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Notes on the interpretation of the Fourier expansion of a time series

A discrete time series, where some property such as the velocity of an atom, is given at times t = 0, h, 2h, 3h, ... Nh, can be Fourier expanded, i.e. represented as a linear combination of sin and cos functions. When the operation is carried out, a list of the expansion coefficients is returned. The expansion coefficients correspond to angular requencies $\omega = \omega_1, \omega_2, ..., \omega_N = 0, \Delta\omega, 2\Delta\omega, 3\Delta\omega, ..., N\Delta\omega$. So, if a peak occurs at coefficient number k in the list, then the angular frequency corresponding to the peak is

$$\omega_k \;=\; (k-1)\;\Delta\omega$$

The smallest non-zero angular frequency, ω_1, that can be obtained from a time series where the total lenght of time is $Nh = T$ corresponds to the term $\sin(2\pi t/T)$, so

$$\omega_2 = \Delta\omega = \frac{2\pi}{T}.$$

So, the angular frequency corresponding to coefficient number k is

$$\omega_k = \frac{2\pi(k-1)}{T}.$$

The frequency is related to the angular frequency by

$$\nu_k = \frac{\omega_k}{2\pi}.$$

From the shape of the peak, it is possible to estimate where the maximum occurrs with higher resolution than the Fourier expansion gives. For example, if the magnitude of the expansion coefficient is equally large for coefficients 13 and 14, then the best estimate for the frequency corresponding to the maximum would be in between, corresponding to $k = 13.5$.

When comparing with the results of the normal mode analysis, it is important to remember that the eigenvalues are ω^2 in inverse time units squared. If the unit of energy is eV, the unit of mass is amu, the unit of length is , then the unit of time is ca. $10^{-15}\ sec = 10\ fsec$.