4 X-ray structural analysis

4.1 Fourier transform and X-ray crystallography

X-ray crystallography is the method with the highest currently available resolution power for structures of large macromolecules and macromolecular complexes. Since the technique of Fourier transform is central to this method, we first deal with some essential aspects of this technique:

4.1.1 Fourier transform

Mathematically the Fourier transform and inverse Fourier transform convert between two domains (spaces), e.g., the domain $\boldsymbol{r}$ (e.g., space or time) and the domain $\boldsymbol{k}$ (e.g., momentum or frequency):

Fourier transform: $$\mathrm{F}(\boldsymbol{k}) = (2\pi)^{-0.5} \int_{-\infty}^{\infty} \mathrm{f}(\boldsymbol{r})\ \mathrm{e}^{-2\pi i \boldsymbol{rk}}\, \mathrm{d}\boldsymbol{r} \tag{4.1}$$

Inverse Fourier transform: $$\mathrm{f}(\boldsymbol{r}) = (2\pi)^{-0.5} \int_{-\infty}^{\infty} \mathrm{F}(\boldsymbol{k})\ \mathrm{e}^{2\pi i \boldsymbol{rk}}\, \mathrm{d}\boldsymbol{k} \tag{4.2}$$

Fig. 4.1 illustrates a one-dimensional Fourier transform: (b) Represents the decomposition of the signal from (a). This decomposition was calculated from the Fourier transform (c). The inverse transform of (c) yields back exactly (a). (d) Is the inverse Fourier transform of the signal of (c) with all phases set to zero instead of using the correct phases. The comparison of (d) with (a) illustrates the importance of the phases in Fourier transform: in order to be able to correctly obtain back the original signal by inverse Fourier transform, both the amplitudes and the phases have to be known.

Three examples in Figs. 4.2–4.4 demonstrate the method of two-dimensional Fourier transform: Fig. 4.2b represents the Fourier transform of the hexagonal arrangement of peaks of Fig. 4.2a. In Fig. 4.3a some of Fourier components with low amplitudes are set to zero, and yet the inverse Fourier transform (Fig. 4.3b) shows that essentially all information is still preserved. Fourier transforming a noisy object, then substituting certain low-amplitude parts of the Fourier transform by zeros, and then inverse-transforming the modified Fourier transform, is an efficient method for noise reduction. Figs. 4.4a and 4.4b show the result when using only a small slice of the Fourier transform for the calculation of the inverse

Fourier transform: significant distortions are observed along the coordinate for which too few Fourier components were utilized for reconstruction.

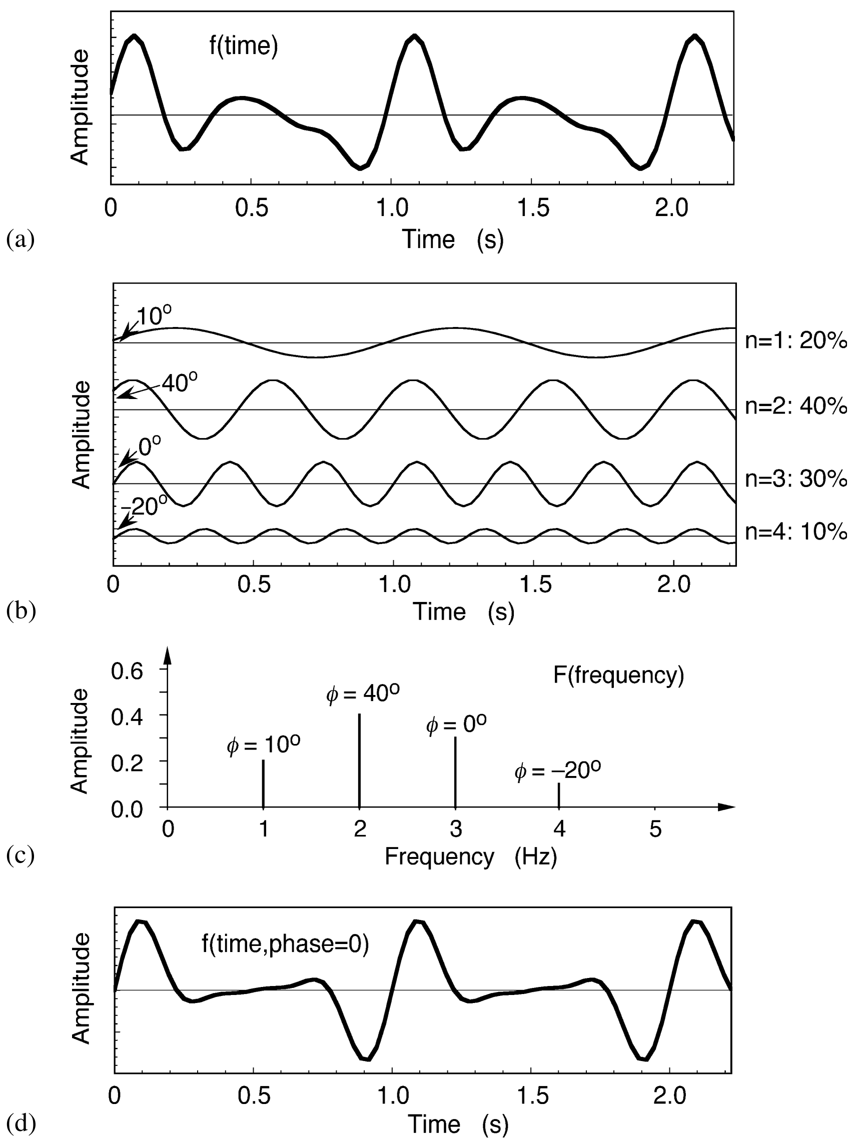

Fig. 4.1 Example for the effect of the loss of phase information on the inverse Fourier transform: With the correct phases, the four frequency components (**b**) add to the sum shown in (**a**). However, when adding the four components with the wrong phase 0, we obtain the wrong sum (**d**). (**c**) Represents the Fourier transform of (**a**). In (**a**), (**b**), (**c**) only a fraction of the function is shown; the complete function is periodical in $(-\infty, \infty)$