Nonlinear Spectroscopy and Bilinear Control Theory

Using light to estimate stuff

NE 155, Spring 2016
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Huh?

Research project!

Prof. Birgitta Whaley (quantum information)

On-and-off since Spring 2015

Computational science: theory + simulations
Goal

Find physical parameters of molecular system

Using spectroscopy!

How?

\[ H(t)\psi(t) = i\hbar \frac{\partial}{\partial t} \psi(t) \]
Idea

Let’s find a space where equations are linear. Then, we invert!

We can recursively expand perturbations:

\[
\frac{\partial \hat{\rho}_n(t)}{\partial t} = \frac{-i}{\hbar} [\hat{H}(t), \hat{\rho}_{n-1}(t)]
\]
Control Theory

Model systems from input-output measurements.

Hamiltonian is time-dependent!

\[ H = H_0 + \mu \cdot \vec{E}(t) \]
Pulses

Experiments use “ultrafast pulses” (femto-sec)

Approximated as rectangular pulse  Or as Dirac delta

http://idav.ucdavis.edu/~okreylos/PhDStudies/Winter2000/BoxFilter.gif

Things simplify!

Now we’re linear!

\[
\begin{align*}
\dot{x} &= Ax \\
\mathbf{x}(t) &= e^{\mathbf{A}t} \mathbf{x}(0)
\end{align*}
\]

To simulate the forward direction, we input A and x(0) to get x(t).
Remember the goal...

Find physical parameters:
- transition dipole
- energy splitting
- energy coupling

It’s harder than expected, but some iterative methods might work.
Code

Part 1: Forward direction
→ Does the simulated data match experiment?

Part 2: Inversion direction
→ Can we get physical parameters from data?