Interactive Tools for Teaching Fourier Transforms

Carlos R. Baiz*

Department of Chemistry, University of Texas at Austin
105 E. 24th St. Stop A5300, Austin, Texas 78712
*cbaiz@cm.utexas.edu

Running title: Interactive Fourier Transforms

Keywords: Fourier; patterns; webcam; lesson; undergraduate

Abstract

Fourier transforms (FT) are universal in chemistry, physics, and biology. Despite FTs being a core component of multiple experimental techniques, undergraduate courses typically approach FTs from a mathematical perspective, leaving students with a lack of intuition on how a FT "works". Here we introduce interactive teaching tools for upper-level undergraduate courses and describe a practical lesson plan for FTs. The materials include a computer program to capture video from a webcam and display the original images side-by-side with the corresponding plot in the Fourier domain. Several patterns are included to be printed on paper and held up to the webcam as input. During the lesson, students are asked to predict the features observed in the FT, and then place the patterns in front of the webcam to test their predictions. This interactive approach enables students with limited mathematical skills to achieve a certain level of intuition for how FTs translate patterns from real space into the corresponding Fourier space.

1. Introduction

Fourier Transforms (FT) are an essential mathematical tool for numerous experimental and theoretical methods. Biophysical characterization techniques, including NMR spectroscopy,(1) infrared spectroscopy,(2) x-ray crystallography,(3) mass spectrometry,(4) and differential scanning calorimetry rely on Fourier transforms for data processing or analysis.(5) Spatial reconstruction algorithms based on Fourier transforms are at the core of modern biomedical imaging applications such as magnetic resonance imaging.(6) Modern molecular dynamics simulation packages implement fast FT algorithms to improve computational accuracy and efficiency.(7) While certain experimental methods such as infrared spectroscopy are nearly universal in undergraduate teaching laboratories, FTs are automatically carried out by internal software libraries using pre-programmed settings which are typically hidden from the user.(8) Developing an intuitive understanding of FTs is therefore essential for undergraduate students to fully grasp the principles behind these techniques. While there are many excellent articles and textbooks on Fourier methods, pedagogical approaches can be highly mathematical,(9-11) introduced within the context of specific techniques,(12) or brief and oversimplified.(13) Thus, it is challenging for students not equipped with strong mathematical skills to understand what a FT "does", and more so to acquire intuition for how a FT translates one function into its conjugate function in the Fourier domain.

Modern pedagogical approaches are designed to develop competency across the entire cognitive spectrum: *Remembering, Understanding, Applying, Analyzing, Evaluating, and Creating.*(14) There is a need for classroom activities that provide students with hands-on experience utilizing Fourier techniques. Students should gain a conceptual understanding of how patterns in one domain are translated into its conjugate domain, as well as more practical knowledge such as intuitively predicting the effect of a Fourier filter. Specifically, it is important for instructors to address advanced learning goals by providing opportunities for students to generate, analyze, and evaluate predictions. Here we present an interactive lesson plan that uses computer software to enable students to predict 2D FTs of various patterns and test their predictions in real time. Figure 1 shows an example of the reciprocal relationship between real and Fourier space where a periodic grid pattern is translated into a series of peaks. The spacing between Fourier peaks is inversely proportional to the spacing between lines in real space.

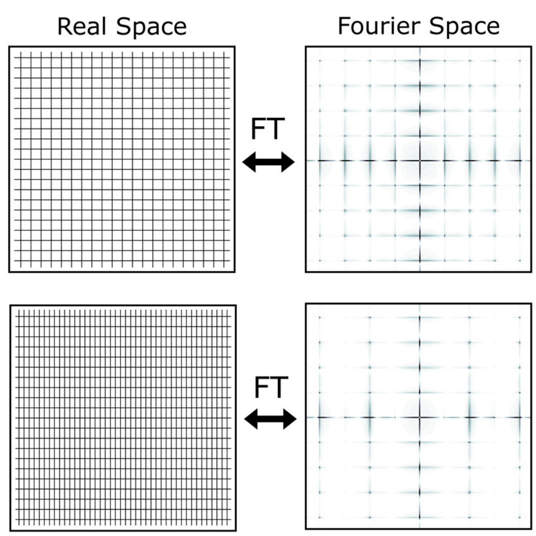

Figure 1– Two example periodic grid patterns (left) alongside their absolute value 2D Fourier Transforms (right). Dark colors represent areas of higher intensity. The upper grid shows a series of equally spaced peaks in the Fourier domain. The lower pair shows the effect of doubling the periodicity along the horizontal axis. The lower FT pattern maintains the spacing of peaks along the vertical but doubles the spacing along the horizontal.

2. Scientific and Pedagogical Background

Fourier transforms are typically introduced in upper-division undergraduate or graduate courses. The typical lecture begins with the concept of Fourier series.(9) Within this approach, a function in one domain, for example, a function in space, (x), is described as a linear combination of functions in a conjugate domain, such as reciprocal space, q:

$$F(x) = \sum_{k=0}^{\infty} A_k \cos(q_k x) + B_k \sin(q_k x), \tag{1}$$

where A_k, and B_k are the Fourier coefficients, which are interpreted as the amplitude of a component with a given periodicity q_k. This mathematical transformation is analogous to a change of basis, where the original function is decomposed into coefficients in reciprocal space, much like a change of coordinate systems in Euclidean space. In this analogy, the Fourier coefficients represent the projections of the original function onto the sine or cosine basis coordinates. In general, there is no information loss in converting between domains since, given a FT, the original function can be recovered by performing the corresponding inverse transformation. Mathematically, the Fourier transform may be introduced as a limit of the Fourier series:

$$F(x) = \int_{-\infty}^{\infty} f(q) \exp\left[-i2\pi(q_x x)\right] dx \cdot \tag{2}$$

Extending Fourier methods to multiple dimensions is seldom introduced in undergraduate courses, despite multidimensional transforms being essential in techniques such as molecular dynamics simulations,(7) x-ray crystallography,(15) or NMR spectroscopy.(16, 17) It is therefore important to expose students to multidimensional FT methods alongside these techniques. Consider a function in the x-y plane; the 2D FT of this function may be interpreted as a one-dimensional FT along the x dimension followed by a second FT along the y dimension, and the result is invariant with respect to the order of operation.

Formally, a two-dimensional FT can be written as a double integral:

$$F(q_x, q_y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x, y) \exp\left[-i2\pi(q_x x + q_y y)\right] dxdy \tag{3}$$

where x and y represent real space and q_x, q_y are the corresponding coordinates in Fourier space. While $F(q_x,q_y)$ is a complex function, its modulus or modulus squared is often displayed for ease of visualization. Further, while the definition above is an integral over all space, numerical algorithms involve sums over discrete data points, analogous to the Fourier series concept introduced above (Eq. 1). The Fast Fourier transform (FFT) algorithm is arguably the most ubiquitous implementation due to its computational efficiency.(8) Numerical FTs are subject to sampling criteria, such as the Nyquist limit, but these concepts are typically outside the scope of introductory courses.(18, 19) The software package described here allows for introducing multidimensional Fourier transforms, together with Fourier filters, as well as more advanced concepts and numerical considerations, such as aliasing.(9)

3. Materials and Methods

a. Software description

The software presented here is written in the MATLAB R2019a (The Mathworks, Natick, MA) programming language. Source code, documentation, and pre-compiled standalone executables for Microsoft Windows and macOS operating systems are available on GitHub (github.com/carlosbaiz/fouriertransforms/). Figure 2 shows a screenshot of the main user interface. The interface displays an image in real-time (Figure 2B), along with its Fourier-transform (Figure 2D). The user control enables adjusting the number of frames displayed per second, the FT horizontal and vertical axis scales, and the colormap scale.

Spectral filtering functions can be applied in the Fourier domain, with the results shown in the reconstructed image. Two filter types are available: 1. Boxcars filter, represented by a circle centered at the origin in the Fourier plane. 2. Gaussian filter, represented by a two-dimensional Gaussian function in the Fourier plane (Figure 2E). These two functions can be applied as low- or high-pass filters. The reconstructed image (Figure 2C) shows the effect of the filter. It is important to note that the displayed Fourier image represents the absolute value, or modulus, of the otherwise complex Fourier plane, but the full complex FT representation is used to reconstruct the real-space function. Therefore, the software cannot be used to illustrate phase effects in the Fourier domain, an important consideration for techniques such as x-ray diffraction crystallography.(20)

In this example, the input pattern is a random distribution of vertically elongated oval shapes (Supplemental Information, Pattern 7). Horizontally elongated rings are observed in the Fourier domain (Figure 2D). These rings are directly related to the size and shape of the ovals. The image illustrates how FTs can extract information related to the molecular shape despite random positions of molecules in real space. For example, the well-known diffraction photograph of partially aligned nucleic acid fibers recorded by Franklin and Gosling showed several diffraction spots arranged in an "X" pattern oriented along the vertical axis, together with oval shaped diffraction rings. The pattern show clear evidence of a helical conformation despite the random translation and partial orientation of the DNA strands.(21) The recorded pattern was later analyzed and the double-helix structure of B-DNA was proposed.(22)

The Supplemental Information includes a set of patterns that can be printed on paper and used as inputs to the FT program in the lesson described below. This program bridges the gap between physical and digital domains by providing a physical "input" in the form of a pattern on paper that becomes digitized. This tool complements a traditional lecture by providing a platform for instructors to address advanced educational goals.(14)

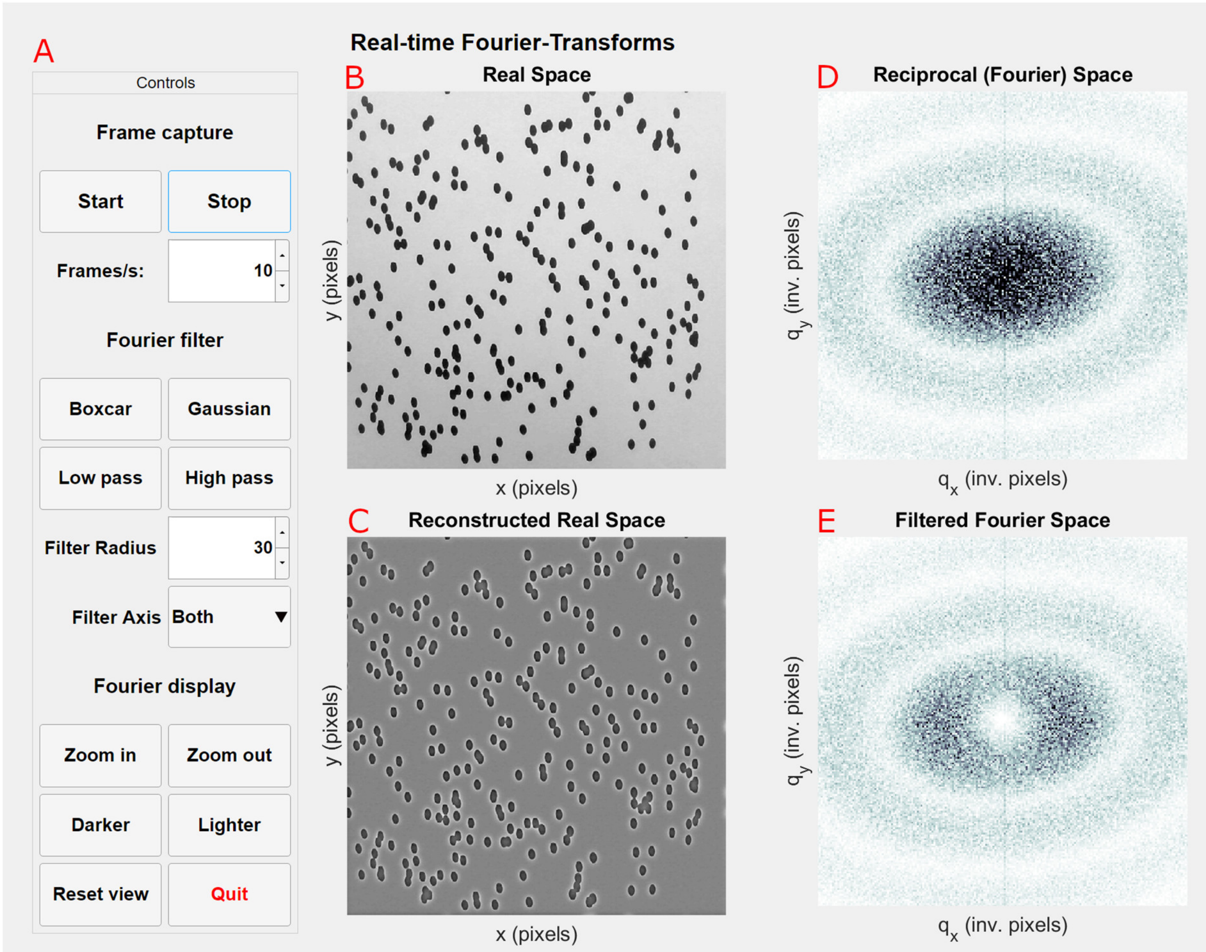

Figure 2– Screenshot of the user interface. ***A.*** *The user control panel includes buttons for starting/stopping the frame acquisition process. Fourier filter settings: type of filter (Boxcar, or Gaussian), Low pass or High pass modes, and filter radius. The filter can be applied in the horizontal dimension, the vertical dimension, or both dimensions simultaneously.* ***B.*** *In the center column, the top figure displays the images captured by the webcam which are converted into grayscale by equally combining the red, green, and blue channels.* ***C.*** *The reconstructed image, obtained by inverse transformation after applying the filter, is displayed below the main image.* ***D.*** *The right-hand column shows the FT of the acquired image using a similar grayscale color map as the original image.* ***E.*** *The filtered FT is included underneath the main FT plot. In this example, a card with a random arrangement of oval-shape dots is held in front of the webcam. The FT plot shows "rings" that contain information on the size and shape of these ovals. The FT plot displays the absolute value for simplicity. The center of the image represents* $q_x=q_y=0$*. In this example, the applied filter is a 30-inverse-pixel high pass Gaussian filter. The reconstructed image lacks the variations in the background that are observed in the original image. The "noise" observed in the FT patterns is due to pixel noise that results from the webcam and background lighting. Proper lighting is recommended for best results. A portable reading light or a desk lamp can be used if classroom lighting is insufficient. In a classroom setting, the computer should be connected to a projector.*

b. Lesson plan

The lesson presented here has a primary learning objective: Students will intuitively understand the reciprocal relationship between real and Fourier space and how periodicity is translated across domains. This lesson should be preceded by a mathematical introduction to Fourier transforms, following the typical approach of upper-level undergraduate textbooks, as outlined in the introduction.(9, 11) The instructor begins the lesson by demonstrating a selection of example patterns, such as the patterns shown in Figure 1. The instructor should describe each pattern in real space and explain the origin of the features observed in the corresponding Fourier space. Certain patterns have direct analogies to specific experiments or experimental techniques, and the instructor may use this part of the lesson to describe analogies to FT applications in biophysics. For example, the helical pattern in Figure 3 produces an "X" that resembles the historic DNA x-ray diffraction pattern first recorded by Franklin and Gosling.(21, 23) Pattern 14 in the Supplemental Information contains a distribution of partially aligned helices, with random tilt angles. The Fourier-transform of this image produces an "X-shaped" pattern with specific peaks displaying lower intensity. Namely, counting outwards from the center of the diffraction pattern, and labeling the center as the first peak, the fourth peaks in "X" are suppressed compared to the others. The suppressed peaks are a well-known characteristic of the diffraction pattern of DNA.(24)

During this part of the lesson, the instructor should emphasize the following concepts: **1.** Real and reciprocal spaces are inversely related. The instruction can demonstrate this relationship in several ways: For example, moving the paper closer to the webcam "zooms in" on the pattern, effectively increasing the period and causing the FT features to move closer to the center of the FT plot. Several patterns with different periodicities are provided in the Supplemental Information. **2.** Periodicity appears as discrete "peaks" in the Fourier domain. Together, these examples help students develop a conceptual foundation for interpreting Fourier transforms in two dimensions. Specific patterns, such as the pair shown in Figure 1 are provided with the dual purpose of illustrating how periodicity in real space is translated into discrete peaks, as well as showing how decreasing the period in real space generates peaks spaced further apart in reciprocal space. **3.** The built-in high and low pass filters can be applied to display how different frequency components are represented in the reconstructed image. The instructor can select specific cutoff frequencies, and toggle high and low pass filters to demonstrate how images can be represented as a sum of low-frequency "smooth" components along with certain high-frequency "sharp" components. The software enables the user to apply filters in either horizonal, vertical, or both dimensions simultaneously. The duration of this first introduction to FTs should typically occupy 15-20 minutes of the lecture period.

During the second half of the tutorial, the instructor hands out a different pattern to each student. Students spend a few minutes studying their assigned pattern and are then asked to predict the expected features in the Fourier domain. Each student then brings their pattern to the front of the classroom, shows it to the class, and describes their predictions. The class is asked if they agree or disagree with the student's interpretation. When students are not in agreement, a short discussion should follow. While the purpose of this exercise is to enable students to apply their knowledge, asking each student to announce their prediction to the entire class provides a valuable opportunity to engage all students including students who are otherwise timid or reluctant to participate. The instructor should refrain from validating or discrediting student's predictions. The student is then asked to hold their assigned pattern up to the webcam to reveal the Fourier features. Following the "experiment", the student is asked to reevaluate their prediction. If the prediction was correct, the concept is further reinforced; if the prediction was incorrect, the instructor may take the opportunity to clarify key misconceptions. For instance, a common misconception is that students fail to predict the inverse relationship between real and reciprocal space. Once the students have observed the patterns, the instructor may also use the opportunity to describe the analogies of certain patterns to the class, such as the DNA helix analog shown in Figure 3.

Finally, as a mastery component of the lesson, students can be given blank sheets of paper and asked to create a new pattern and predict the FT features. During this portion of the lecture, students are encouraged to work in small groups, where they can discuss the concepts, and create patterns that give rise to interesting FT features. Students can make simple modifications to the existing cards, such as drawing one pattern over another one or can draw entirely unique patterns. Since FTs are linear transformations when two patterns are superimposed in real space, in general, an overlay of the two individual FT patterns is observed in reciprocal space. Note that the modulus of the complex FT function is displayed in the program for ease of visualization, artifacts may therefore be present as a result of not displaying the real and imaginary components separately.

The entire lesson should last approximately one class period, about 45 minutes. The described lesson is ideal for a class size of 10-15 students. In larger classes, students may work together in groups of two or more. This pedagogical tool addresses learning outcomes across all levels of the cognitive spectrum, Remembering, Understanding, Applying, Analyzing, Evaluating, and Creating, ensuring that students achieve full competency in this topic.

Mastery of the material can be tested in exams or homeworks by designing exercises that require students to match a real-space pattern with the corresponding Fourier pattern or to predict the effect of a Fourier filter in the reconstructed image. For example, a student may be given an image with a superimposed periodic pattern and asked to explain how FTs can be used to suppress the pattern and recover the original image. Students are asked to explain their thought process for a more in-depth evaluation of their conceptual understanding.

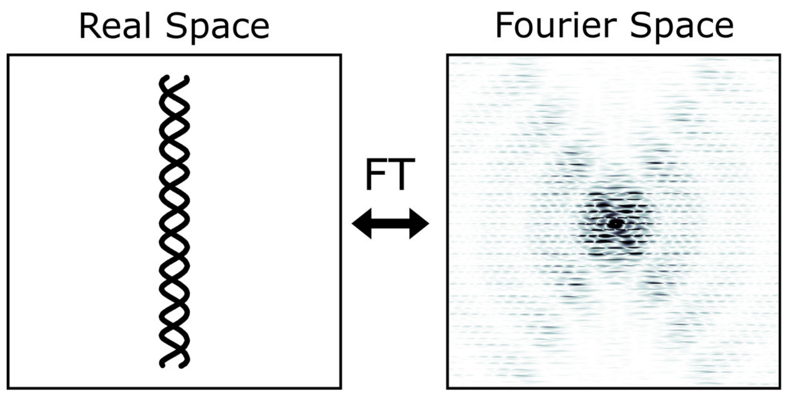

Figure 3– The image on the left resembles a 2D projection of the helical structure of B-DNA. The Fourier domain shows an X-like shape analogous to the crystal x-ray diffraction pattern. The "rings" observed in the pattern are a result of the curved edges used to represent the 2D projection of each turn. The helix was generated using the PyMOL molecular graphics program. See S1 Pattern 12.

4. Results

This lesson plan described here has been implemented in the curriculum of two courses at the University of Texas at Austin, an upper-level undergraduate course in Biophysics and a graduate-level course in Time-Dependent Quantum Mechanics and Spectroscopy. Students have been responsive to the lesson, and together with a traditional lecture on Fourier transforms, this interactive activity has been successful for communicating the "concept" of Fourier transforms beyond the traditional mathematical approach that is commonly used. The activity is compatible with student-centered pedagogical approaches such as flipped classroom environments. In addition to the material covered, group work, advanced hands-on predictions, and teamwork are important elements of the lesson that are difficult to address using a more traditional approach.

5. Conclusion

We have presented an interactive lesson plan developed around a real-time FT program to develop competency and intuition among upper-level undergraduate and graduate students. The lesson illustrates the use of consumer technology to perform "experiments" in the classroom and bridge the gap between the digital and physical worlds. Instructors may adopt the lesson across different courses in the physical sciences. Previous experience shows that students are not only responsive to this approach but find the lesson instructive and enjoyable.

6. Author Contributions

CRB designed and implemented the lesson plan, wrote the software, designed the patterns, and wrote the manuscript.

7. Acknowledgments

The author acknowledges Prof. Kevin Kubarych (University of Michigan, Ann Arbor) for the original idea for the program. Jennifer C. Flanagan (University of Texas at Austin) compiled tested the software for the macOS platform. The work has been generously supported by the Welch Foundation (F-1891), as well as by the National Science Foundation through grants BIO-1815354 and CHE-1847199. We thank the students at the University of Texas at Austin for useful feedback on the software and lesson plan.

8. References

1. Becker, E. D. 1999. High resolution NMR: theory and chemical applications. Elsevier.
2. Low, M. J. D. 1969. Infrared Fourier transform spectroscopy. Analytical Chemistry 41(6):97A-108a.
3. Galli, S. 2014. X-ray crystallography: One century of nobel prizes. Journal of Chemical Education 91(12):2009-2012.
4. Hu, Q., R. J. Noll, H. Li, A. Makarov, M. Hardman, and R. Graham Cooks. 2005. The Orbitrap: a new mass spectrometer. Journal of mass spectrometry 40(4):430-443.
5. Danley, R. L. 2003. New modulated DSC measurement technique. Thermochimica acta 402(1-2):91-98.
6. Liang, Z.-P., and P. C. Lauterbur. 2000. Principles of magnetic resonance imaging: a signal processing perspective. SPIE Optical Engineering Press.
7. Darden, T., D. York, and L. Pedersen. 1993. Particle mesh Ewald: An N· log (N) method for Ewald sums in large systems. The Journal of chemical physics 98(12):10089-10092.
8. Frigo, M., and S. G. Johnson. 2005. The design and implementation of FFTW3. Proceedings of the IEEE 93(2):216-231.
9. Butz, T. 2006. Fourier transformation for pedestrians. Springer.
10. Bialek, W. 2012. Biophysics: searching for principles. Princeton University Press.
11. Bracewell, R. N. 1986. The Fourier transform and its applications. McGraw-Hill New York.
12. Zaccai, N. R., I. N. Serdyuk, J. Zaccai, and G. Zaccai. 2017. Methods in Molecular Biophysics. Cambridge University Press.
13. Phillips, R., J. Theriot, J. Kondev, and H. Garcia. 2012. Physical biology of the cell. Garland Science.
14. Krathwohl, D. R., and L. W. Anderson. 2009. A taxonomy for learning, teaching, and assessing: A revision of Bloom's taxonomy of educational objectives. Longman.
15. Patterson, A. L. 1934. A Fourier series method for the determination of the components of interatomic distances in crystals. Physical Review 46(5):372.
16. Williams, K. R., and R. W. King. 1990. The Fourier transform in chemistry—NMR: Part 3. Multiple-pulse experiments. Journal of Chemical Education 67(4):A93.
17. Williams, K. R., and R. W. King. 1990. The Fourier transform in chemistry—NMR: Part 4. Two-dimensional methods. Journal of Chemical Education 67(5):A125.
18. Steel, C., T. Joy, and T. Clune. 1990. Teaching FFT principles in the physical chemistry laboratory. Journal of Chemical Education 67(10):883.
19. Ramirez, R. W. 1975. The FFT: Fundamentals and concepts. Tektronix.
20. Taylor, G. L. 2010. Introduction to phasing. Acta Crystallographica Section D: Biological Crystallography 66(4):325-338.
21. Franklin, R. E., and R. G. Gosling. 1953. Molecular configuration in sodium thymonucleate. Nature 171(4356):740.

22. Watson, J. D., and F. H. Crick. 1953. Molecular structure of nucleic acids. Nature 171(4356):737-738.
23. Lucas, A., P. Lambin, R. Mairesse, and M. Mathot. 1999. Revealing the backbone structure of B-DNA from laser optical simulations of its X-ray diffraction diagram. Journal of chemical education 76(3):378.
24. Nelson, P. 2017. From photon to neuron: Light, imaging, vision. Princeton University Press.