Computational Physics III: Fourier transforms and analysis

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Problem 1

Discrete Fourier transform

The Fourier transform is a mathematical operator that changes the way a complex valued function defined over the real space $\mathbb{R}^n$ is described, by describing the function in terms of the frequencies that it contains. Formally, the Fourier transform of a function f is defined as follows:

$$\mathcal{F}(f)(\mathbf{k}) := \hat{f}(\mathbf{k}) = \int_{\mathbb{R}^n} f(x) \cdot e^{-2\pi i \mathbf{k}\cdot\mathbf{x}} d\mathbf{x}, \tag{1}$$

where $\mathbf{k}$ is an element from the so-called Fourier space, or frequency space, and $\mathbf{x} \in \mathbb{R}^n$. For the sake of simplicity, in what follows, we will focus only on the 1-dimensional case, so the Fourier transform reads

$$\mathcal{F}(f)(k) := \hat{f}(k) = \int_{R} f(t) \cdot e^{-2\pi i k t} dt. \tag{2}$$

The discrete Fourier transform aims at computing the integral from Eq.(2) over a discrete set of points. To do so, one needs to discretize the real and the Fourier spaces, that is describe f over a discrete set of points $f \to f(t_n)$, $n \in \mathbb{N}$. However, in order for the discrete transform to be implemented numerically, the function can only be described on a finite set of points. Choosing the same number of grid points (N) for both the real and Fourier spaces, the discrete formulation of Eq.(2) reads

$$\hat{f}[m] = \sum_{n=0}^{N-1} f[n] e^{-2\pi i m n / N}, \tag{3}$$

where $f(t_n) = f[n]$ and $\hat{f}(k_m) = \hat{f}[m]$. Then, the numerical implementation of the above Eq.(3) is straightforward, and the algorithm is shown below:

Discrete Fourier transform algorithm

Listing 1: Matlab script for the discrete Fourier transform algorithm

```
function discrete_fourier = mydft(F)
    N    = length(F);   % spatial domain
    temp = zeros(size(F));
    for m = 0:(N-1)     % Fourier space variable
        for n = 0:(N-1) % real space variable associated to domain of F
            temp(m+1)= temp(m+1) + F(n+1)*exp(-2*pi*1j*m*n/N);
        end
    end
    discrete_fourier = temp;
end
```

Problem 2

NMR spectroscopy

The structure of molecules and solids can be determined by mean of NMR spectroscopy. To do so, the transitions between different quantum states of nuclear spins (of protons) in an externally applied magnetic field are studied. More precisely, the spins are excited by radio-frequency waves and their relaxation is recorded. The recorded signal is called the free-induction decay (FID). The Fourier transform of the FID yields the NMR spectrum.

Problem 3

Radix-2 FFT algorithm

Problem 4

Fourier Ptychography

Fourier ptychograpghy enables to overcome the problem of limited resolution in conventional optical microscopy by generating a wider aperture, that is by allowing a wider range of angles under which the light can be captured by the microscope. Indeed, denoting the resolution by $\mathcal{R}$, one gets the following relation:

$$\mathcal{R} \propto \frac{\lambda}{n\sin(\theta)}, \tag{4}$$

where λ is the wavelength of the incoming light, n the refractive index of the lens and θ the maximum angle of acceptance. It is then trivial that increasing θ will increase $\mathcal{R}$.

In order to understand the Fourier ptychography algorithm, let us recall how a typical optical microscope works. Considering that the studied object can be represented by a 2-dimensional complex function O, that is the real space image is given by $O(x, y)$, where (x, y) is an appropriate coordinate choice. Thus, the reciprocal (Fourier space) image is given by $\mathcal{F}(O)(k_x, k_y) \cdot a(k_x, k_y)$, where $\mathcal{F}$ represents the Fourier transform operator and a an amplitude transfer function of finite radius. The latter can be approximated by a low-pass filter of radius r_c, mapping to 1 below r_c and 0 otherwise. The real image is then reconstructed after the light passes through the second lens, and the detector will record an intensity $I \propto |\mathcal{F}^{-1}\Big(\mathcal{F}(O)(k_x, k_y)\cdot a(k_x, k_y)\Big)|^2$.

In Fourier ptychography, the process is slightly different since instead of using perpendicular plane waves $\propto e^{ik_{zi}z}$ as illumination sources, several images are taken with tilted light sources $\propto e^{ik_{xi}x}e^{ik_{yi}y}e^{ik_{zi}z}$. Then by the transfer theorem from Eq.(**??**), the Fourier transform is shifted as follows:

$$\mathcal{F}(O)(k_x - k_{xi}, k_y - k_{yi}), \tag{5}$$

and hence, the intensity recorded by the microscope verifies

$$I \propto \left|\mathcal{F}^{-1}\Big(\mathcal{F}(O)(k_x - k_{xi}, k_y - k_{yi}) \cdot a(k_x, k_y)\Big)\right|^2. \tag{6}$$

The cutoff circle has then been shifted by (k_{xi}, k_{yi}) and some higher frequencies were involved in the image formed. Thus, taking several images under tilting angles enables to reconstruct the Fourier transform with a higher cutoff radius, and enhance the resolution.

Numerical implementation of Fourier ptychography algorithm

In the next part, the following reconstruction algorithm will be used:[IS16]

1. Start with a (complex) guess function I and compute $\mathcal{F}(I)$.
2. Restrict $\mathcal{F}(I)$ to a circle in Fourier space, centered around (k_{xi}, k_{yi}) multiplying it by a cutting function: $\mathcal{F}(I) \to \mathcal{F}(I)_c = \mathcal{F}(I) \cdot C_{(k_{xi},k_{yi})}$

3. Take its inverse Fourier transform $\mathcal{F}^{-1}(\mathcal{F}(I)_c)$
4. Retain the phase but replace the magnitude by the experimental one
5. Perform the Fourier transform of the resulting object and use it to replace the values of $\mathcal{F}(I)$ inside the cutoff circle
6. Repeat the previous steps for the the circles in Fourier space, that is for different values of (k_{xi}, k_{yi})
7. Repeat the previous algorithm till convergence is reached

References

[IS16] Toshitaka Idehara and Svilen Petrov Sabchevski. Gyrotrons for high-power terahertz science and technology at FIR UF. *Journal of Infrared, Millimeter, and Terahertz Waves*, 38(1):62–86, oct 2016.