Volume Visualization of Bose-Einstein Condensates

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Abstract

Theoretical aspects of Bose-Einstein condensates are investigated by conducting computer simulations of their behavior. Scientific visualization techniques are employed in order to examine the large amount of data generated by simulation. Visualization of this simulated data demonstrates theoretical predictions, influences the research process, accelerates scientific understanding, and stimulates further investigation.

1 Introduction

An active area of research in the physics community is the study of Bose-Einstein condensation. Predicted decades ago, but not produced in the laboratory until recently, a Bose-Einstein condensate (BEC) is an exotic state of matter that exists only at low temperatures [5]. Because the interactions between the atoms are well-understood, the properties of BECs may be modeled by computer simulations based on first principles. Furthermore, researchers employ scientific visualization techniques in order to examine the large amount of data generated by simulation.

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1.1 BEC Background

A BEC is a coherent collection of particles obeying Bose-Einstein statistics and all occupying the same quantum mechanical state. Since the particles in a BEC are all described by the same quantum mechanical wave function, they behave as a single quantum entity. Closely related macroscopic quantum phenomena include superfluidity and superconductivity [4]. Though the existence of a BEC was postulated early in the previous century [3, 8], it was not until 1995 that Bose-Einstein condensation was achieved in the laboratory using magnetically confined alkali atoms [7]. For an extremely dilute gas of atoms relevant to current experiments, the transition to such a state occurs at submicrokelvin temperatures [14]. Indeed, the coldest temperature achieved to date, three billionths of a degree above absolute zero, is required in order to form a BEC of ^{85}Rb atoms [6].

1.2 Motivation

One focus of physics research at the National Institute of Standards and Technology (NIST) is the behavior of magnetically trapped BECs of alkali atoms that are subjected to rotation. One of the long-standing conjectures of many-body physics is that BECs of interacting particles should be a superfluid, with properties similar to those of liquid ^{4}He(II) [13]. One key prediction is that the confined BEC forms quantized vortices when subjected to an external torque. To explore this possibility, researchers at

NIST perform computer simulations of BECs in rotating magnetic traps. Two experimental groups confirm that vortices may be produced this way in confined BECs [17, 18, 1], though there remain some interesting discrepancies between theory and experiment [12]. Because of the large amount of data generated by simulation and the inherently small size of vortices in condensates, visualization provides not only an effective method for the detection of quantized vortices, but also for the investigation of vortex dynamics in these systems.

2 Visualization Process

Currently, visualization techniques are as much an art as a science. Principles and algorithms that further the science of visualization, as opposed to the art of visualization, have significant value.

For this work, the visualization process includes three main activities:

1. analysis of researcher needs, conventions, and requirements in order to ensure a meaningful presentation of the data,

2. assignment of colors and opacities to the data, and

3. rendering of the data to produce a final image.

2.1 Data Presentation

Computer simulation of the BEC wave function generates complex-valued data on a three-dimensional Cartesian grid. After final processing by the simulation program, the grid contains 200 data points along each dimension (see Figure 1). It is a convention among physicists who study BECs to express this complex-valued data in polar form. For a complex number at a grid point, the square of the radial component (or amplitude) of the complex number corresponds to the "density" of the BEC wave function and the angular component corresponds to the "phase" of the BEC wave function.

2.2 Color and Opacity Assignment

Color and opacity are assigned to each grid point based on the data value at that grid point. The goal is to assign color and opacity in a manner that exhibits features of interest. Opacity is the degree to which a grid point absorbs light that passes through it. For this work, all grid points in three dimensions have zero opacity, i.e., complete transparency. In two dimensions, the concept of opacity does not apply.

2.2.1 Qualitative Description

Color is assigned to a grid point as a function of the density and phase at that grid point. Since phase is the angular component of a complex number, it is natural to associate phase with a color circle[1] (see Figure 2). Under this association, a phase of 0 corresponds to red, a phase of $2\pi/3$ corresponds to green, and a phase of $4\pi/3$ corresponds to blue. Density is associated with brightness. Since vortices correspond to localized suppressions of the condensate wave function, zero-density regions are rendered brightest in order to exhibit vortex structures.

The function that assigns color to grid points is called a *transfer function*. A sample transfer function expressing a density-brightness association is shown in Figure 3. Specification of transfer functions can be challenging; even small misjudgments may produce a final image that is all but useless. The specification of appropriate transfer functions is an active area of research within the scientific visualization community [19]. For this work, transfer functions are determined empirically.

2.2.2 HSV Color Model

An HSV (hue, saturation, value) color model is ideal for implementing the color scheme described above. With an HSV color model, density is mapped to value (the degree of brightness) and phase is mapped to hue (the degree of red-, green-, or blueness) (see Figure 4). Saturation (the degree of pastelness) is held constant; all grid points are fully saturated.

[1] or perhaps more appropriately, a "hue circle"

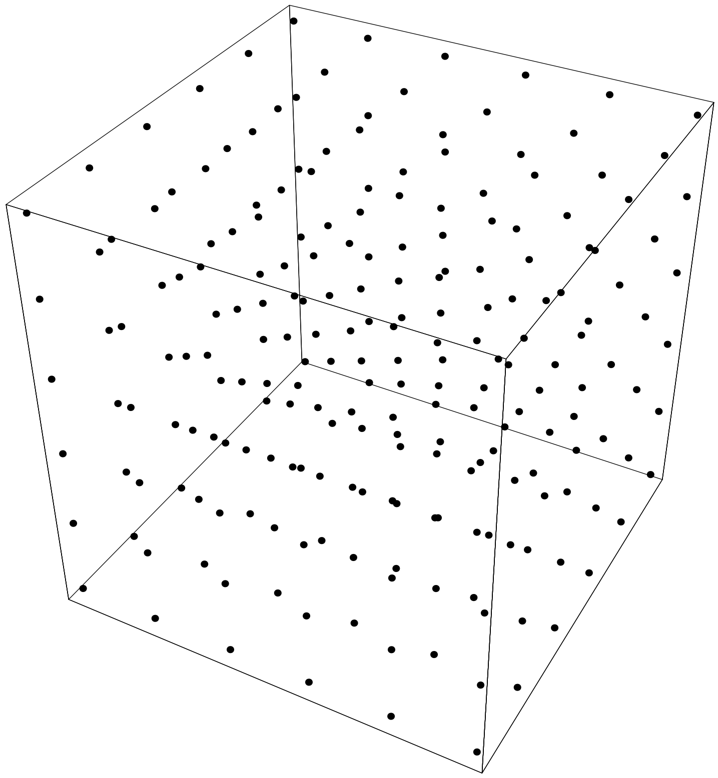

Figure 1: Cartesian grid of simulated BEC data.

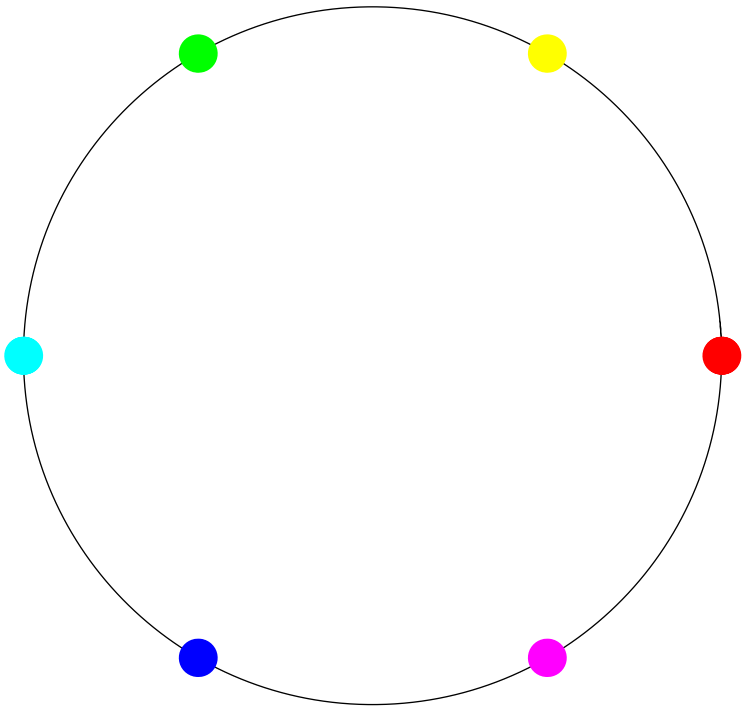

Figure 2: Color circle displaying six hues (counterclockwise from right: red, yellow, green, cyan, blue, magenta).

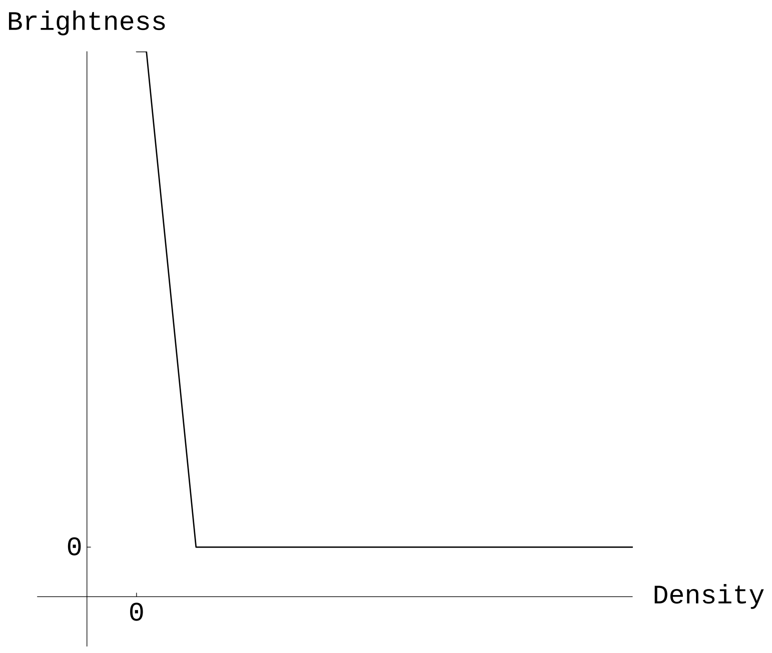

Figure 3: Transfer function expressing a density-brightness association. Brightness decreases (in a specified manner) as density increases.

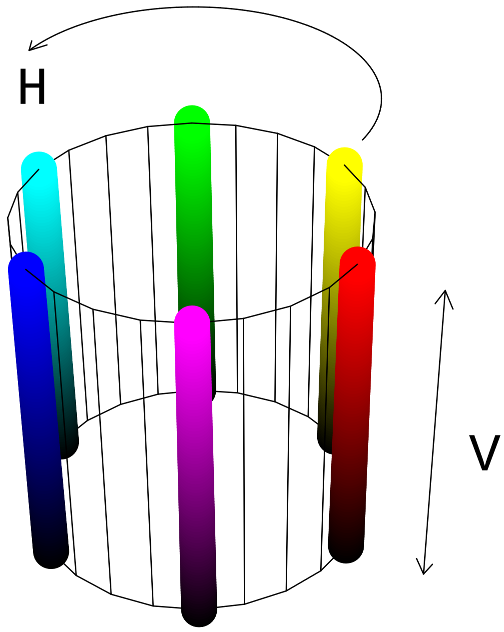

Figure 4: HSV color model.

2.3 Rendering

After the assignment of color and opacity, the data set is rendered. OpenDX[2] (Open Visualization Data Explorer) is the application software used for rendering. The rendering step produces an image of the data based on inputs such as color, opacity, and (virtual) camera position. In the three-dimensional case, a "dense emitter" rendering model is used. This rendering model assumes that each point in space both emits and absorbs light. As noted above, for this work, all grid points in three dimensions are completely transparent and thus do not absorb any light.

2.3.1 Two-Dimensional Data

Figure 5 displays a rendering of two-dimensional data obtained from a three-dimensional data set. In this case, low-density regions are dark and high-density regions are bright. Vortices appear as dark, approximately round spots at the confluence of various colored regions. Figure 5 shows twelve vortices. A tight, circular trip around a vortex takes one through a complete color circle.

2.3.2 Three-Dimensional Data

Figure 6 displays a rendering of three-dimensional data. In this case, low-density regions are bright and high-density regions are dark. Vortices appear as bright, tornado-like, vertical bands. Figure 6 shows twelve vortices. Note that the brightness mapping for three-dimensional data is the reverse of the brightness mapping for two-dimensional data. Therefore, vortices appear as bright bands in three dimensions instead of dark spots as in two dimensions. Some care is taken in the rendering of the three-dimensional data in order to prevent uninteresting, low-density, outer regions from obscuring the inner vortex structures.

[2]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.

3 Impact

Visualization of simulated BEC data demonstrates theoretical predictions, influences the research process, accelerates scientific understanding, and stimulates further investigation.

3.1 Results

Visualization demonstrates the following theoretical results for BECs:

- the existence of quantized vortex array structures within a trapped, rotating BEC, and
- the spontaneous decay of a soliton into concentric, quantized vortex rings (a "snake instability") within a trapped, non-rotating BEC.

3.2 Feedback Loop

Visualization provides a feedback loop in the sense that visualization results influence subsequent research activities. The feedback process may occur at the initial, intermediate, or final stages of a particular study. For example, renderings of three-dimensional data from early BEC simulations display a low-density equatorial ring (see Figure 7). The equatorial ring has no physical significance; it is the result of an error in the simulation program. In this case, visualization serves as a debugging tool: visualization exposes a flaw in the simulation program and correction of that flaw eliminates the equatorial ring. As another example, final visualization results influence the direction of further laboratory experiments; see the quotation in Section 3.4.

3.3 Publications

BEC images from this work appear in a number of publications in order to illustrate and augment the accompanying text in those publications. These images also appear beside photographs of actual BECs produced in the laboratory as a comparison between theory and experiment. Examples of publications containing BEC images from this work include *Physics Today* [4, cover page and p. 38], *Parity* [15,

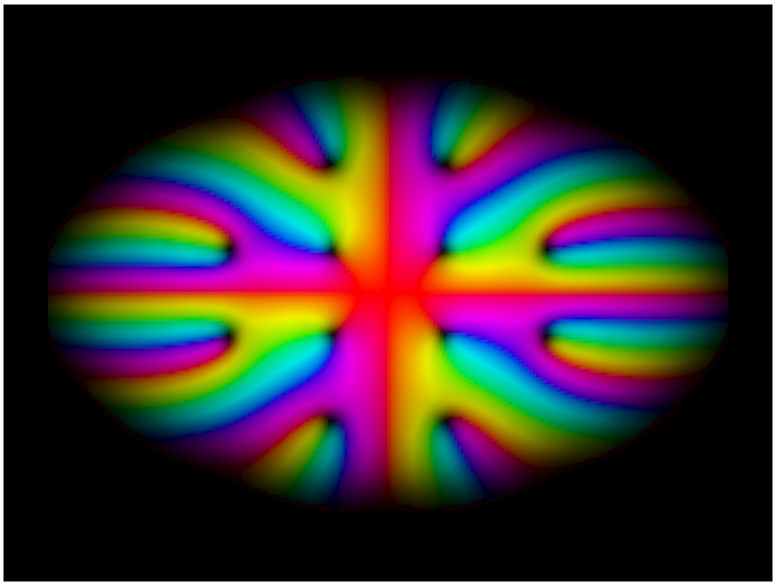

Figure 5: Rendering of 2D data. High-density regions are bright.

cover page], *Science* [16, p. 898], *Scientific American* [5, p. 68], and *Optics & Photonics News* [10, cover page and p. 38].

3.4 Research Stimulation

Visualization of BECs stimulates further investigation of BECs. Regarding the relationship between theory and experiment in the study of BECs, a member of the research team writes [11]:

> You might be interested to know that we followed up our original observation of this snake instability by a great deal of further simulations and calculations, and wrote up the results in a recent article [9] that features some nice still images also rendered in the same way. Experimentalists at JILA, namely postdoc Brian Anderson and supervisor Eric Cornell, read the article and decided to attempt to generate these vortex rings in condensates in exactly this way. They have confirmed all the predictions, and we are in the process of writing up a joint theory-experimental paper [2] on the subject.

4 Conclusion

Visualization of BECs, especially in three dimensions, enhances and accelerates the investigation of this exotic state of matter. Visualization is an integral part of the simulation process and a key component of modern, collaborative research efforts. In this work, visualization enables scientific discoveries that may be difficult to achieve by other methods in a reasonable period of time.

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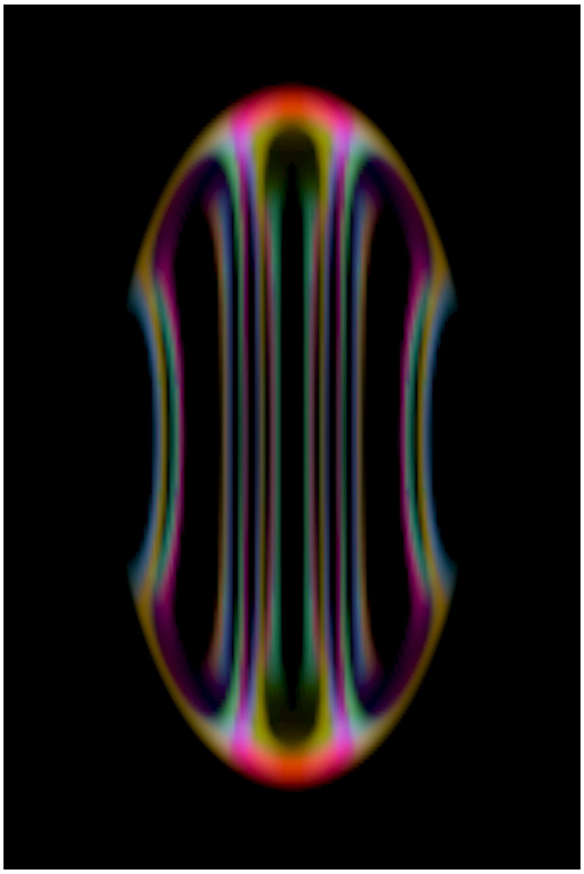

Figure 6: Rendering of 3D data. Low-density regions are bright.

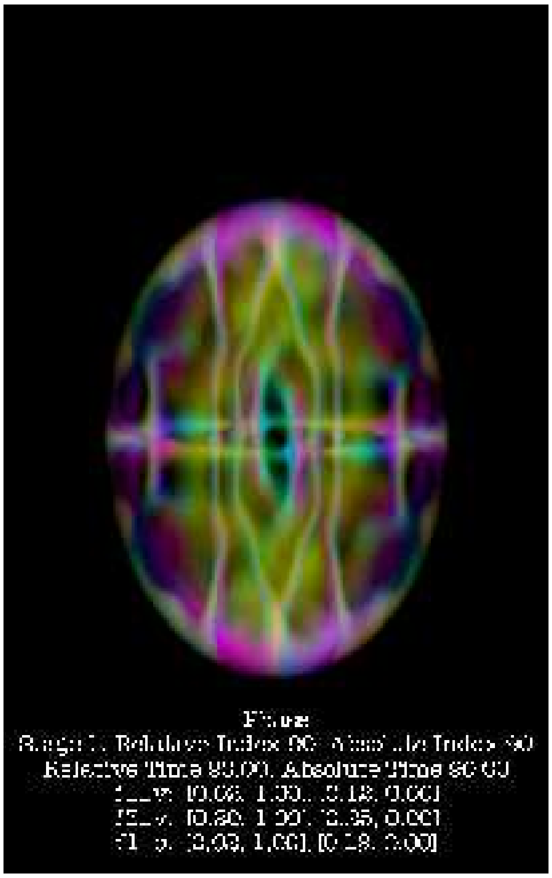

Figure 7: Rendering of 3D data displaying equatorial ring.

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