Solving the FMO

Here is the Hamiltonian describing a single excitation in the FMO complex from the latest work by Fleming: A. Ishizaki and G. R. Fleming, Proc. Natl. Acad. Sci. U.S.A. 106, 17255 (2009).

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The units are wavenumbers, i.e. cm^{-1}.

$$V = \begin{pmatrix} 12410 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 12530 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12210 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12320 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12480 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12630 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 12440 \end{pmatrix}$$

$$K = \begin{pmatrix} 0 & 87.7 & -5.5 & 5.9 & -6.7 & 13.7 & 9.9 \\ 87.7 & 0 & -30.8 & -8.2 & -0.7 & -11.8 & -4.3 \\ -5.5 & -30.8 & 0 & 53.5 & 2.2 & 9.6 & -6.0 \\ 5.9 & -8.2 & 53.5 & 0 & 70.7 & 17.0 & 63.3 \\ -6.7 & -0.7 & 2.2 & 70.7 & 0 & -81.1 & 1.3 \\ 13.7 & -11.8 & 9.6 & 17.0 & -81.1 & 0 & -39.7 \\ 9.9 & -4.3 & -6.0 & 63.3 & 1.3 & -39.7 & 0 \end{pmatrix}$$

$$KX = X\lambda \tag{1}$$

$$X = \begin{pmatrix} -0.2713781 & 0.4351370 & 0.1155647 & -0.0691068 & -0.1655553 & 0.8267552 & 0.0891404 \\ 0.2052872 & 0.6427755 & -0.5419359 & 0.4112510 & 0.2403535 & -0.0998430 & -0.1188969 \\ -0.6613888 & -0.2678740 & -0.0013524 & 0.6699533 & 0.0359892 & 0.0090086 & -0.2014764 \\ 0.3611684 & -0.3199886 & 0.0562502 & 0.3630684 & 0.4654431 & 0.3438680 & 0.5452517 \\ 0.2988589 & 0.1865958 & 0.7071748 & 0.2002269 & 0.2491240 & 0.0240024 & -0.5225318 \\ 0.4316540 & -0.3916357 & -0.3371893 & 0.1443333 & -0.4043355 & 0.3766622 & -0.4694742 \\ -0.2017213 & -0.1874828 & -0.2756656 & -0.4295554 & 0.6865415 & 0.2138464 & -0.3828575 \end{pmatrix}$$

$$\mathrm{diag}(\lambda) = \begin{pmatrix} -143.85474 & -92.22032 & -42.55453 & 0.95012 & 54.82277 & 94.65536 & 128.20133 \end{pmatrix}$$

A. units

In spectroscopy, the wavenumber $\tilde{\nu}$ of electromagnetic radiation is defined as

$$\tilde{\nu} = 1/\lambda \tag{2}$$

where λ is the wavelength of the radiation in a vacuum. The wavenumber has dimensions of inverse length and SI units of reciprocal meters (m^{-1}). A wavenumber can be converted into quantum-mechanical energy E in J or regular frequency ν in Hz according to

$$E = hc\tilde{\nu} = 1.9865 \times 10^{-23}\,\mathrm{J\,cm} \times \tilde{\nu} = 1.2398 \times 10^{-4}\,\mathrm{eV\,cm} \times \tilde{\nu}, \tag{3}$$

$$\nu = c\tilde{\nu} = 2.9978 \times 10^{10}\,\mathrm{Hz\,cm} \times \tilde{\nu} \tag{4}$$

Note that here wavenumber and the speed of light are in cgs units.

B. plot

We are interested in the population of the localized sites, given some starting state.

$$U(t) = Xe^{-it\lambda}X^\dagger \tag{5}$$

Let ψ_q be the localized wave function for the q^{th} BChl in the particle basis and let

$$\Pi_i \psi_q = \delta_{iq} \tag{6}$$

We start the system in particle basis ψ_i and want the probability of finding the particle in the q^{th} BChl

$$\mathrm{Prob}_q(t) = \mathrm{Tr}\left(\Pi_q |U(t)\psi_i\rangle\langle\psi_i U(t)|\right) = \mathrm{Tr}\left(\Pi_q U(t) \Pi_i U^\dagger(t)\right) = |\langle\psi_q|U(t)\psi_i\rangle|^2 \tag{7}$$

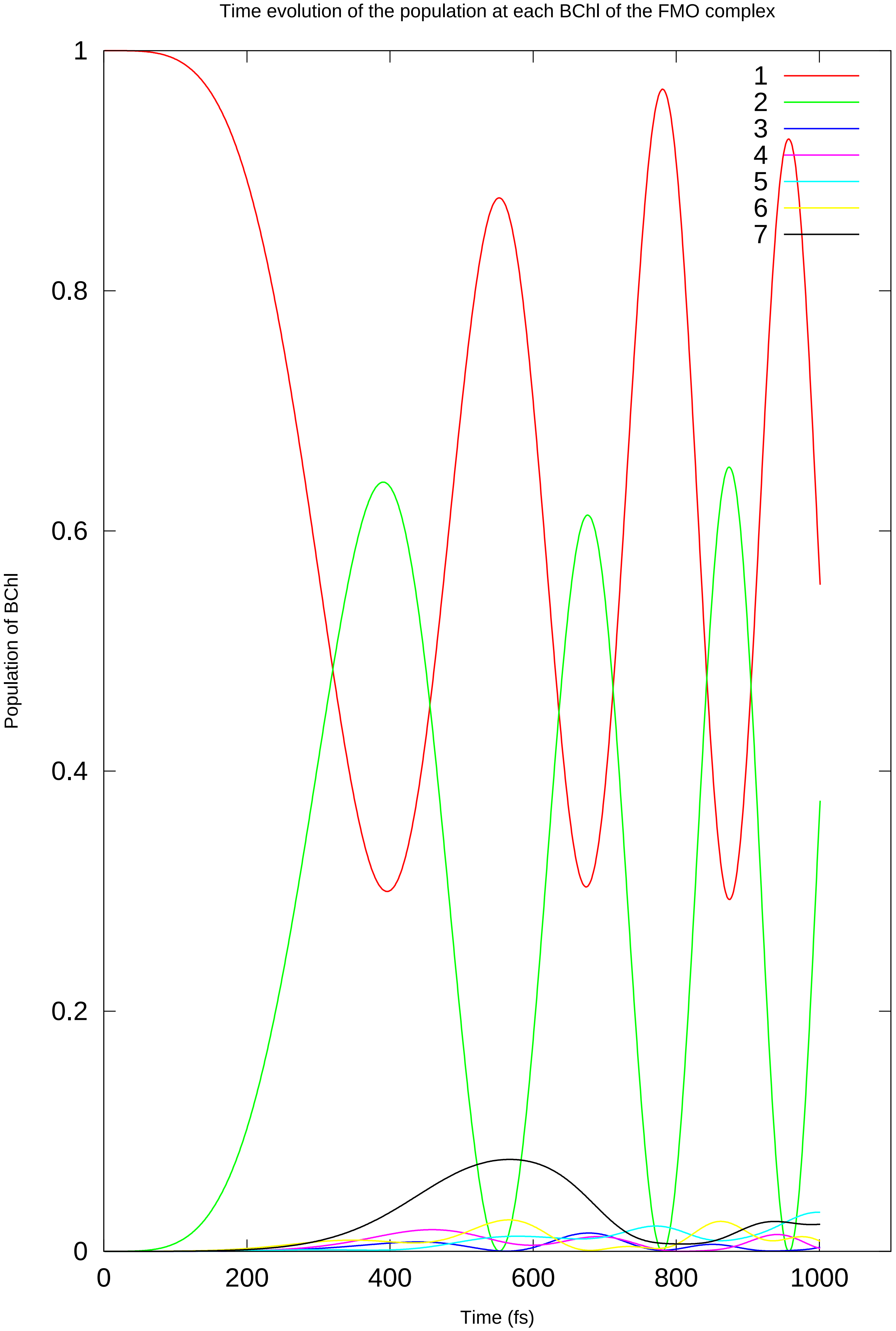

FIG. 1: Time evolution with initial state BChl-1 $|1\rangle$.