Computational quantum mechanics, the coupled channel method

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Introduction

We describe a component in a computational physics course dealing with simulations of time-dependent quantum mechanical systems. The goal was to increase the effective understanding of quantum mechanics by studying problems in a less theoretical but more visual and intuitive manner. Conceptual difficulties are manifold. Also unhelpful is the fact that few meaningful time-dependent problems are analytically solvable. In this poster we present numerical simulations of bound systems interacting with external fields. Specifically, we discuss the interaction between an oscillating laser field and a particle in a box. However, the method is universal.

The coupled channel method

We found the coupled-channel method commonly used in atomic physics calculations to be useful. In this method, the Schroedinger equation is solved in a basis set, reducing it to a set of ordinary differential equations. The advantages of the method are that it can be directly applied to many time-dependent problems, and it can use higher order numerical solutions to ODEs typically developed fairly early in a computational physics course. Thus, space is continuous, only time is discretized. Briefly:

Let $H = H_0 + V(t)$ be the total Hamiltonian, H_0 the unperturbed Hamiltonian, and $V(t)$ the perturbation. Then the total wave function of the system can be expanded as

$$\psi(x,t) = \sum_n a_n(t) u_n(x) \exp(-iE_n t/\hbar),$$

where $a_n(t)$ is the expansion coefficient and $u_n(x)$ is the eigenfunction of H_0,

$$H_0 u_n = E_n u_n, \quad E_n \text{ is the eigenenergy.}$$

Defining $\omega_{mn} = (E_m - E_n)/\hbar, V_{mn}(t) = \langle m|V|n\rangle$, and substituting $\psi(x,t)$ into $H\psi = i\hbar\partial\psi/\partial t$ yields

$$\frac{da_m(t)}{dt} = -\frac{i}{\hbar}\sum_n a_n(t) V_{mn}(t) \exp(i\omega_{mn} t).$$

This is the final result. It consists a set of coupled ODEs that can be solved (e.g., using Runge-Kutta) subject to the initial conditions that

$a_1(0)=1$ (initial state), and $a_n(0)=0$ for n>1

Example

We choose the simple electron-in-a-box as our system (box width = 2 angstrom) and apply an oscillating laser pulse to it. The laser pulse has a center frequency and an envelope as shown in Fig. 1.

The laser pulse

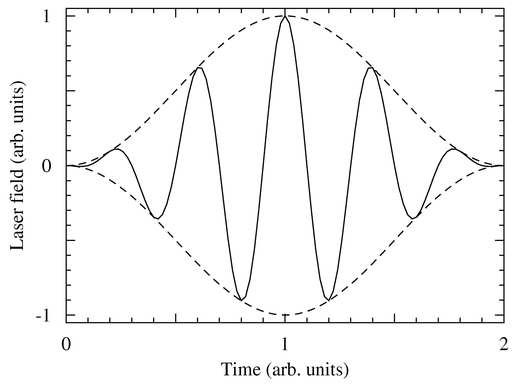

Fig. 1. The interaction is assumed to be a laser pulse with a sinusoidal oscillation modulated by an envelope. The center frequency, the field magnitude, and its duration are adjustable parameters as in

$$F(t) = F_0 \sin^2(\pi t/\tau)\cos(\omega_L t),\ 0 \le t \le \tau.$$

Results

Below we show results for various field parameters. The results are presented graphically with explanations and brief discussions in the figure captions. Box units (b.u.) are used.

In box units (b.u.), length=1 angstrom, energy=37.5 eV

Resonant transition

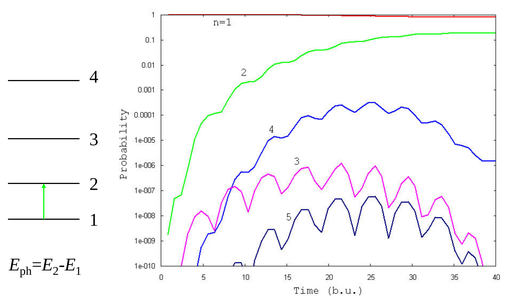

Fig. 2. Occupation probability as a function of time. The center frequency is resonant with the transition energy between the ground state (*n*=1) and the first excited state (*n*=2). The field is relatively weak and the duration short. Five states are included in the simulation, but only *n*=2 state – which is dipole allowed – has any significant probability (more apparent on a linear scale, not shown here). Two-state approximation should hold.

Dipole-forbidden transition

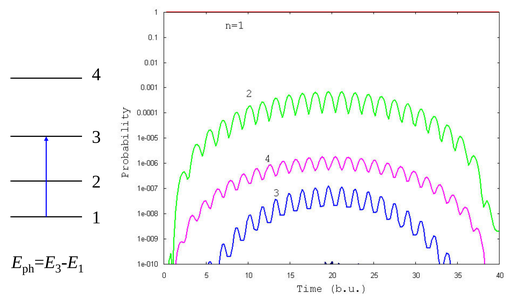

Fig. 3. Occupation probability as a function of time. The center frequency is now tuned such that it is resonant with the transition energy between the ground state (*n*=1) and the second excited state (*n*=3). The field is relatively weak and the duration short. Again, five states are included in the simulation.
There is very little probability of excitation to the *n*=3 state. This is because to first order, the transition between 1 and 3 is dipole forbidden. Due to the identical parity of states 1 and 3, the transition matrix element $V_{13}(t)$ is zero. Only second or higher order effects cause the excitation with an insignificant probability.
The *n*=2 state is dipole-allowed, and has a small probability of excitation due to broadening. Since this transition is of first order, it has the largest excitation probability despite the fact that it is non-resonant.

Particle density

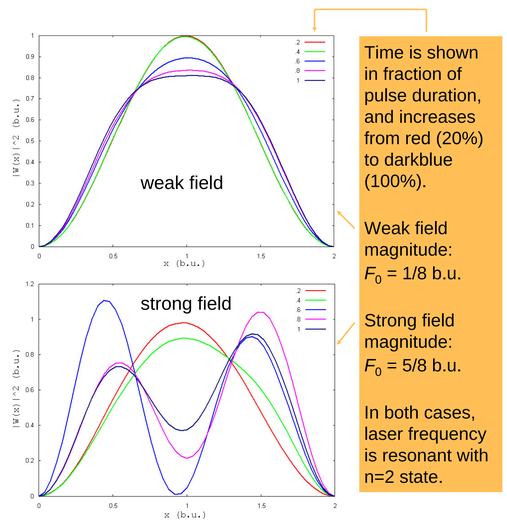

Fig. 4. Particle densities as a function of time.

Rabi flopping

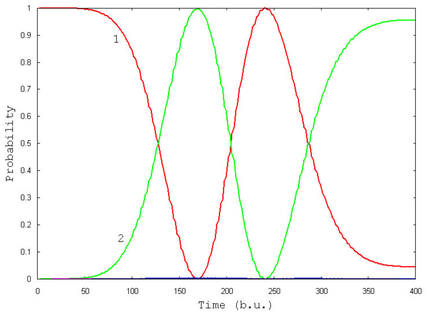

Fig. 5. Occupation probability of the ground and the first excited states as a function of time for a long laser pulse. At the beginning, the ground state steadily depletes while the excited state gradually builds up. Thereafter, the two states flip-flops back and forth at the Rabi frequency. This occurs in real atomic/optical systems. There is no abrupt transition.
One can check two approximations here: the two-state approximation and the rotating wave approximations (RWA). Both work well, producing solutions of no unnoticeable deviations on the scale shown above.

Energy transfer

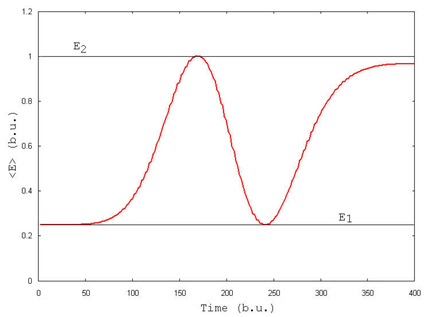

Fig. 6. The average energy of the system as a function of time during Rabi flopping. The energy varies continuously between the two states as expected.

Conclusions

The coupled channel method offers several advantages:

- no further discretization of the spatial coordinates required
- suitable to common situations where numerical solutions to ODEs are introduced
- easy to use in many time-dependent problems
- able to produce meaningful results and to help with conceptual understanding