OPTI 571L Lab 6: Atom Diffraction and Interference I.

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In this lab you will numerically model and graphically display the process of atom diffraction and interference as atom waves propagate through slits and gratings. This lab is based on four published experimental papers, and you will construct routines that simulate the processes of these papers. The first paper and simulation investigates diffraction of an atomic beam upon passing through a material slit. The second simulation involves the atomic Talbot effect. The third covers a Young's double slit apparatus for atoms. The final simulation is of an atomic interferometer with standing waves of laser light that serve as beamsplitters.

The simulations are all very similar to one another; after your first simulation is successfully written (which shouldn't take too much time), the others should follow quickly. In each, you will take a 1D wave function that corresponds to an atomic plane wave after it passes through a narrow slit. Through a series of FFT and IFFT operations, you will calculate the wave function as it propagates through free space, and is incident on amplitude masks or phase gratings.

Keywords: Atom optics, atom diffraction, atom interferometer, atom beam propagation, Fourier transforms for wavefunctions, single-slit diffraction, double-slit diffraction.

I. BACKGROUND

One approach to simulating atom beam diffraction past a narrow slit uses a propagator and integral approach. That approach is suitable for studying far-field diffraction, but becomes numerically difficult when calculating wave function propagation over short distances. You may explore that approach in a separate lab. Here, we will use Fourier transforms instead of the wave function propagator and integration approach.

Consider a quantum state $|\Psi(t_0)\rangle$ that can be represented as a 1D wave function $\Psi(x, t_0)$ over the position coordinate x. These quantities are defined at time t_0. For a free particle, the quantum state at time t is given by $|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle$, where

$$U(t, t_0) = \exp\{-iP_x^2\,(t - t_0)/2m\hbar\},$$

m is the mass of the particle, and P_x is the x-direction momentum operator. Because P_x takes the form of a multiplicative function in the momentum representation, it is easiest to evaluate the wave function $\Psi(x, t)$ by first expressing the initial state in the momentum representation (i.e., the Fourier transform of $\Psi(x, t_0)$), then multiplying this function by the momentum representation of $U(t, t_0)$, which is equal to $\exp\{-ip_x^2\,(t-t_0)/2m\hbar\}$. Here, p_x is the 1D momentum coordinate. Finally, an inverse transform on the result produces $\Psi(x, t)$. If this method is applied repeatedly for small time steps dt, one can approximate the continuous change of Ψ in time. For the case of a monochromatic (single deBroglie wavelength) atomic beam propagating through an apparatus along the direction z with a z-momentum of p_z, this result is equivalent to a 2D wave function $\Psi(x, z = t\,p_z/m)$, where the different points along the spatial dimension z correspond to different points in time. This is the quantity that you will calculate in each of the simulations of this lab, displaying the 2D probability density distribution $|\Psi(x, z)|^2$ in each case.

Generally, when using FFT routines in this type of approach to model wave function propagation, one must pay careful attention to the spatial grid: the grid increment dx is inversely proportional to the maximum momenta that will be contained within the plane-wave expansion (via the FFT), and the real-space grid length will be inversely proportional to the momentum increment dp between neighboring plane-wave components of the Fourier transform. For this reason, you will need to use a spatial grid that corresponds to spatial scales much larger than that the overall width (in x) of the wave function with which you are working. You will be able to test this constraint with your code, and build experience that should help in future work with Fourier transforms performed using FFT routines.

In your routines, you can neglect the calibration of $\Psi(x, z)$ in order to make it useful for calculating atom number or flux. Thus as long as your FFT routines preserve normalization, you don't need to worry about making sure your wave functions are always suitably normalized.

II. DIFFRACTION OF AN ATOMIC BEAM DUE TO A NARROW SLIT

This simulation is an alternative approach to that taken in the special project of the same topic often given in OPTI 570A. The simulation is based upon the experiment of Ref. [1]. Find and download this paper for reference, and read or skim the paper to familiarize yourself with the setup and the results. In your simulation, you will calculate probability density distributions that

correspond to those of Figs. 2 and 3 of the paper.

A. Procedure in detail

For this simulation, construct a MATLAB routine that first defines physical constants and experimental parameters. Since the different simulations that you will write use different atomic masses, it is convenient to define the neutron mass as a constant and then to scale this to the relevant atomic mass via the number of nucleons in the atoms of each experiment.

Other than the atomic mass of ^{39}K, the relevant parameters in this first simulation that you will need are the distance from the source to the diffracting slit (0.96 m), the distance from the slit to the detector (1 m), the width of the source slit (use 2.5 nm), the width of the diffracting slit (nominally 25.4 μm, but you will vary this), and the deBroglie wavelength 0.175×10^{-10} m.

In setting up the spatial grid, consider the range over which you will want to plot results; for the data of Figs. 2 and 3, for example, this would be from -40 μm to 40 μm. To start with, you should choose a spatial grid with N points that has a range $x_{max} = Ndx$ that is about 100 times this maximum range of interest. Next, create a uniform spatial grid with $x_j = (j-1)dx - x_{max}/2, j = 1, 2, \ldots N$; for a 1D problem like the one of this simulation, you can try $N = 2^{14}$ points, and vary this number after your code is running properly to find a suitable number of grid points (the FFT routines work best when the number of points in the spatial grid is a power of 2). Now create the corresponding momentum grid using $p_j = (j-1)dp - p_{max}/2, j = 1, 2, \ldots N$, where $dp = 2\pi\hbar/x_{max}$ and $p_{max} = 2\pi\hbar/dx$.

You should now define a time evolution operator dU in the momentum representation using your p grid, where this operator spans a short increment of time dt. Better yet, for a given deBroglie wavelength λ_{dB}, define this operator for an increment of space dz, where $dt = dz/v$, and v is the velocity associated with λ_{dB} for an atom of mass m.

Next, define an initial wave function $\psi_0(x)$ that will represent the state of a particle immediately after the diffracting slit. In the paper of Leavitt and Bills, the numerical data of Fig. 2 assumed an initial point source placed 0.96 m before the diffracting slit, hence a spherical wave was incident on the slit. Alternatively, you can consider a plane wave incident on the slit. You will explore both of these choices for your simulation. The simpler one is the plane wave; in this case, $\psi_0(x)$ is just a square wave (a RECT function) with a width that corresponds to the diffracting slit. To determine $\psi_0(x)$ for the case of a spherical wave, you should create a square wave with a narrow width (25 nm for instance), and create an evolution operator that corresponds to 0.96 m propagation. In this case, the wave function immediately after the slit can now be determined via something like the following:

```
psi0spherical = slit.*iftptox(U.*ftxtop(psi0source,dx,hbar),dp,hbar);
```

Here, `ftxtop` is a user-defined function that calculates the Fourier transform (via FFT), preserving normalization, of an input array `psi0source`. To produce a momentum-space wave function, values for $\hbar$ and dx are also passed to the function. The output is multiplied (element by element) with the operator for evolution over distance 0.96 m. The user-defined routine `iftptox` returns this final array back to position-space via IFFT, whereupon the result is multiplied by an array `slit` that is equal to 1 for points within the range of the diffracting slit, and equal to zero outside of this range. You can create your own functions `ftxtop` and `iftptox` or obtain these from the course website.

Now, calculate the wave function $\Psi(x, z)$ at each point z within a range from $z = 0$ (for the initial wave function $\psi_0(x)$) to $z = 1$ m, corresponding to the position of the detector in the experiment. For your initial calculation, try 100 points in this range. Specifying this range of z values and the number of points will determine dz, used in the incremental evolution operator dU discussed above. With a `for` loop, obtain the 2D array $\Psi(x, z)$.

Display the following results. In one figure, use `imagesc` to show $|\Psi(x, z)|^2$ for the entire range of z values used, and for x limited to only the region of interest, not the entire range of x values used in the calculation. In a different figure or subplot, plot $|\Psi(x, z)|^2$ vs x corresponding to $z = 1$ m. This plot should be somewhat similar to that of Fig. 2 in the paper. If not, look at your 2D image of $|\Psi(x, z)|^2$ and try to determine what might be going wrong based on your physical insight of what the diffraction pattern should look like vs z.

B. Questions

1. Is your x grid suitably defined? If you increase or decrease the range of x or the spacing dx by a factor of 2, you should see very little quantitative or qualitative changes to your results. This is a quick check to see whether or not your grid might be limiting your calculations, or if there might be too many points (and thus cause your code to run unnecessarily slow).

2. Your results for spherical wave input to the diffracting slit should quantitatively resemble Fig. 2, but the plane wave input will not quantitatively correspond to the figure, even though it will look qualitatively similar.

Conceptually, why is there a difference between the two cases?

3. Change the source (not diffracting slit) width to be 2.5 μm, and consider spherical wave input to the diffracting slit. Make the diffraction slit width 6.35 μm and 2.54 μm, corresponding to cases (3) and (4) of Fig. 3. Your results should look similar to those of this figure. However, for case (1), there is a significant difference between the result in the figure and the result you should obtain. Why is this the case? Examine the paragraph below Fig. 3 to see how the Fig. 3 results were obtained, and compare with your procedure.

III. ATOMIC MATTER WAVE TALBOT EFFECT

Download and examine Ref. [2] to familiarize yourself with the Talbot effect, and the experimental parameters of this experiment with atoms. The experiment involved a spherical wave incident on the grating, but as before, allow for either a spherical wave or a plane wave to be incident on your grating so that you can compare the two results. The Talbot effect experiment was performed with helium atoms; the atomic mass and other experimental parameters that were inputs in your previous routine will need to be suitably adjusted.

Set up a routine that calculates the wave function $\Psi(x, z)$ behind a grating, using the grating parameters of the paper. You can treat this grating as having a periodicity that extends across your entire x distribution (rather than the finite grating described in the paper). For your first calculation, assume plane-wave input with $\lambda_{dB} = 45$ pm. Don't forget to account for the grating open fraction of 10%. Now, instead of trying to reproduce the figures in the paper, make a 2D image of $|\Psi(x, z)|^2$ where visible values of x range from -15 μm to 15 μm, and z ranges from 0 to 2 m. The pattern of the resulting 2D image is called a Talbot carpet. You may need to re-scale the colors in the figure by over-saturating the regions with large values of $|\Psi(x, z)|^2$ in order to better emphasize regions with low values of $|\Psi(x, z)|^2$. Calculate the Talbot length L_T and verify that the grid pattern repeats in $|\Psi(x, z)|^2$ at $z = L_t$.

Now calculate the Talbot carpet for an input spherical wave, using the parameters of the paper for the source slit width and the distance from the slit to the grating. If you gradually make the slit-grating distance longer and longer in your calculation, you can appreciate conceptually the effect of spherical wave vs plane wave sources, the effective Talbot length described in the paper, and the approximation of a spherical wave as a plane wave for distances far from the spherical wave source.

Examine the effects of changing the open fraction of the grating, or using a plane wave input with a gaussian envelope that spans only a few grating spacings. Discuss your results.

IV. YOUNG'S DOUBLE SLIT EXPERIMENT WITH ATOMS

Download and read Ref. [3]. Simulate the propagation of the atomic wave function from the source to the detector, interrupting propagation half-way through so that you can account for the double-slit mask. Use $\lambda_{dB} = 1.03 \times 10^{-10}$ m, and source slit, double slit, and distance parameters that correspond to those of the experiment. Then make a 2D plot of $|\Psi(x, z)|^2$ for which the results of atom diffraction and interference are visible. Display a cross section of $|\Psi(x, z)|^2$ corresponding to the detector position, and check your results to see if they reproduce Fig. 5 reasonably well.

V. ATOM WAVE INTERFEROMETER

Download and examine Ref. [4], where standing waves of light were used as phase gratings. Build a routine that simulates the atom interferometer, using the parameters described in the paper. Use a square-wave envelope for plane-wave input into the first grating at $z = 0$, and calculate $\Psi(x, z)$ up to $z = 0.5$ m, the position of the third grating in the paper. Notice that the maximum phase shifts of the first and third phase gratings are not identical to the maximum shift from the second grating.

Make a 2D plot of $|\Psi(x, z)|^2$. Observe what happens as you change the width of the input source: if the source width is reduced by a factor of 2, what happens to the arms of the interferometer? Do they become better defined, or worse? What happens as you adjust the maximum phase shifts due to the phase gratings?

If you wish to take this calculation further, you can build into your model the part of the apparatus that corresponds to the detector, then integrate over the detector opening to obtain a number that is proportional to the total number of atoms reaching the detector. Once this is done, you can insert a phase shifter into one arm of the device, and plot the number of atoms detected (or a value proportional to this) vs the phase shift. Alternatively, you can adjust the position of the 3rd grating to reproduce Fig. 2.

This is a relatively simple atom interferometer. Advances in atom interferometry have led to the creation of devices capable of measuring extremely small forces and rotations. With the routine that you have just developed, you have built the basic framework needed to analyze such devices.

[1] J. A. Leavitt and F. A. Bills, "Single-slit diffraction pattern of a thermal atomic potassium beam," *Am. J. Phys.* **37**, 905 (1969): https://aapt.scitation.org/doi/10.

1119/1.1975924

[2] S. Nowak, Ch. Kurtsiefer, T. Pfau, and C. David, "High-order Talbot fringes for atomic matter waves," *Opt. Lett.* **22**, 1430 (1997): https://www.osapublishing.org/ol/abstract.cfm?uri=ol-22-18-1430

[3] O. Carnal and J. Mlynek, "Young's double-slit experiment with atoms: A simple atom interferometer," *Phys. Rev. Lett.* **66**, 2689 (1991): https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.66.2689

[4] E. M Rasel, M. K. Oberthaler, H. Batelaan, J. Schmiedmayer, and A. Zeilinger, "Atom Wave interferometry with diffraction gratings of light," *Phys. Rev. Lett.* **75**, 2633 (1995): https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.75.2633