Visualization of Bose-Einstein Condensates

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Abstract

A Bose-Einstein condensate (BEC) is a state of matter that exists at extremely low temperatures. BECs are currently under investigation by the research community through both numerical simulation and laboratory experiments. The central goal of this visualization project is to create a graphical representation of data from a BEC simulation. In particular, the visualization of vortices within the BEC is of primary interest to the researchers.

1 Introduction

A Bose-Einstein condensate (BEC) is a state of matter that exists at extremely low temperatures. Researchers at the National Institute of Standards and Technology are studying BECs confined in magnetic traps through numerical simulation as well as laboratory experiments. Numerical simulation of BECs is addressed by solving for the appropriate wave equation. The wave function of a BEC corresponds to the ground state of a macroscopic quantum object. In other words, a collection of atoms in a BEC behaves as a single quantum entity. One aspect of BECs that is under study is the evolution of the BEC wave function when the trapped BEC is subjected to rotation. Upon rotation, vortices may form within the BEC. These vortices are of interest because of their theoretical implications on the nature of BECs [1].

2 Background

The researchers are studying the behavior of a BEC that obeys the partial differential equation

$$i\partial_\tau \psi(\mathbf{r},\tau) = [T + V_{\text{trap}} + V_{\text{H}} - \Omega L_z]\psi(\mathbf{r},\tau)$$

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where $\mathbf{r}$ denotes position in $\mathbf{R}^3$, τ denotes time, and $i = \sqrt{-1}$. A full explanation of the terms T, V_{trap}, V_{H}, and ΩL_z is beyond the scope of this paper [2, 3]. However, a brief description is that they reflect two aspects of the BEC simulation: (1) the physics of a trap that contains the BEC, and (2) the rotation of the BEC around the z-axis. The rotation of the BEC around the z-axis induces the formation of vortices within the trap.

The solution of the above equation is a complex-valued function. For the purposes of visualization, we can treat the solution ψ as the mapping

$$\psi(\mathbf{r}, \tau) : \mathbf{R}^3 \times \mathbf{R} \to \mathbf{C}.$$

It is customary for the researchers to express the complex values of ψ in the polar form $z = (\sqrt{\rho}, \theta)$ where $\rho = |\psi(\mathbf{r}, \tau)|^2$. That is, $\psi(\mathbf{r}, \tau) = \sqrt{\rho}e^{i\theta}$. The researchers refer to $\rho = \rho(\mathbf{r}, \tau)$ as "density," and $\theta = \theta(\mathbf{r}, \tau)$ as "phase."

Let ϕ be the function

$$\phi : \mathbf{C} \to D \times P$$

where $D = [0, \infty)$, $P = [0, 2\pi]$, and $\phi(\sqrt{\rho}e^{i\theta}) = (\rho, \theta)$. Then

$$\phi \circ \psi : \mathbf{R}^3 \times \mathbf{R} \to D \times P$$

maps position and time into density and phase.

The data set produced by the simulation is the result of computing $\phi \circ \psi$ on a three-dimensional grid at a collection of times. That is, for each position in $\mathbf{R}^3$ and for each time τ, there are two associated scalar quantities: density and phase. In addition, a vector field can be generated by computing the gradient of the phase.

3 Researcher Requirements

The central goal of this visualization project is to create a graphical representation of the function $\phi \circ \psi$ that displays the qualities and characteristics of the associated BEC. In particular, vortices in the BEC are the principal features of interest. Several other visualization requirements include:

- Color choices that reflect the standard practice of the researchers. In particular, the phase values in the interval $[0, 2\pi]$ must be mapped to a corresponding color circle.
- Easily identified vortices. Vortices occur where the density approaches zero in a localized region.
- Suppression of noisy data in outlying, low-density areas. Noise is an artifact of the simulation program that generates the data.
- Display of the vector field derived from the gradient of the phase.
- Images of two- and three-dimensional data.

4 Approach

The general approach centers on the following points:

- An HSV color model is a natural choice given the requirement for the representation of the phase data.
- Two side-by-side images are needed: one for density and one for phase.
- The images are generated by specifying vector-valued functions to map the density-phase space to a hue-saturation-value-opacity space.

In particular, to generate a density image, a vector-valued function $\mathbf{f}$ is defined as

$$\mathbf{f}(\rho, \theta) : D \times P \to H \times S \times V \times O$$

where H, S, V, and O denote hue, saturation, value, and opacity spaces, respectively. We take $H = S = V = O = [0, 1]$. In addition, we follow the convention that hue values of 0, 1/3, 2/3, and 1 correspond to red, green, blue, and red, respectively. Further, a value of 1 corresponds to maximum saturation, maximum value, and maximum opacity. The component functions of $\mathbf{f}$ are denoted by f_h, f_s, f_v, and f_o.

Similarly, a function $\mathbf{g}$ is defined to generate a phase image. Its domain and range are the same as for $\mathbf{f}$ and its component functions are analogous.

5 Implementation

The implementation task is an iterative process of selecting definitions for the component functions (f_h, g_h, etc.) and analyzing the generated images. The application platform selected is IBM Visualization Data Explorer.

Work begins with the two-dimensional data. The simulation program generates two-dimensional data by integrating the three-dimensional data along the z-axis. To visualize this two-dimensional data, the component functions are defined as

$$\begin{array}{ll} f_h(\rho,\theta) = \frac{2}{3}(1 - \rho/\rho_1) & g_h(\rho,\theta) = \theta/2\pi \\ f_s(\rho,\theta) = 1 & g_s(\rho,\theta) = 1 \\ f_v(\rho,\theta) = 1 & g_v(\rho,\theta) = 1 \\ f_o(\rho,\theta) = 1 & g_o(\rho,\theta) = 1 \end{array}$$

where ρ_1 is the maximum density of an entire data set. The corresponding image is shown in Figure 1. There are a number of shortcomings with this image. First, the vortices in the density image (the twelve small, blue dots), do not show up well and are too small. Second, vortices do not show up in the phase image at all. This is a direct consequence of the above definition of $\mathbf{g}$ as a function of θ only; i.e., ρ does not appear in the definition of any component function of $\mathbf{g}$. Third, the red areas on the outer portion of the phase image are essentially simulation noise and should be suppressed. (The simulation program sets the phase to 0 when the density is very low.)

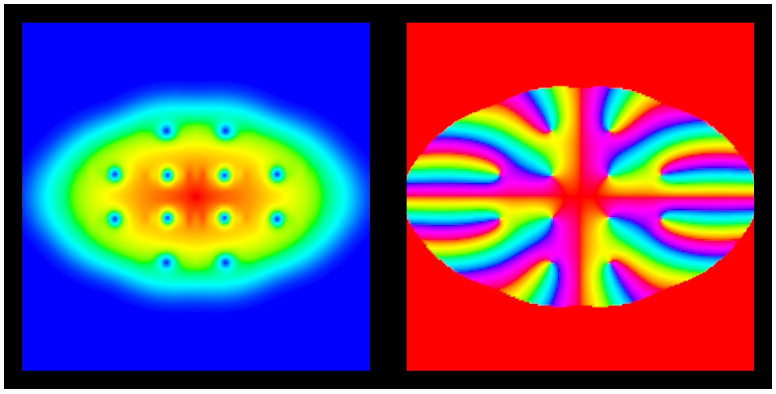

Figure 1: Density (left) and phase (right).

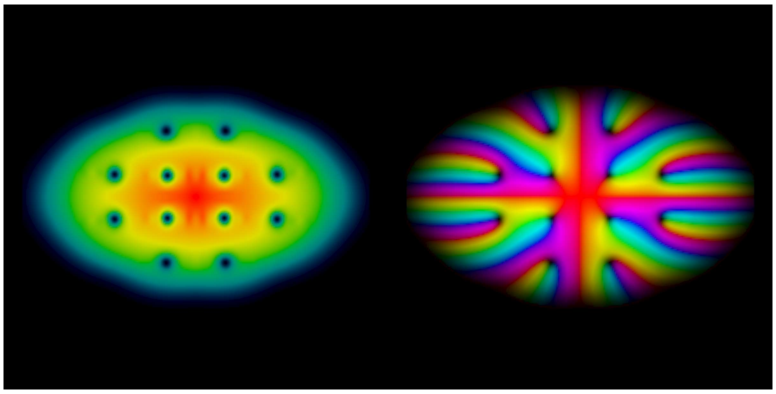

Figure 2: Density (left) and phase (right). Chromatic value is a *linear* function of density.

All three of the above shortcomings are addressed by redefining f_v and g_v as

$$f_v(\rho, \theta) = g_v(\rho, \theta) = \rho/\rho_1.$$

The result is that high-density areas are bright, while low-density areas, such as vortices, fade to black. The corresponding image is shown in Figure 2.

Although the above redefinition improves the situation, the result is still not satisfactory. The vortices need to be enlarged to enhance their prominence within the image. To accomplish this objective, f_v and g_v are further redefined as

$$f_v(\rho, \theta) = g_v(\rho, \theta) = (\rho/\rho_1)^p$$

where $p > 1$. Due to the nature of the function x^p, $p > 1$, on the interval $[0, 1]$, low-density areas are "over-suppressed," while high-density areas retain most of their brightness. The corresponding image, with $p = 2$, is shown in Figure 3.

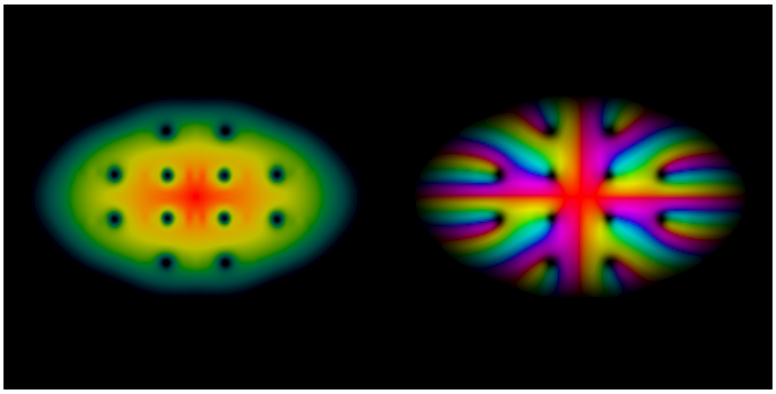

Figure 3: Density (left) and phase (right). Chromatic value is a *nonlinear* function of density.

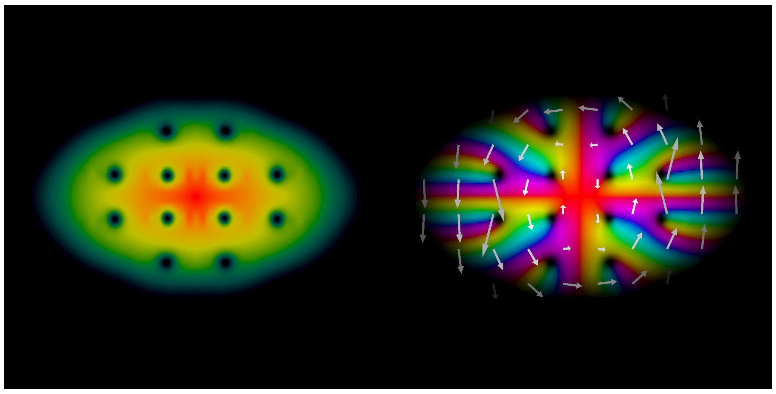

Figure 4: Density (left) and phase (right). Arrow glyphs represent the gradient.

Arrow glyphs are added to the final phase image to represent the vector field derived from the gradient of the phase data. The glyphs are colored as gray values from white to black to avoid overlap with the colors used for the phase data. The brightness of each glyph follows directly from g_v. The adorned image is shown in Figure 4.

6 Future Work

Work on visualizing a three-dimensional volume of density and phase data is in progress. Initially, the strategy was to define the opacity functions, f_o and g_o, in a manner similar to the value functions, f_v and g_v. The intent was that low-density areas would be dark and transparent, while high-density areas would be bright and opaque. This approach proved to be unsatisfactory. The essential problem is that the features of interest, namely the vortices, share the same low-density characteristic as the uninteresting block of material surrounding the central core. What is needed is a way to discriminate between these interesting and uninteresting regions. The new approach, currently under implementation, is to redefine the functions **f** and **g** such that their domain is $D \times P \times \mathbf{R}^3$ instead of just $D \times P$. In other words, **f** and **g** take position into account, thus providing a mechanism to focus on regions where the vortex structures are present.

7 Disclaimer

Certain commercial equipment and software may be identified in order to adequately specify or describe the subject matter of this work. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the equipment or software is necessarily the best available for the purpose.

References

[1] David Feder, Barry Schneider, William Reinhardt, William George, Peter Ketcham, Terence Griffin, and Charles Clark. Generation of solitons and vortices in Bose-Einstein condensates by trap rotation and optical imprinting. JILA, University of Colorado, February 1999. Workshop on Bose-Einstein Condensation and Degenerate Fermi Gases.

[2] David L. Feder, Charles W. Clark, and Barry I. Schneider. Nucleation of vortex arrays in rotating anisotropic Bose-Einstein condensates. Submitted to Physical Review Letters.

[3] David L. Feder, Charles W. Clark, and Barry I. Schneider. Vortex stability of interacting Bose-Einstein condensates confined in anisotropic harmonic traps. Submitted to Physical Review Letters.