Solving the Maxwell-Bloch equations for resonant nonlinear optics using computers

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Outline

1. What is resonant nonlinear optics?
2. The Maxwell-Bloch equations
3. Solving the equations on computers
4. Outlook: connection / thoughts with the present problem

What is resonant nonlinear optics?

Resonant nonlinear optics

- A medium with discrete absorption lines
- Monochromatic light field(s) resonant with the transition(s)
- Strong light, substantial effect on atomic quantum states
- Medium optically dense - substantial back-action on light

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Some applications:

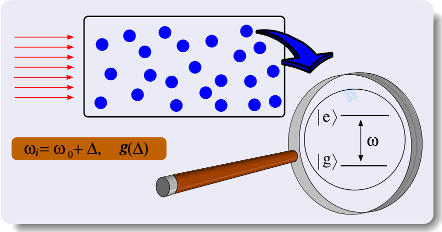
- Quantum communication
- Quantum computing
- Deterministic single-photon source, optical quantum memories

To be more specific:

Typical system: Transparent crystal + dopants (rare-earth ions)

Large inhomogeneous broadening!

$\sigma_\Delta \gg 1/\tau_p \Rightarrow$ ensemble description must be used



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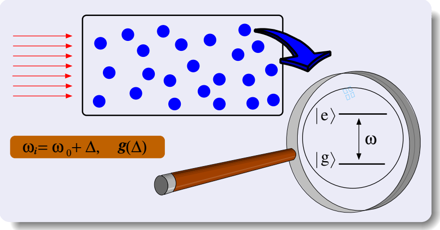

Light: Maxwell (1D)

$$\left(c^2 \frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial t^2} \right) E(z,t) = \frac{1}{\varepsilon_0} \frac{\partial^2}{\partial t^2} \mathcal{P}(z,t)$$

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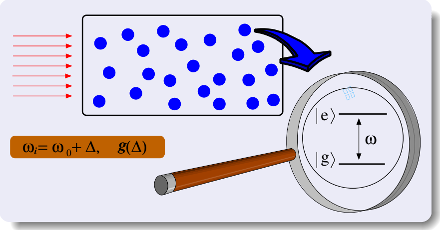

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$$i\hbar\partial_t \Psi = (\hat{H}_a - \hat{d}E)\Psi$$

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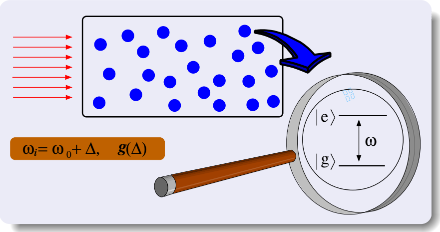

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$$\Updownarrow$$

Macroscopic polarization

$$\mathcal{P}(z,t) = \int g(\Delta) \langle \hat{d} \rangle d\Delta$$

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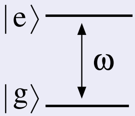
The simplest case

Two-level atoms



rotating frame atomic Hamiltonian:

$$\hat{H}_a = \hbar\Delta|e\rangle\langle e|$$

$$|\psi\rangle = \alpha(t)|g\rangle + \beta(t)|e\rangle$$

Slowly varying envelope approximation (μs, ns pulses):
$E(z,t) = \varepsilon(z,t)e^{i(kz-\omega t)}$
$\partial_t\varepsilon \ll \omega\varepsilon$ and $\partial_z\varepsilon \ll k\varepsilon$
delayed time: $t = t' - z/v_g$

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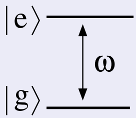

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$\Longrightarrow$

Maxwell-Bloch equations:

Schrödinger part:

$$\partial_t\alpha(z,t) = i\frac{\varepsilon^* d}{2\hbar}\beta(z,t)$$

$$\partial_t\beta(z,t) = i\frac{\varepsilon d}{2\hbar}\alpha(z,t) - i\Delta\beta(z,t)$$

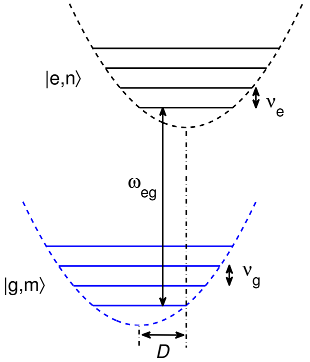
(Bloch form: u, v, w)
Maxwell part:

$$\partial_z\varepsilon(z,t) = i\frac{\alpha_D\hbar}{d\pi g(0)}\mathcal{P}(z,t)$$

$$\mathcal{P}(z,t) = \int g(\Delta)\alpha^*(z,t;\Delta)\beta(z,t;\Delta)d\Delta$$

A more elaborate case

Vibrational sublevels



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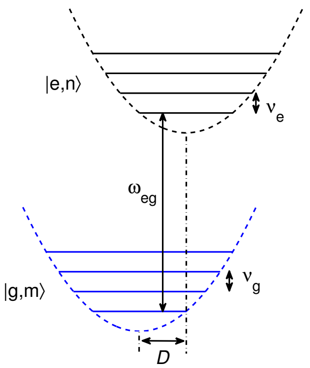

Multiple sublevels:

$$|\psi\rangle = \sum_m \alpha_m(t)|g, m\rangle + \sum_n \beta_n(t)|e, n\rangle$$

Multiple fields:

$$E(z, t) = \sum_l \varepsilon_l(z, t)e^{i(kz-\omega_l t)}$$

More equations & transition elements (Franck-Condon factors) but ...
... nothing is conceptually different!
In general solvable with computers.

The problem at a glance...

Difficulties:

- atoms & field(s) in spatially extended domain
- coupled dynamical systems (neither plays a subordinate role, no χ)
- nonlinear
- inhomogeneous broadening $\Rightarrow$ statistical ensemble must be computed

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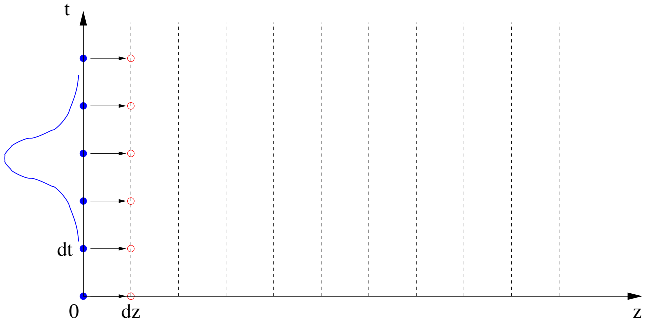
Convenient properties:

- Maxwell: $\partial_z \varepsilon(z,t) = i \frac{\alpha_D \hbar}{d \pi g(0)} \mathcal{P}(z,t)$ ... an ODE! (Albeit with embedded ODE-s for the ensemble on the RHS)
- Schrödinger: ODE if $\varepsilon(t)$ is known
- $\Rightarrow$ ODE methods can be used, numerous libraries available (GNU Octave/Matlab, C++, etc.)
- Computation of ensemble can be parallelized.

Straightforward strategy: $\varepsilon(t)$ on boundary given, solve on a space-time grid



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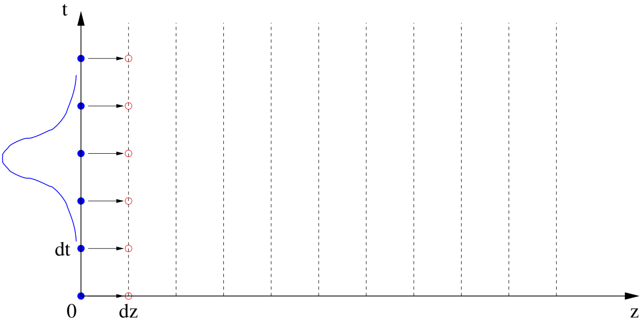


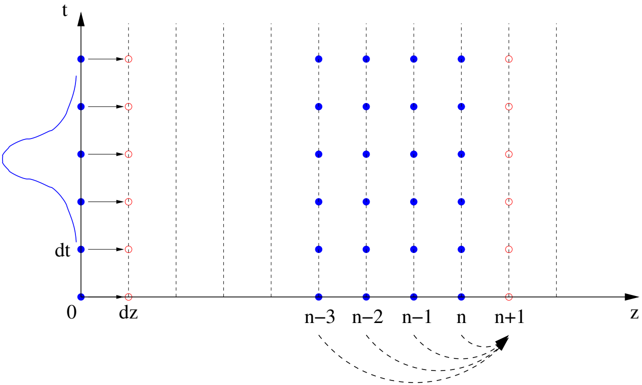
algorithm outline

For each step to advance $\varepsilon(z, t)$ from z to $z + dz$ do:

1. For each atom in the ensemble:
   - Compute $\alpha_j(t), \beta_j(t)$ using $\varepsilon(z, t)$ (Solve ODEs)
2. Compute $\mathcal{P}(t)$ (i.e. $\partial_z \varepsilon(z, t)$)
3. Compute $\varepsilon(z + dz, t)$

Maxwell: expensive RHS ⇒ linear multistep methods (Adams-Bashforth)

- Less evaluations of RHS (no midpoint)
- Methods correct to any order exist (4th order a perfect compromise)
- Uses more memory



Schrödinger: any convenient ODE method can be used (adaptive methods best to treat wide range of Δs).

Steps ❶ and ❷

$$\left.\begin{array}{r}\text{Integrate Sch. to get } \alpha(t), \beta(t) \\ \text{Increment } \mathcal{P}\end{array}\right\} \Leftarrow \text{can be parallelized easily!}$$

Steps 1 and 2

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- Multiple CPU threads (multicore machines, cloud environment):
  - relatively easy to program (openMP, even Matlab)
  - sizeable work delegated to each thread $\rightarrow$ efficient work
  - $\mathcal{P}$ must be incremented in a thread safe manner!
  - groups of atoms best to fill L1 cache, (with similar Δ!)

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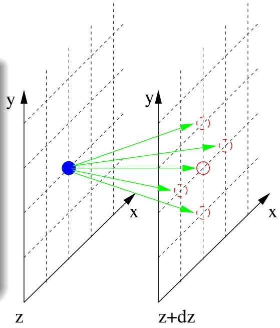
- GPU:
  - can be much faster but ...
  - much more fine-grained, more difficult to code to fully exploit potential
  - requires a different strategy - advance all atoms together
  - fastest if all relevant variables fit into RAM of a single GPU card

Single run for meaningful problems on single GPUs or 4-8 core (virtual) machines $\sim$ 1 - 10 hours.

Outlook: some thoughts / questions on plasma creation

Fields:

- $L = 10$ m $\rightarrow$ transverse structure, real PDE
- 3D field, much more data.
- plasma, time dependent density $n_e(r, t)$
- anisotropy?
- $\tau_p = 100$ fs . . . SVEA?



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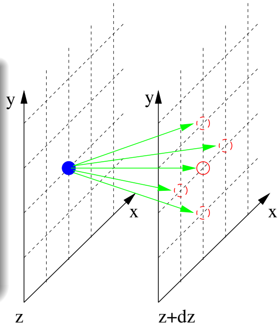

Atoms:

- bound levels + continuum ... „low dimensional" description?
- $g(\Delta) \ll \tau_p$, no ensemble required