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

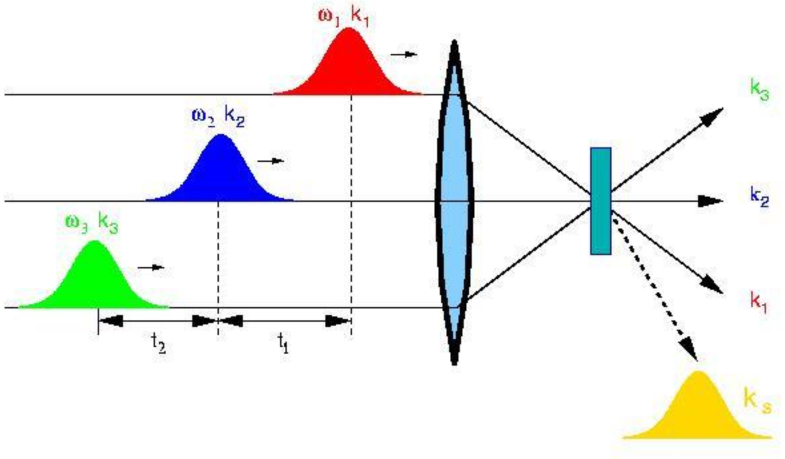
Find physical parameters of molecular system

Using spectroscopy!

How?

$$H(t)|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

http://cdn.phys.org/newman/gfx/news/hires/2013/schrodingerequation1.jpg



https://www.mbi-berlin.de/de/research/projects/3.1/topics/history/Subproject5/p3_experiment.jpg

Idea

Let’s find a space where equations are linear.

Then, we invert!

$$\underbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}}_{b}$$

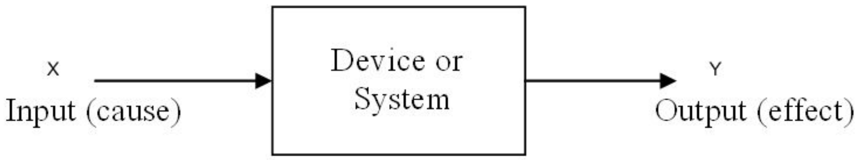
http://i.stack.imgur.com/hx8PR.png

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.



http://1.bp.blogspot.com/_U3umjVzCXTA/TJ2qDnhANMI/AAAAAAAAAPk/AHIC2YGuO1U/s1600/I-O-block+diagram.gif

$$\dot{\vec{x}} = A\vec{x} + B\vec{u}$$

$$\vec{y} = C\vec{x} + D\vec{u}$$

https://users.ece.cmu.edu/~koopman/des_s99/control_theory/stateq.gif

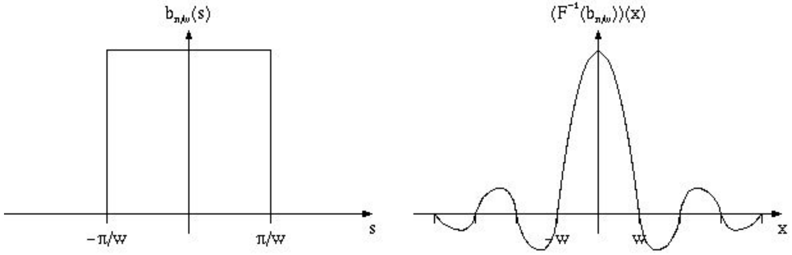
Hamiltonian is time-dependent!

$$H = H_0 + \mu \cdot \vec{E}(t)$$

Pulses

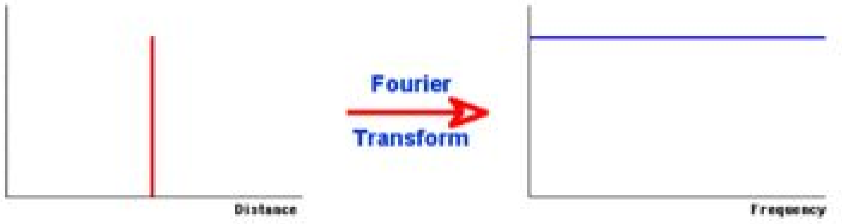
Experiments use “ultrafast pulses” (femto-sec)

Approximated as
rectangular pulse



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

Or as
Dirac delta



https://upload.wikimedia.org/wikibooks/en/thumb/c/c2/NM16_10.gif/380px-NM16_10.gif

Things simplify!

Now we're linear!

$$\dot{x} = Ax$$

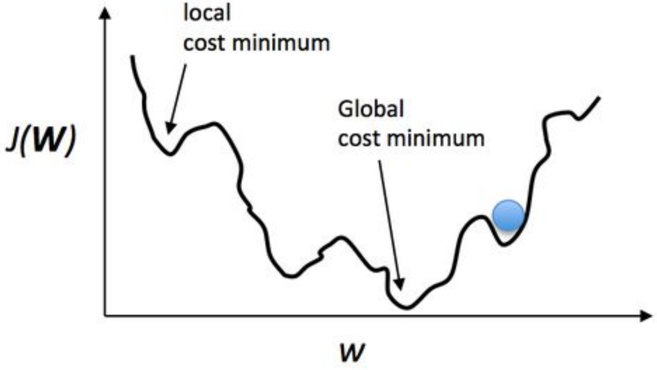
$$x(t) = e^{At}x(0)$$

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

Remember the goal...

Find **physical parameters:**

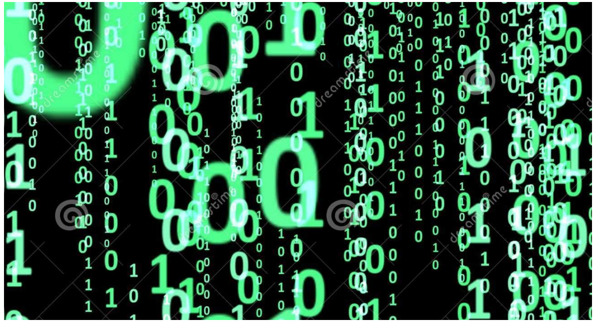
- transition dipole
- energy splitting
- energy coupling



http://sebastianraschka.com/images/faq/visual-backpropagation/nonconvex-cost.png

It's harder than expected, but some iterative methods **might** work.

Code



http://thumbs.dreamstime.com/z/binary-code-abstract-background-animation-digits-falling-downwards-against-black-42622233.jpg

Part 1: Forward direction

→ Does the simulated data match experiment?

Part 2: Inversion direction

→ Can we get physical parameters from data?