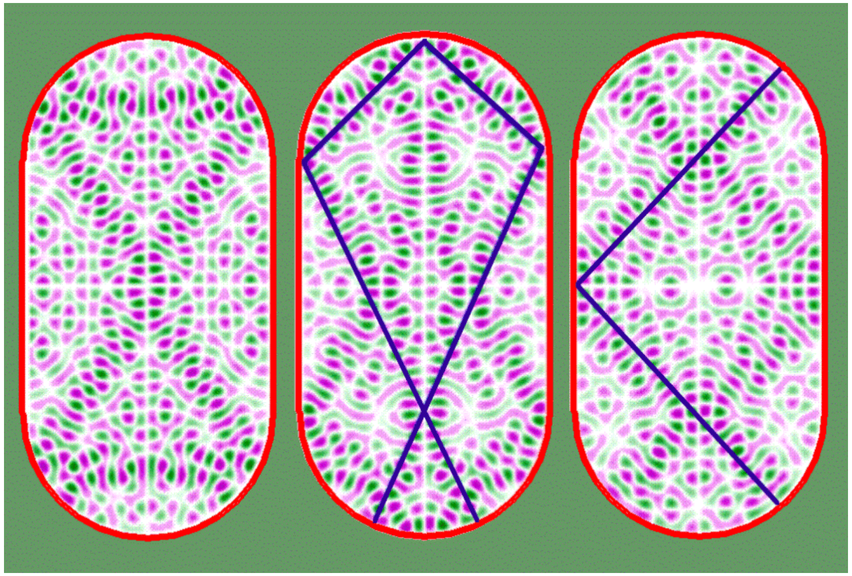
- Understanding the connections between classical chaos theory and quantum physics leads to beautiful and very deep mathematics, including number theory and the complex zeros of the Riemann zeta function,

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p\ prime} \frac{1}{1 - p^{-s}}$$

Scar Theory

- It came as a surprise (1984) that some quantum eigenfunctions of ergodic classical systems are not ergodic and scarred (high probability) along closed geodesics – periodic orbits. This is still under investigation.





Discover and theory of scars

- Scars were discovered graphically, by plotting eigenfunctions. This was done with a computer program implementing a new mathematical approach to finding them.
- Then, the theory of why they appear was given, using asymptotic semiclassical arguments for time domain quantum mechanics and its Fourier transform.

Many body

- Another realm, many body physics, is truly intractable; models of the real thing must be used. They are better than the exact answer anyway, because we get an intuitive grasp.
- The search for "emergent phenomena" in many body models is mathematical; pure or computational.

More Feynman quotes

- “If all mathematics disappeared today, physics would be set back exactly one week,”
- To which a mathematician replied
  “True – if you mean the week that God created the Universe!”
- “Shut up and calculate” (attributed to Feynman, but David Mermin claims it).

The mathematical challenges

- All but the simplest quantum systems are far too difficult to understand exactly.
- The super-challenges facing quantum physics are explaining ***emergent phenomena***, like superconductivity, an unexpected many body effect.

MATHEMATICAL FRONTIERS
Mathematics of Quantum Physics

Xiaosong Li,
University of Washington

Harry and Catherine Jaynne Boand Endowed Professor of Chemistry

co-Associate Chair for Graduate Education

Electron's Dance

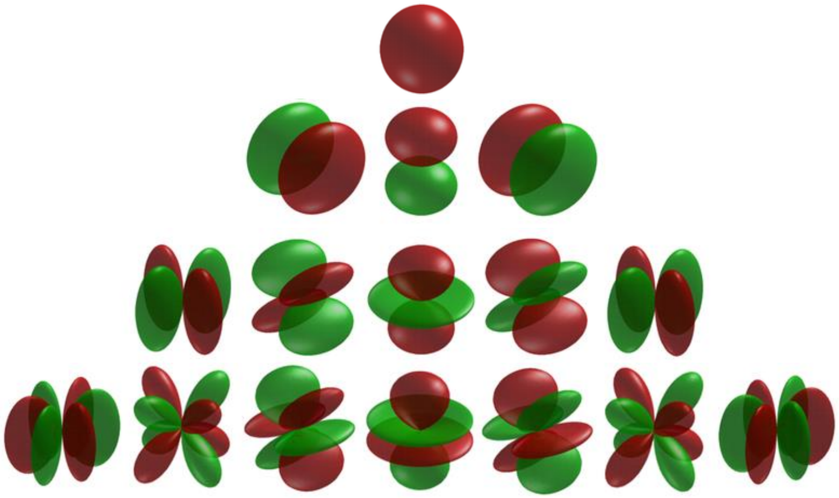
What do Electrons Look Like in Molecules?

Quantum Physics

– from math to electron wave functions

$$\hat{H}\Psi = E\Psi$$

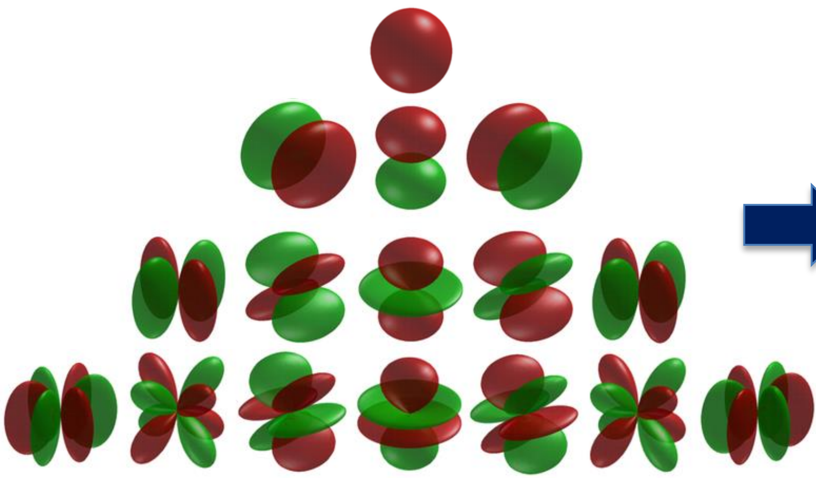
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}$$

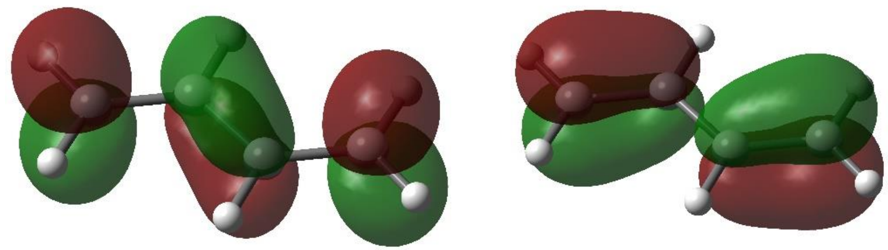


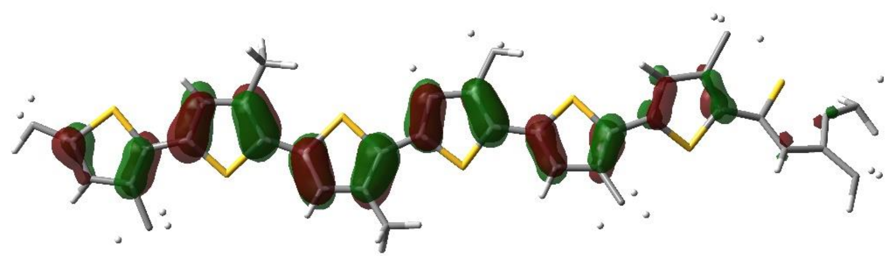
What do Electrons Look Like in Molecules?

Quantum Physics

– from atoms to molecules







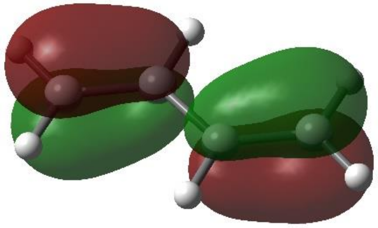
$$\phi$$

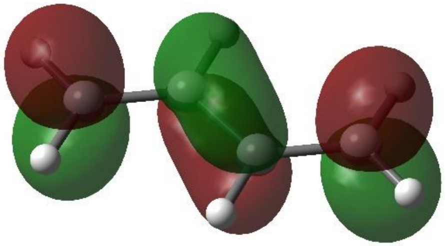
$$\psi = \sum_i c_i \phi_i$$

What do Electrons Look Like in Molecules?

Time-Dependent Quantum Physics

– from quantum physics to spectroscopy



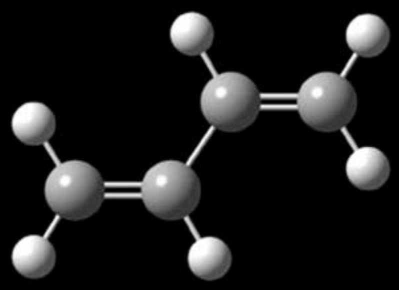


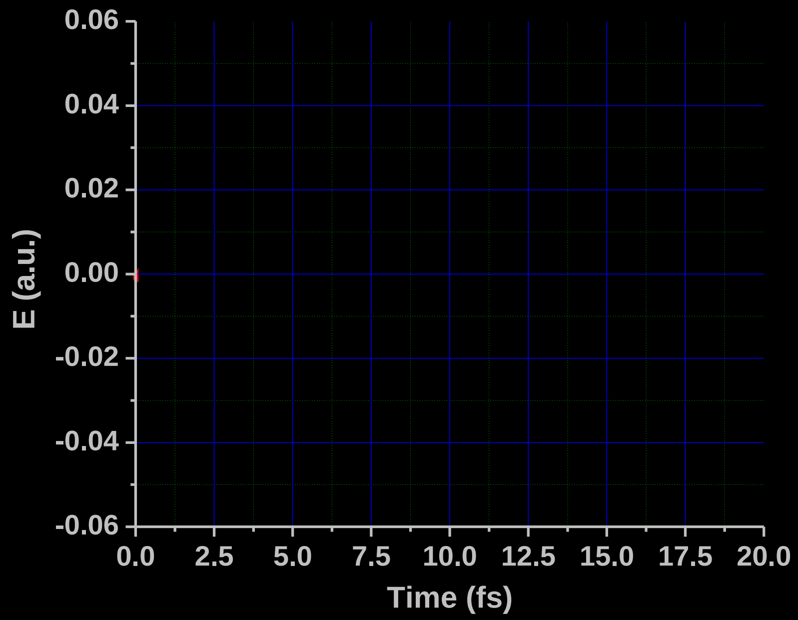
$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

$$\psi(x,t) = e^{-\frac{iEt}{\hbar}}\psi(x)$$

From Quantum Physics to Spectroscopy

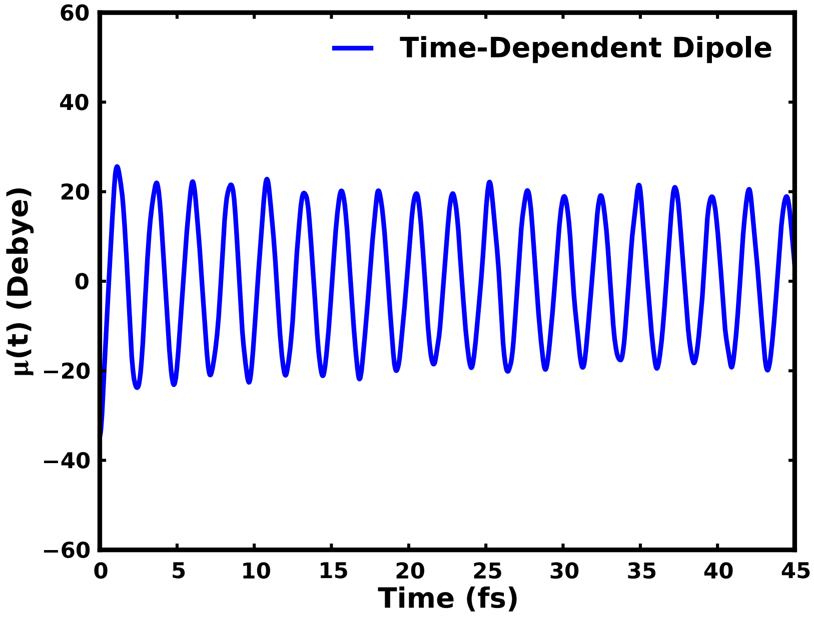
$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \qquad \psi(x,t) = e^{-\frac{iEt}{\hbar}}\psi(x)$$

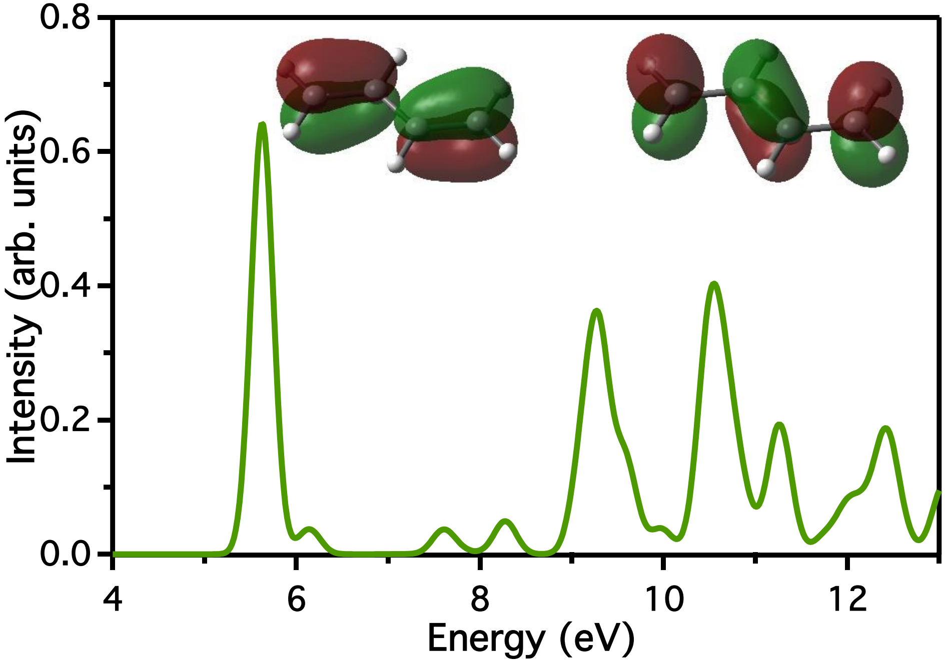




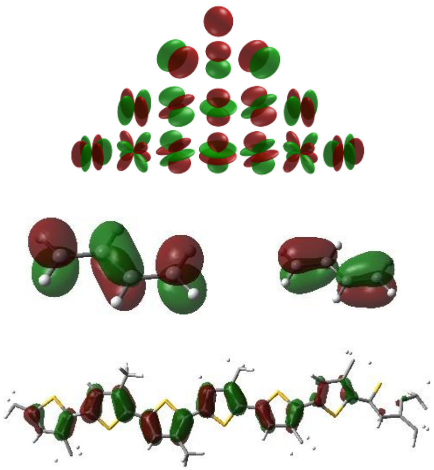
Electron Dynamics and Spectroscopy

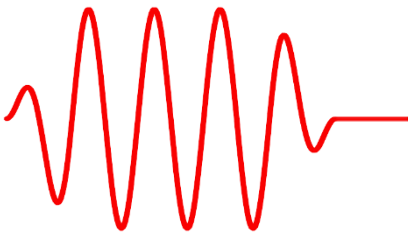
$$\mu(t) = \langle \psi(x,t) | \hat{x} | \psi(x,t) \rangle \rightarrow \mu(\omega)$$

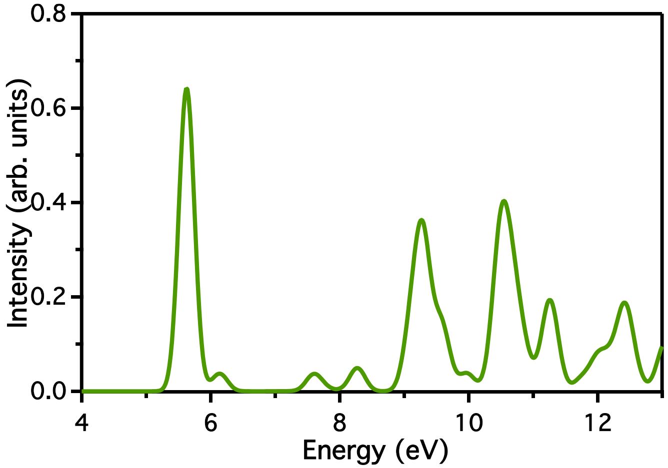




From Time-Dependent Quantum Theory to Spectroscopy





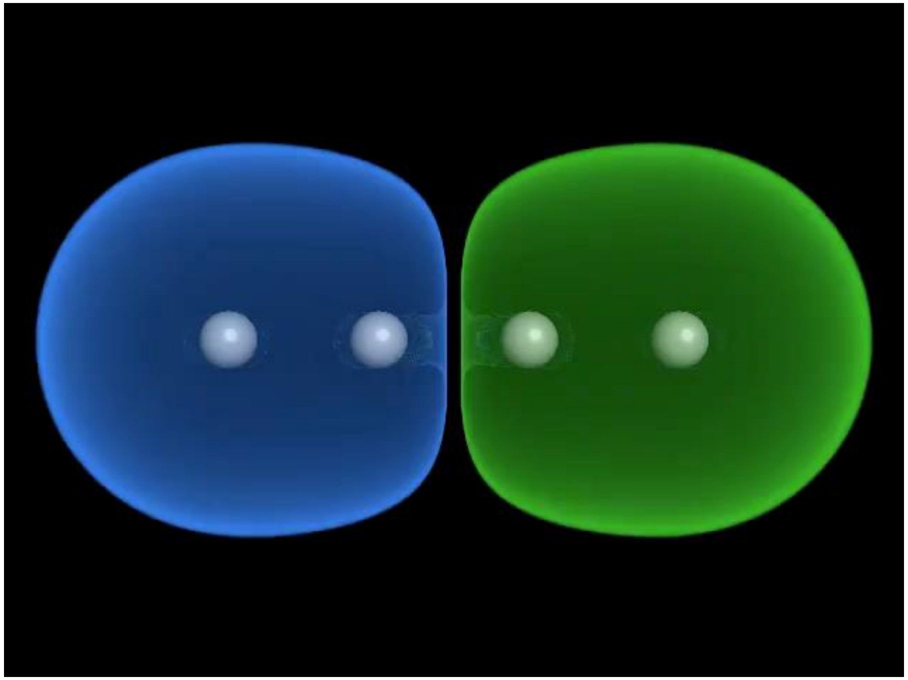


$$\psi(x,t)$$

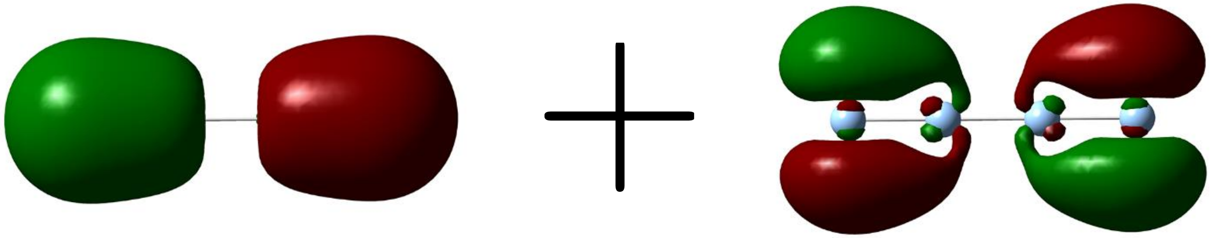
$$\hat{H}$$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

Photophysics of Superposition State

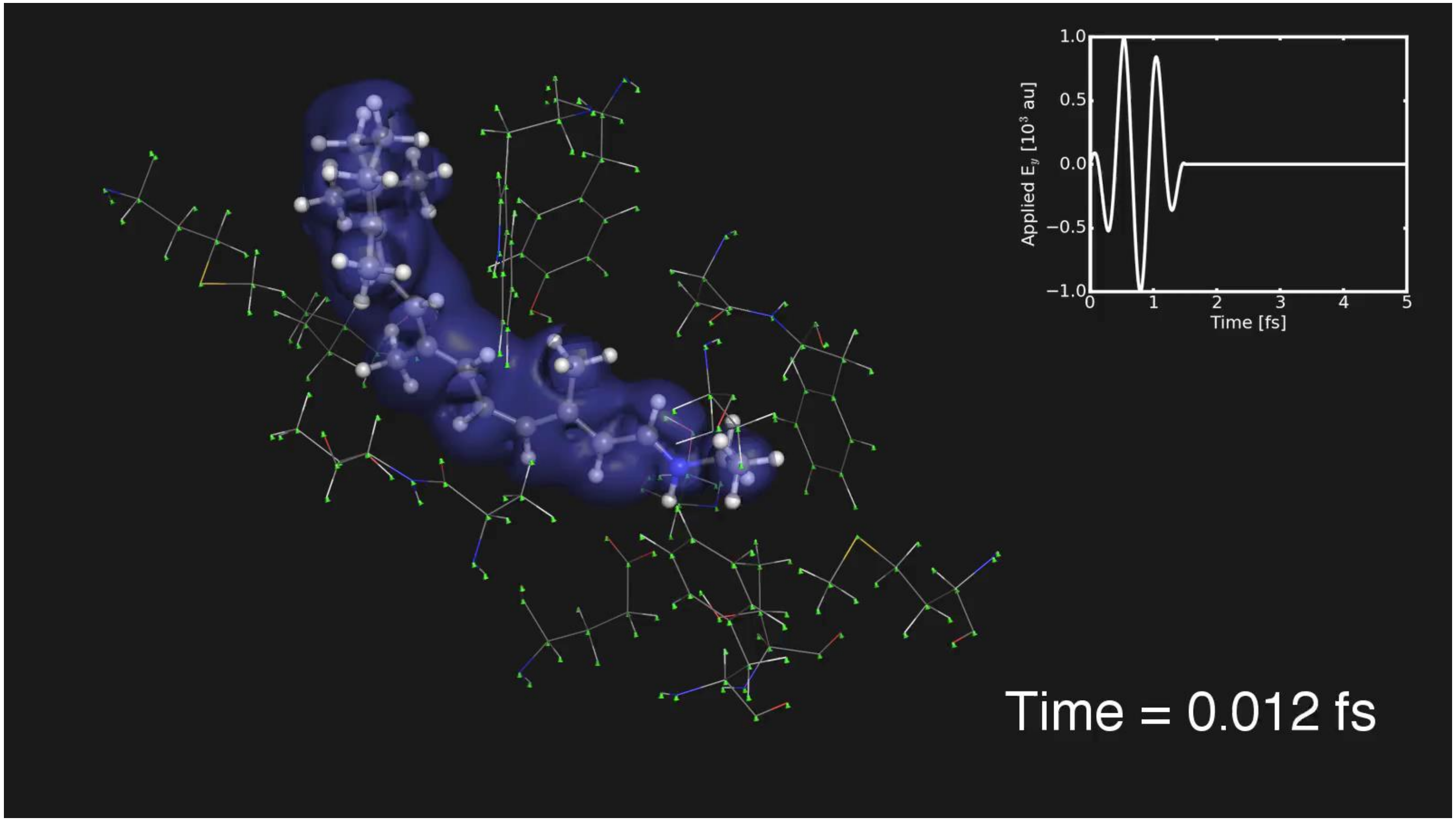


$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

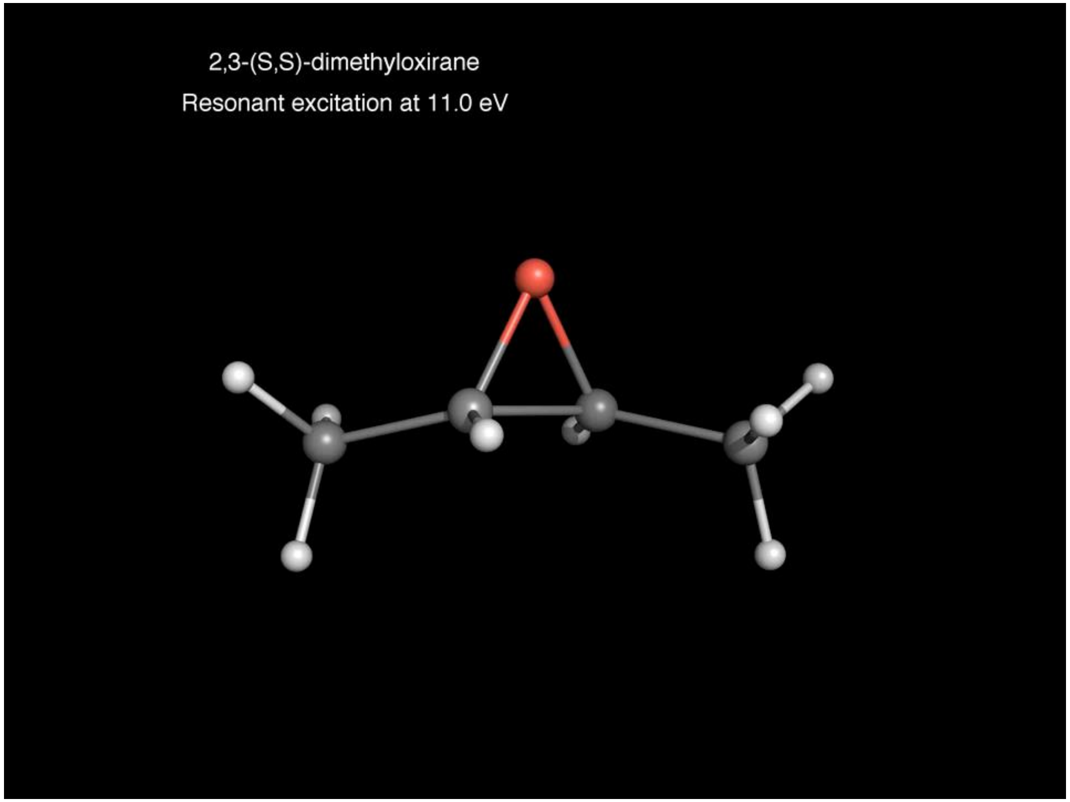


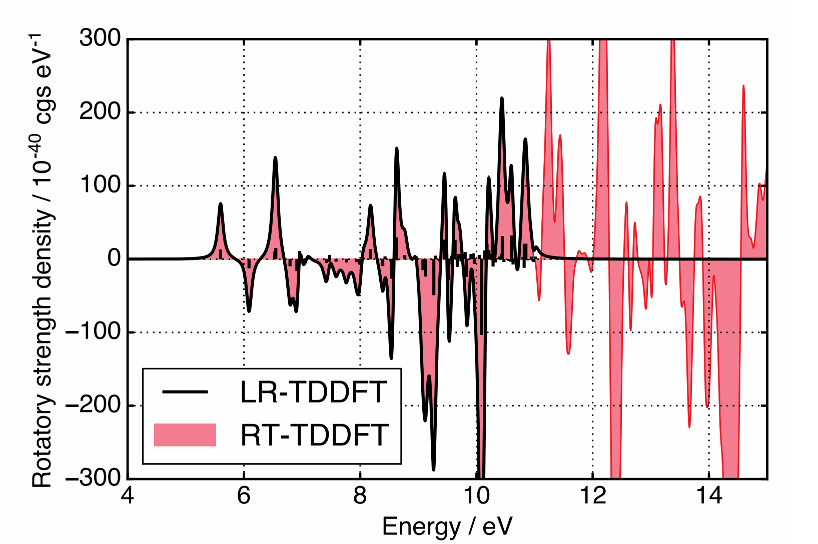
Mixed Quantum-Classical Mechanics

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \qquad \hat{H} = \hat{H}_{QM} + \hat{V}_{eff}$$



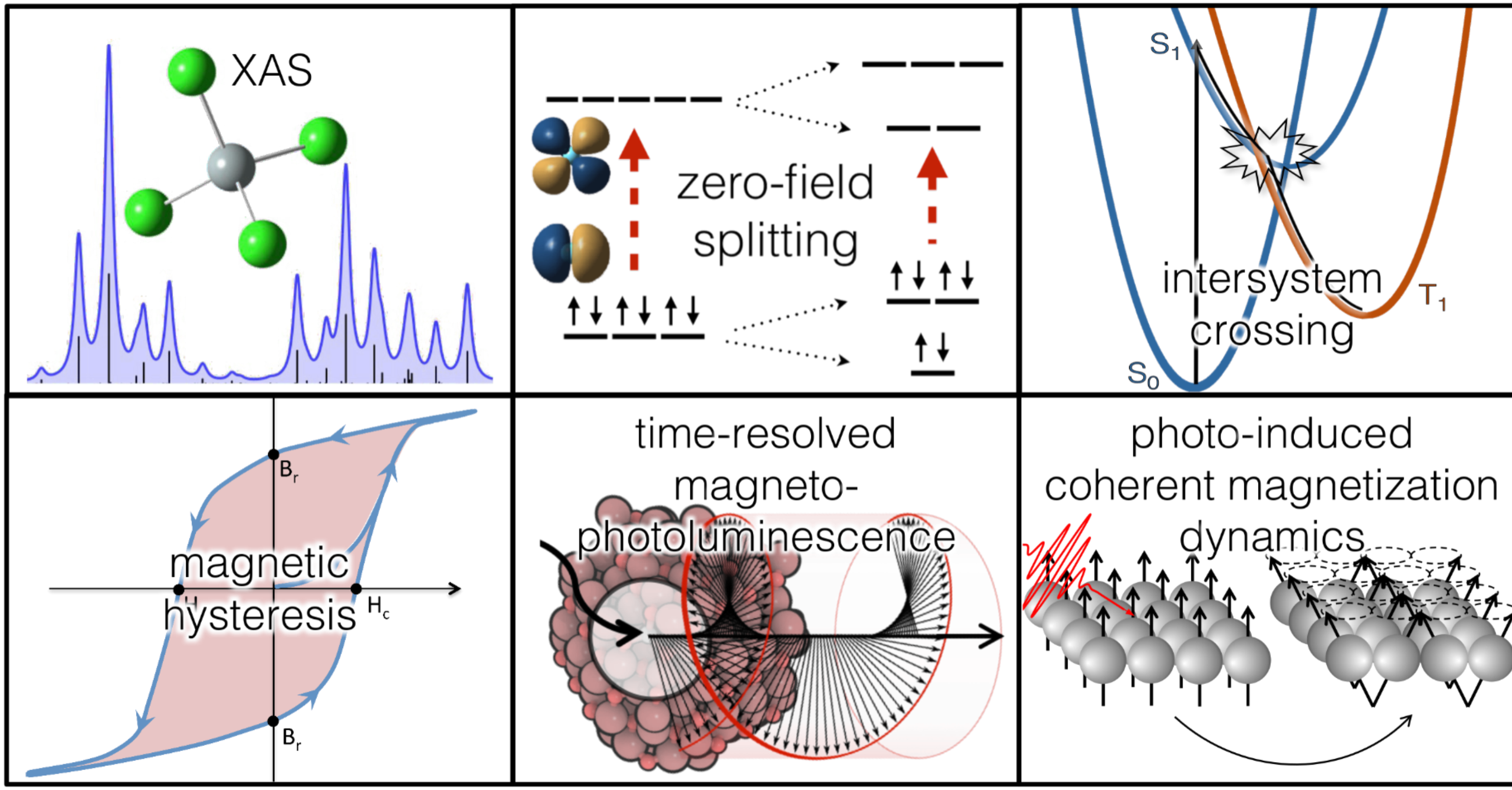
Photophysics of Chirality





$$-2\sum_{j\neq n}\frac{\omega}{\omega_{jn}^2-\omega^2}\mathrm{Im}\left(\langle\psi_n|r_\beta|\psi_j\rangle\langle\psi_j|m_\alpha|\psi_n\rangle\right)$$

Spin-Physics



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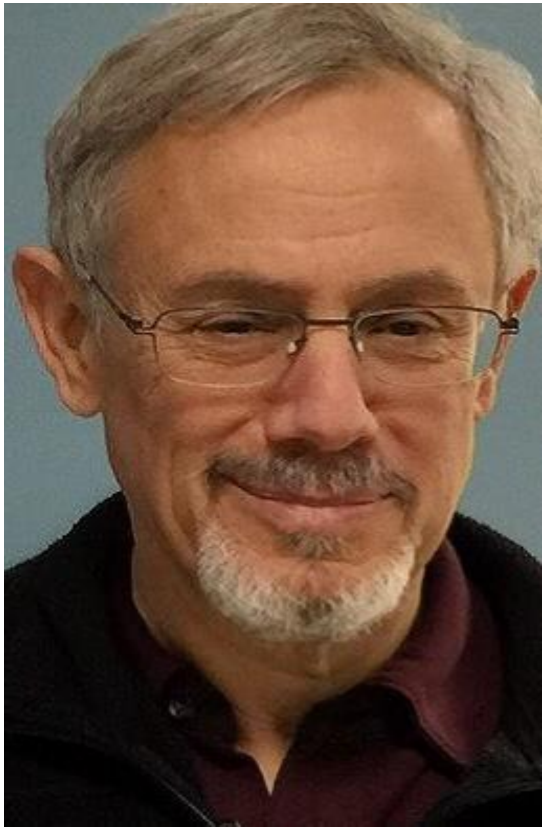

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