Solution of time-dependent problems in quantum mechanics

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Website for book

- Codes for many of this week's topics can be found at the following link:

  https://sites.google.com/site/varga1kalmanbook/

- See Chapter 5 for the code I'll discuss today

Why do we need time dependence?

- We're often interested in time-dependent phenomena
- Usually, time-independent methods just give you information about the ground state
    - they can sometimes give TD, but only approximately
- Our approach: We solve the time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = H\Psi(t).$$

Methods of time propagation

- Direct integration of TDSE
  - Euler, Runge-Kutta, etc.

- Application of the time evolution operator
  - Taylor expansion, Crank-Nicholson, etc.

- Either way: use ground state as initial state $\Psi(x, 0)$, then time-develop the wavefunction to get $\Psi(x, t)$

Direct integration of the TDSE

We can use the standard definition of the derivative to write

$$\frac{\partial \Psi}{\partial t} = \frac{\Psi(t+\Delta t) - \Psi(t)}{\Delta t} = \frac{H\Psi(t)}{i\hbar}$$

which gives

$$\Psi(t+\Delta t) = \frac{\Delta t}{i\hbar} H\Psi(t) + \Psi(t) + \mathcal{O}((\Delta t)^2)$$

Using a symmetric form of the derivative,

$$\frac{\partial \Psi}{\partial t} = \frac{\Psi(t+\Delta t) - \Psi(t-\Delta t)}{2\Delta t} = \frac{H\Psi(t)}{i\hbar}$$

we get a more accurate method:

$$\Psi(t+\Delta t) = \frac{2\Delta t}{i\hbar} H\Psi(t) + \Psi(t-\Delta t) + \mathcal{O}((\Delta t)^3)$$

We can do even better: Runge-Kutta

Let

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

$$\mathbf{x}(t) = (\Psi(x_1, t), \Psi(x_2, t), \ldots, \Psi(x_N, t))$$

The RK method approximates the solution by

$$\mathbf{x}(t+\Delta t) \equiv \mathbf{x}(t) + \frac{1}{6}\left[f(\mathbf{y}_1, \tau_1) + 2f(\mathbf{y}_2, \tau_2) \right.$$
$$\left. + 2f(\mathbf{y}_3, \tau_3) + f(\mathbf{y}_4, \tau_4)\right]\Delta t + \mathcal{O}((\Delta t)^5)$$

where the terms are given by

$$\begin{aligned}
\mathbf{y}_1 &= \mathbf{x}(t), & \tau_1 &= t \\
\mathbf{y}_2 &= \mathbf{x}(t) + \frac{1}{2} f(\mathbf{y}_1, \tau_1)\Delta t, & \tau_2 &= t + \frac{1}{2}\Delta t \\
\mathbf{y}_3 &= \mathbf{x}(t) + \frac{1}{2} f(\mathbf{y}_2, \tau_2)\Delta t, & \tau_3 &= t + \frac{1}{2}\Delta t \\
\mathbf{y}_4 &= \mathbf{x}(t) + f(\mathbf{y}_3, \tau_3)\Delta t, & \tau_4 &= t + \Delta t.
\end{aligned}$$

Code for RK4 method

```
! fourth-order Runge-Kutta
! step 1
call Hamiltonian_wavefn(psi,t,H_Psi)
rk(:,1)=dt*H_Psi(:)
.
.
.
! step 4
psi(:)=psi0(:)+rk(:,3)
t=t0+dt
call Hamiltonian_wavefn(psi,t,H_Psi)
rk(:,4)=dt*H_Psi(:)
! together
psi(:)=psi0(:)+(rk(:,1)+rk(:,4))/6.0+(rk(:,2)+rk(:,3))/3.0
```

Another approach: the time evolution operator

We can solve the TDSE using

$$\Psi(t + \Delta t) = U(t + \Delta t, t)\Psi(t)$$

where the **time evolution operator** is given by

$$U(t + \Delta t, t) = \mathrm{e}^{-\frac{i}{\hbar} H \Delta t}$$

To use this approach one has to approximate the exponential operator

Approximations to the time evolution operator

- We can simply Taylor expand the exponential:

$$e^{-iH\Delta t/\hbar} \approx \sum_{n=0}^{N} \left[\frac{(-i\Delta t/\hbar)^n H^n}{n!} \right]$$

Truncating the series breaks unitarity, so small time steps are needed.

- The Crank-Nicholson scheme approximates the exponential as

$$e^{-\frac{i}{\hbar}H\Delta t/\hbar} \approx \frac{1 - \frac{i\Delta t}{2\hbar}H}{1 + \frac{i\Delta t}{2\hbar}H}$$

Unitary, so can use longer time steps. But the inverse is expensive.

Code for Taylor method

```
! Taylor expansion coefficients
do i=1,N_p
  Taylor(i)=(-zI*dt)**i
  do j=1,i
    Taylor(i)=Taylor(i)/j
  end do
end do

! calculate the Hamiltonian, H_time at time t
call time_dependent_hamiltonian(t)

! Taylor expansion of exp(-iHdt)
psip=psi
do power=1,N_p
  psip=matmul(H_time,psip)
  psi=psi+Taylor(power)*psip
end do
```

Example: Free Gaussian wave packet

The time development of a free Gaussian wave packet is analytically solvable:

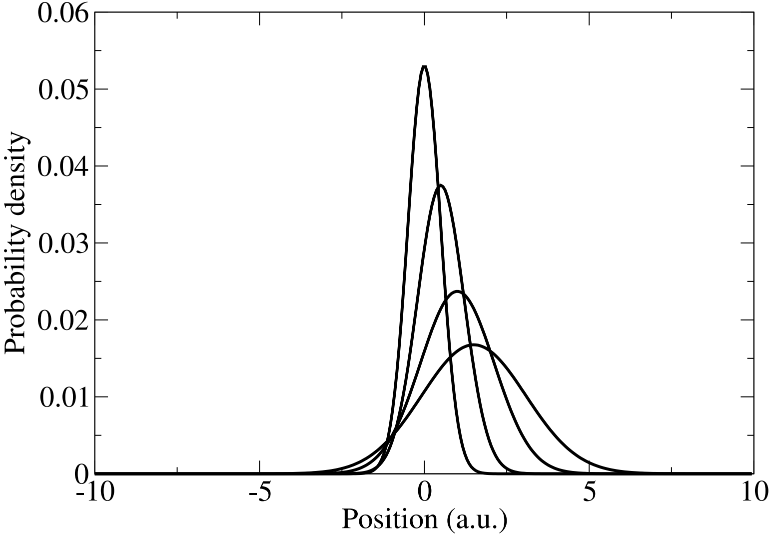
$$\psi(x,t) = \sqrt{\frac{\sigma}{\sqrt{\pi}(1+i\Omega t)}}\,\mathrm{e}^{-\frac{\sigma^2}{2}\frac{(x-vt)^2}{1+i\Omega t}}\,\mathrm{e}^{ik_0(x-vt)}$$

where $v = \hbar k_0/m$ and $\Omega = \hbar\sigma^2/m$
As time goes by, the center of the packet moves with the classical speed v, but the width of the packet $w(t)$ increases

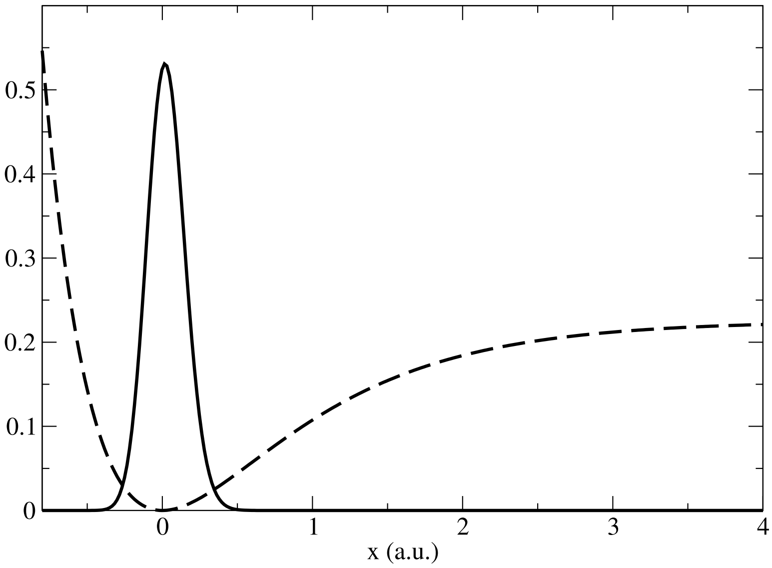
$$w^2(t) = \frac{(1+\Omega^2 t^2)}{\sigma^2}.$$

The spreading occurs more rapidly if Ω is large, that is, if the original width $w(0) = 1/\sigma$ is small

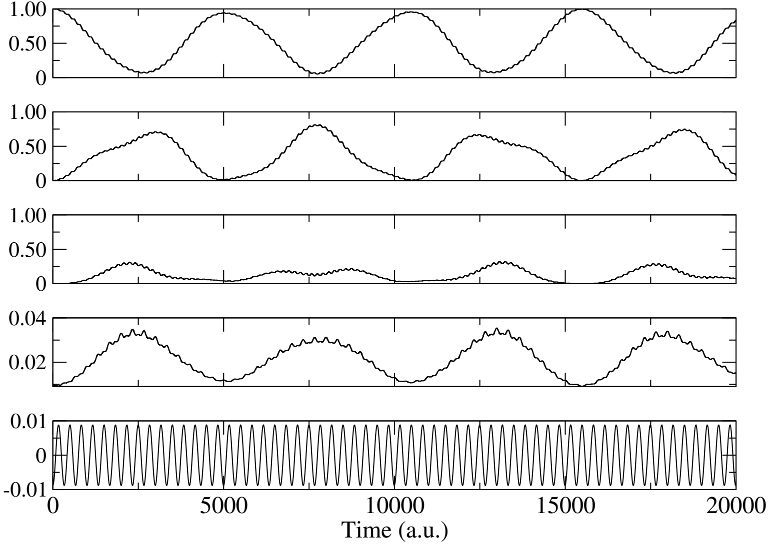
Wave packet vs. time



Example: Particle in a time-dependent potential



Small perturbation



Larger perturbation