1. Time-dependent perturbation theory

We study a charged harmonic oscillator in an external electric field. The corresponding Hamiltonian reads

$$\begin{aligned} H &= H_0 + H_1 \\ H_0 &= \hbar\omega_0 \left(a^\dagger a \; + 1/2\right) \\ H_1 &= qE_0 f(t)\hat{X} \\ &= qE_0\sqrt{\frac{\hbar}{2m\omega_0}}\left(a^\dagger + a\;\right) f(t) \\ &:= \hbar\omega_1 \left(a^\dagger + a\;\right) f(t)\;. \end{aligned}$$

The unperturbed Hamiltonian H_0 has orthonormal eigenvectors $|n\rangle$ and eigenvalues

$$E_n = \hbar\omega_0 \left(n + 1/2\right) \qquad \text{with } n = 0, 1, \ldots$$

Moreover, we have

$$\begin{aligned} \langle m|a\;|n\rangle &= \sqrt{n}\;\delta_{m+1,n} = \sqrt{\max(n,m)}\,\delta_{m+1,n} \\ \langle m|a^\dagger|n\rangle &= \sqrt{n+1}\;\delta_{n+1,m} = \sqrt{\max(n,m)}\,\delta_{n+1,m} \end{aligned} \tag{1}$$

.

In the eigen basis of H_0, the time-dependent Schrödinger equation reads:

$$i\hbar\frac{d}{dt}\vec{c}(t) = H(t)\;\vec{c}(t)\;.$$

The matrix elements of the Hamiltonian are

$$H_{mn}(t) = \hbar\omega_0(n+1/2)\;\delta_{mn} + \hbar\omega_1 f(t)\;\delta_{|m-n|,1}\;\sqrt{\max(n,m)}$$

or rather

$$H(t) = \frac{\hbar\omega_0}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 \\ 0 & 0 & 0 & 7 & 0 \\ 0 & 0 & 0 & 0 & 9 \end{pmatrix} + \hbar\omega_1 f(t)\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

In order to solve the differential equation numerically, we consider a small time step Δt

$$\vec{c}(t+\Delta t) = \overbrace{\left(\mathbf{1} - \frac{i}{\hbar} H(t)\Delta t\right)}^{V} \vec{c}(t) + O(\Delta t)^2$$

This differencing scheme is not unitary and the norm $\|c(t)\|$ is not conserved. Alternatively, we write

$$\vec{c}(t+\Delta t) = \overbrace{\frac{\mathbf{1} - \frac{i}{\hbar} H(t)\Delta t/2}{\mathbf{1} + \frac{i}{\hbar} H(t)\Delta t/2}}^{U} \vec{c}(t) + O(\Delta t)^2 \tag{2}$$

The matrix U is obviously unitary and hence $\|c(t)\| = 1 \forall t$. We rewrite eq.2 into

$$\left(\mathbf{1} + \frac{i}{\hbar} H(t)\Delta t/2\right) \vec{c}(t+\Delta t) = \left(\mathbf{1} - \frac{i}{\hbar} H(t)\Delta t/2\right) \vec{c}(t) \tag{3}$$

which also known as Crank-Nicholson method. Since both matrices are tri-diagonal, the set of linear equations can easily be solved by *TridiagonalSolve.* Initially (at time zero) the system be in the ground state of the unperturbed harmonic oscillator, i.e. $\vec{c}(0) = (1, 0, \ldots, 0)^T$.

- Solve the time dependent Schrödinger equation numerically for the following time dependencies

$$\begin{aligned} f(t) &= 1 \\ f(t) &= \cos(\omega_2 t) \qquad . \end{aligned}$$

- Plot c_i for the lowest 5 indices.
- Determine $\langle \hat{x}(t) \rangle$. (Hint: Use eq.1)
- Compare $\langle \hat{x}(t) \rangle$ with $x(t)$ of a classical system.
- Compare the result with time-dependent perturbation theory.
- Study the dependence on the parameters ω_1, ω_2, on the cutoff n_max and on the size of Δt.

Remember:

$$\begin{aligned} p_{i \to f} &= \frac{2}{\hbar^2} |H_{if}|^2 \frac{\sin(\frac{\omega_{if}}{2} t)^2}{\omega_{if}} \\ \omega_{if} &= \omega_0 (n_f - n_i) \ . \end{aligned}$$

Analyze the probability $p_n(t)$ to find the System at time t in the n-th excited state. For time dependencies, it is useful to measure time in units of $1/\omega_0$, which corresponds to setting $\omega_0 \to 1$, $\omega_1 \to \tilde{\omega}_1 = \frac{\omega_1}{\omega_0}$, and $\omega_2 \to \tilde{\omega}_2 = \frac{\omega_2}{\omega_0}$