Exercise 2: 4th-order Runge-Kutta method

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Convention

Atomic unit (Hartree) is used in the calculation, with a unit of time = 2.419e-2 fs, a unit a energy = 27.21 eV. Plots of the wavefunctions are made in SI unit. Error analysis is done again in atomic unit.

Workflow

Calculation	Error Analysis	Results
Ex2_RK4.py	error.py	global_ERR
Ex2_RK4_variables.py	error_plot.py	ERR.h5 (typical data)
RK4.f90 (→ made into module: RK4.cpython-39-x86_64-linux-gnu.so)		

Inputs are stored in "Ex2_RK4_variables.py", which is imported from the main python script "Ex2_RK4.py". Similar to what I did in exercise 1, this script can either do all the calculations on its own, or call fortran90 module "RK4_func" from "RK4.f90". Extra effort is made to inspect the global error of the 4th-order Runge-Kutta method. Typical data of error accumulation are stored in "ERR.h5", and the global errors (actually $\frac{\text{global error}}{\text{T}}$) are stored in "gloabal_ERR".

- Problem: Solve Schrödinger equation with $H = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix}$

This can be easily diagonalized by hand to obtain the eigenstates and eigenenergies:

$$\frac{E_1+E_2}{2} - \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}, \qquad \psi_1 = \left(-V, \frac{E_1-E_2}{2} + \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)^T$$

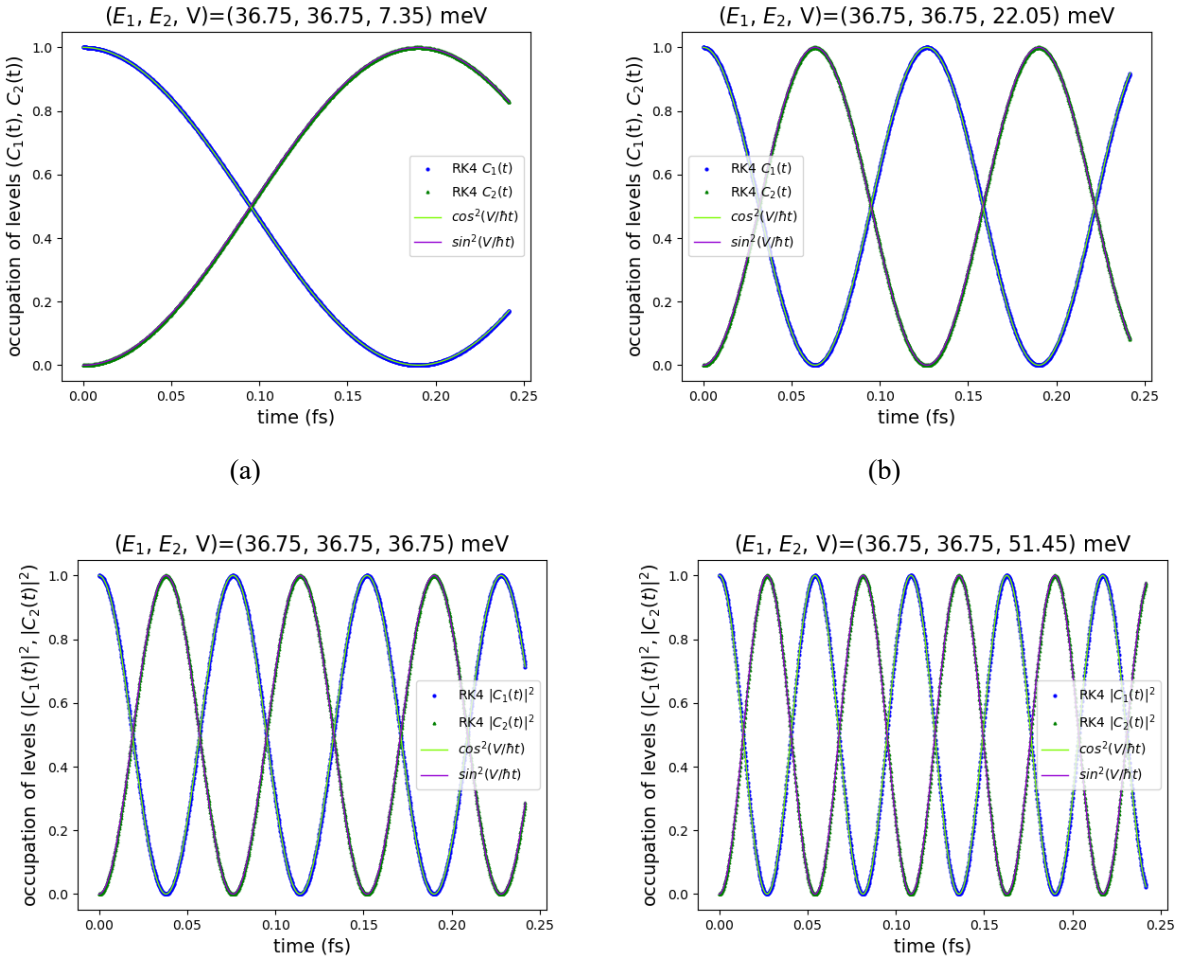
$$\frac{E_1+E_2}{2} + \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}, \qquad \psi_2 = \left(-V, \frac{E_1-E_2}{2} - \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)^T$$

- $E_1 = E_0 = E_2, \psi(0) = (1,0)^T$

Basis $\{\psi_1, \psi_2\} = \{(-V, V)^T, (-V, -V)^T\} \parallel \left\{\frac{1}{\sqrt{2}}(-1,1)^T, \frac{1}{\sqrt{2}}(1,1)^T\right\}$

$$\psi(t) = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \cdot \exp\left[\frac{1}{i\hbar}(E_0 - V)t\right] + \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \exp\left[\frac{1}{i\hbar}(E_0 + V)t\right] = \exp\left[\frac{E_0 t}{i\hbar}\right]\begin{pmatrix} \cos\frac{V}{\hbar}t \\ \mathrm{i}\sin\frac{V}{\hbar}t \end{pmatrix}$$

$$\begin{pmatrix} |C_1(t)|^2 \\ |C_2(t)|^2 \end{pmatrix} = \begin{pmatrix} \cos^2\frac{V}{\hbar}t \\ \sin^2\frac{V}{\hbar}t \end{pmatrix}$$



(a) (b)

(c) (d)

Figure 1 From (a) ~ (d), the off-diagonal element V = 0.2, 0.6, 1.0, 1.4 respectively, whereas $E_1 = E_2 = 1$, Δt = 0.01, total simulation time T = 10 (Hartree atomic unit), $\psi(0) = (1,0)^{\mathrm{T}}$

Level occupation results obtained via 4th-order Runge-Kutta method match well with $\left(\cos^2\frac{V}{\hbar}t, \sin^2\frac{V}{\hbar}t\right)^T$. Oscillation of occupation between the two levels becomes faster as V increases. at least through inspection. In order to know how well they match, further analysis is required.

- $V \ll |E_1 - E_2|, \psi(0) = (1,0)^T$

Basis $\{\psi_1, \psi_2\} \approx \left\{\left(-V, \frac{E_1-E_2}{2} + \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)^T, \left(-V, \frac{E_1-E_2}{2} - \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)^T\right\}$

$$= \left\{\left(-V, \frac{\Delta E}{2}\left(1 + \left(1 + \frac{2V^2}{\Delta E^2}\right)\right)\right)^T, \left(-V, \frac{\Delta E}{2}\left(1 - \left(1 + \frac{2V^2}{\Delta E^2}\right)\right)\right)^T\right\} = \left\{\left(-V, \Delta E + \frac{V^2}{\Delta E}\right)^T, \left(-V, -\frac{V^2}{\Delta E}\right)^T\right\}$$

$$\parallel \left\{\left(-\frac{V}{\Delta E}, 1 + \frac{V^2}{\Delta E^2}\right)^T, \left(1, \frac{V}{\Delta E}\right)^T\right\}$$

$$\psi(t) = \psi_1 \exp\left[\frac{1}{i\hbar}\left(\frac{E_1+E_2}{2} - \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)t + \phi_1\right] + \psi_2 \exp\left[\frac{1}{i\hbar}\left(\frac{E_1+E_2}{2} + \sqrt{\left(\frac{E_1-E_2}{2}\right)^2 + V^2}\right)t + \phi_2\right]$$

$$\psi(t) \approx -\frac{V}{\Delta E}\left(1+2\frac{V^2}{\Delta E^2}\right)^{-1}\psi_1 \cdot \exp\left[\frac{1}{i\hbar}\left(E_0-\left(\frac{\Delta E}{2}\right)\left(1+\frac{2V^2}{\Delta E^2}\right)\right)t\right]+\left(1+\frac{V^2}{\Delta E^2}\right)\left(1+2\frac{V^2}{\Delta E^2}\right)^{-1}\psi_2 \cdot \exp\left[\frac{1}{i\hbar}\left(E_0+\left(\frac{\Delta E}{2}\right)\left(1+\frac{2V^2}{\Delta E^2}\right)\right)t\right]$$

$$\approx \begin{pmatrix}\frac{V^2}{\Delta E^2}\\ -\frac{V}{\Delta E}\end{pmatrix}\exp\left[\frac{1}{i\hbar}\left(E_0-\left(\frac{\Delta E}{2}\right)\left(1+\frac{2V^2}{\Delta E^2}\right)\right)t\right]+\left(\frac{1}{\frac{V}{\Delta E}}\right)\exp\left[\frac{1}{i\hbar}\left(E_0+\left(\frac{\Delta E}{2}\right)\left(1+\frac{2V^2}{\Delta E^2}\right)\right)t\right]$$

$$\begin{pmatrix}|C_1(t)|^2\\ |C_2(t)|^2\end{pmatrix} \approx \begin{pmatrix}1-2\frac{V^2}{\Delta E^2}\left(1-\cos\frac{\Delta E}{\hbar}\left(1+\frac{2V^2}{\Delta E^2}\right)t\right.\\ 2\frac{V^2}{\Delta E^2}\left(1-\cos\frac{1}{\hbar}\left(\frac{\Delta E}{2}\left(1+\frac{2V^2}{\Delta E^2}\right)\right)t\right)\end{pmatrix}$$

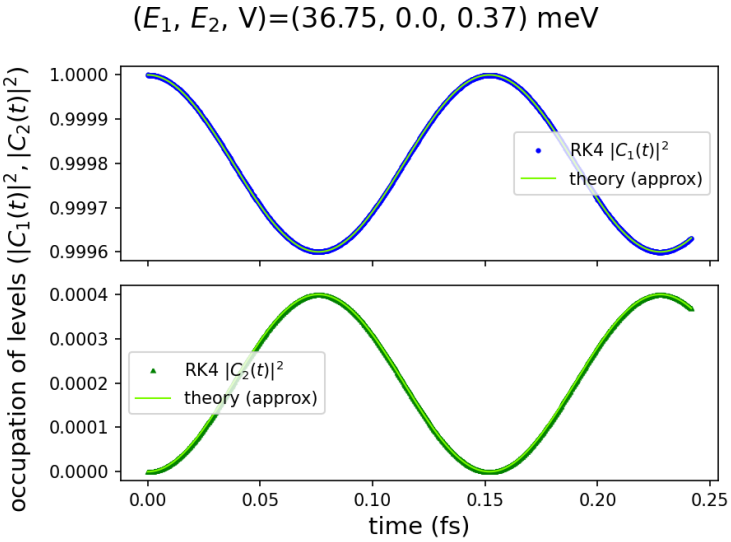


Figure 2 the off-diagonal element V = 0.01 respectively, whereas $E_1 = 1, E_2 = 0$, Δt = 0.01, total simulation time T = 10 (Hartree atomic unit), $\psi(0) = (1,0)^{\mathrm{T}}$. Theoretical plot is calculated from the approximation obtained above.

At this limit, perturbation is weak and the initial wavefunctions would stay largely at its initial state. Simulation again seems to agree well with the theoretical (approximated) solution.

- Examination of error

Although a straightforward expression can be obtained by hand more easily with approximation, the exact solution can be even more easily obtained without approximation by computer.

$$\psi(t) = \psi_1 \exp\left[\frac{1}{i\hbar}\left(\frac{E_1+E_2}{2}-\sqrt{\left(\frac{E_1-E_2}{2}\right)^2+V^2}\right)t+i\phi_1\right]+\psi_2 \exp\left[\frac{1}{i\hbar}\left(\frac{E_1+E_2}{2}+\sqrt{\left(\frac{E_1-E_2}{2}\right)^2+V^2}\right)t+i\phi_2\right]$$

where we choose ϕ_1, ϕ_2 such that $\psi_1 e^{i\phi_1}+\psi_2 e^{i\phi_2} = \psi(0)$.

$$e^{i\phi_1} = C_1(0) = \frac{\langle\psi(0)|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle}, e^{i\phi_2} = C_2(0) = \frac{\langle\psi(0)|\psi_2\rangle}{\langle\psi_2|\psi_2\rangle}$$

Then calculate occupation:

$$\begin{pmatrix}C_1(t)\\ C_2(t)\end{pmatrix} = |\psi(t)|^2$$

As such, simulation of arbitrary parameters can be compared with the exact solution. Now that, theoretically speaking, the Runge-Kutta method has a global error that scales at most as $(\Delta t)^4$, I tried to verify this in the program. Let's define the deviation of the simulation result from exact solution as:

$$\text{global error} \equiv \sqrt{(\Delta\psi)^2(t)} \equiv \sqrt{\frac{\langle\psi - \psi_{exact}|\psi - \psi_{exact}\rangle}{\langle\psi_{exact}|\psi_{exact}\rangle}}$$

In most cases, the accumulation of error is perfectly linear. To fully exploit the information contained in the data, I decide to do a linear fit and obtain the rate of error accumulation.

$$\text{slope} = \text{global error} / T$$

Doing so avoids the randomness in local error and can hopefully provide a more accurate picture. I expect the slope to scale with Δt in the same way as the global error does, i.e., $(\Delta t)^4$.

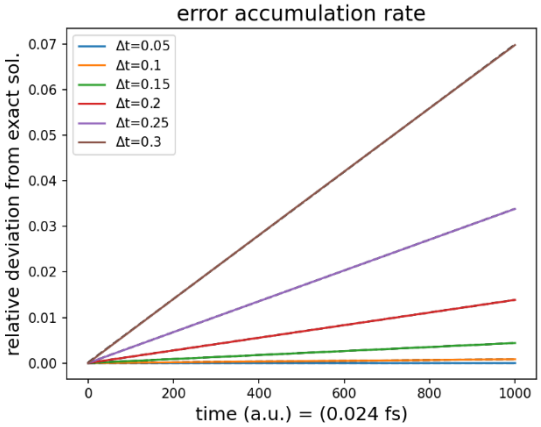
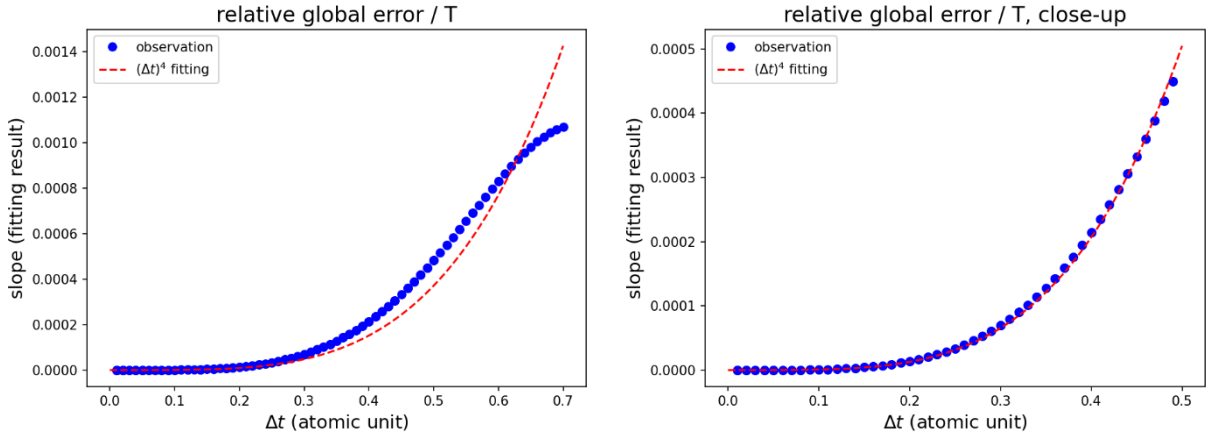


Figure 3 Error as a function of simulation time $E_0 = 0.01$, T=1000, (Hartree atomic unit). Black dashed lines, almost covered by the observed data, are the linear fits.



(a) (b)

Figure 4 relative global error (defined above) divided by T v.s. time step Δt. (Parameters identical with those in Fig. 3) (a) $\Delta t = 0\sim0.7$, (b) $\Delta t = 0\sim0.5$, and the fitting is restricted to this range as well.

Note that the global error no longer follows $(\Delta t)^4$ as Δt goes beyond than 0.5, possibly because the error terms that scales as $(\Delta t)^5$ and even higher powers start to play an nonnegligible role. In the $(\Delta t)^4$ regime, assuming

$$\text{Local Error} = a(\Delta t)^5, \text{ i.e., Global Error} = aT(\Delta t)^4$$

With the fitting in Fig 4(b) gives:

$$\text{Global Error} / T = 0.008078(\Delta t)^4$$

It is thus be inferred that parameter a = 0.008078, i.e., the algorithm would become increasingly precise for the calculation of $\psi(T)$ as Δt becomes finer. However, the improvement is not that significant as $\Delta t < 0.01$ in practice, as be seen in Table 1. This could arise from the limit set by roundoff error. As a result, one may choose $\Delta t = 0.01\sim0.1$ to achieve the

best precision at a reasonable time cost.

Table 1 representative slopes at various Δt (atomic unit)

Δt	slope	Δt	slope
0.001	6.96E-08	0.01	4.75E-08
0.002	7.26E-08	0.1	8.20E-07
0.003	4.40E-08	0.2	1.39E-05
0.004	8.28E-08	0.3	6.98E-05
0.005	5.41E-08	0.4	2.14E-04
0.006	5.15E-08	0.5	4.82E-04
0.007	6.29E-08	0.6	8.31E-04
0.008	7.82E-08	0.7	1.07E-03
0.009	6.02E-08		