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VISUALIZING BOSE–EINSTEIN CONDENSATES

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BOSE–EINSTEIN CONDENSATES ARE THE COLDEST SUBSTANCES EVER MADE. ALONG WITH THIS DISTINCTION, BECS HAVE OTHER INTRIGUING PROPERTIES: FOR EXAMPLE, THEY BEHAVE MUCH LIKE LIGHT DOES IN AN OPTICAL FIBER. IN FACT, many research groups have produced "atom lasers" formed from traveling BECs. They also behave similarly to superfluids, much like liquid helium or superconductors. By studying BECs, we've gained important insights into much more complicated, but closely related, systems.

BECs created from dilute alkali vapors were first produced in the laboratory in 1995[1–4] using laser cooling and trapping techniques developed over the past 20 years. Creating a BEC requires temperatures between one billionth and one millionth of a degree above absolute zero.

Once the cooling technology became available, an explosion of research in the area followed; over 30 experimental groups around the world have made BECs. However, BECs are not a new idea. Satyendra Nath Bose and Albert Einstein predicted the Bose–Einstein condensation phenomenon in dilute ideal gases over 75 years ago.[5–7]

In this article, we present a method for visualizing numerical simulations of BECs, discuss the visualization process, which includes selecting a color scheme and the application of a volume rendering model, and describe our visualization's impact on associated scientific research.

Quantum Vortices

Laboratory-produced BECs aren't quite as simple as the ones Bose and Einstein originally predicted because they are made from real alkali atoms, not ideal gases. For instance, unlike an ideal gas, atoms can't pass through one another. They interact strongly, and attract each other if they get too close together. Thus, keeping the gas dilute enough is very important; otherwise, you would end up with a lump of metal instead of a BEC. Conversely, the atoms also repel each other if kept sufficiently far apart, and it's this repulsive interaction that gives rise to the most interesting properties of BECs. For more on the physical intricacies of BECs, see the "Quantum Degeneracy and BECs" sidebar.

One of the most interesting phenomena exhibited by superfluids is the formation of quantum vortices. When an ordinary fluid is rotated—for example, when you stir milk into a cup of coffee—a large vortex, or depression, is formed in the center. But a superfluid, by its very nature, wants to flow without friction. This means that if you tried to stir it with a spoon, it would attempt to flow around the spoon with no resistance. Of course, there are some limitations on its ability to do so, and the result is the formation of tiny quantum vortices, each with a quantized amount of superflow around it.

These quantum whirlpools are produced in BECs by rotating the magnetic trap in which the BEC is contained—much like trying to stir your coffee by squeezing the cup and spinning yourself around. BECs range from a millimeter to a centimeter in size, so you'd think it should be easy to detect the vortices simply by shining light on the cloud, taking a photograph, and noting the tiny holes in the picture where the atom density has gone to zero in the vortex cores.

Unfortunately, in spite of many efforts, it wasn't until several years after BECs were first formed that researchers saw quantum vortices in gases made of a single species of atom.[8] (The first quantum vortices in BECs were produced in two-species gases, so that one species filled the core of the vortex formed in the other species. This made the vortex large enough to image, but the cloud as a whole had no density depression in the vortex core.) The inability to see single-species gas quantum vortices wasn't properly understood until full three-dimensional numerical simulations and visualizations of rotating BECs began to emerge in the 1990s. These simulations demonstrated that the rotation frequencies needed to produce quantum vortices were higher than previously expected.

The visualizations also revealed that the vortices themselves were generally

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quite curved. Due to the small size of the vortices, this curvature meant that any photograph of the entire BEC wouldn't detect the holes because the position of the holes changes down the line of sight, thus the cloud itself would obscure the vortices.

Vortices were finally imaged experimentally using two techniques. At École Normale Supérieure, Jean Dalibard's group found that if they released the atoms from their trap and allowed the BEC to expand, the vortex cores were magnified sufficiently to be detectable.[9,10] This approach works well when the number of atoms isn't too large, on the order of a few hundred thousand. Wolfgang Ketterle's BEC, however, contained several million atoms; his solution was to pump a thin section of the cloud into another quantum state using a laser and then image only that slice.[11]

Quantum Degeneracy and BECs

A Bose–Einstein condensate forms when a gas of particles obeying Bose–Einstein statistics, bosons, becomes *quantum degenerate*. In his 1924 doctoral thesis, Louis de Broglie proposed that all particles possess a quantum wave nature in addition to a quantum particle nature. When viewed as a wave, a particle has an associated quantum wavelength. This quantum wavelength is inversely proportional to the particle's mass and temperature, so the colder the temperature and the lighter the mass, the longer the quantum wavelength. Particles with long quantum wavelengths more readily manifest their wavy character.

Quantum degeneracy occurs when the quantum wavelength becomes comparable to the average spacing between particles. In practice, this means either very high particle densities or very cold temperatures. Metals are good conductors because the electrons carrying the charge are quantum degenerate, which is possible at room temperatures due to the high electron densities.

Two kinds of particles exist in the known universe: bosons and fermions, the latter of which obey Fermi–Dirac statistics. (In certain artificial two-dimensional systems, such as semiconductor heterojunctions, particles can actually have fractional statistics, intermediate between bosons and fermions. These instances give rise to the fractional quantum Hall effect at low temperatures and high magnetic fields.) Bosons, which have integer values of something called *spin*, include photons (the quantum particles of light). Fermions, which have half-integer spin, include the electrons, protons, and neutrons making up ordinary atoms.

Atoms themselves are either bosons or fermions, depending on the total number of their fermion constituents: an even number of fermions gives a bosonic atom. For example, hydrogen is a boson, with one proton and one electron. In fact, most efforts to produce a BEC over the past two decades focused on hydrogen, and in 1998, a hydrogen BEC was finally produced in the laboratory by Dan Kleppner and Thomas Greytak's group at Harvard University.[1] Hydrogen was long considered a good candidate because of its light mass.

In principle, the gas needed to be only a few thousandths of a degree above absolute zero to become a BEC. But achieving these temperatures in hydrogen proved to be very difficult, and efforts turned instead to alkali atoms where laser cooling could be used. Alkali atoms are much heavier than hydrogen, however, so the temperatures needed to reach BEC are perhaps 100 times lower.

Reference

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Numerical Simulation

We can numerically model the formation of quantum vortices in BEC superfluids by solving differential equations very similar to those used to model ocean or air currents. The main differences are the total lack of friction and the inclusion of terms that take the quantum nature of the atoms into account.

All the atoms in a BEC are in a single quantum state (which is why it's called quantum degeneracy). This state is represented by a wave function ψ, which is a complex number characterized by two values: a density ρ and a phase ϕ, so that $\psi = \sqrt{\rho e^{i\phi}}$. Here, $i = \sqrt{-1}$ is the imaginary unit, so that exp $(i \times 0) = 1$ and exp $(i \times \pi) = -1$. The density gives the cloud's overall profile, expressing the average number of atoms in a given time. The phase is a quantum mechanical variable that defines the superfluid flow: the superfluid velocity v is proportional to the gradient of the phase $v \propto \nabla\phi$.

Visualization

The product of the numerical simulation of BEC vortex formation we used is a data set containing 8 million complex numbers expressed in polar form. The data values represent the wave function ψ on a three-dimensional grid with 200 grid points in each dimension. Visualization provides a way to examine this data set at a high conceptual level.

Process

The visualization process includes three main activities:

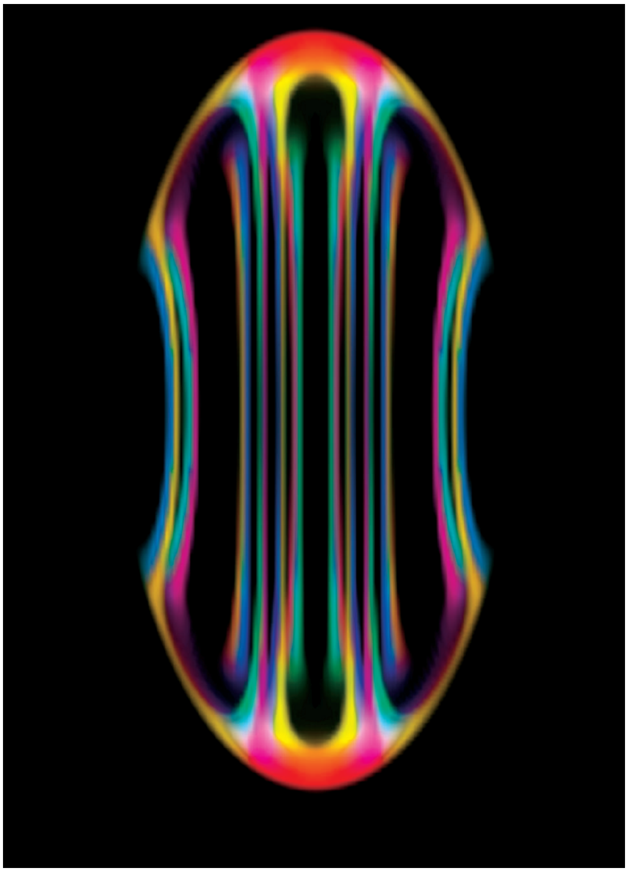

Figure 1. A volume rendering of Bose–Einstein condensate wave function data. The various colors reflect the changing phase of the wave function throughout the condensate.

- A review of the requirements and conventions of physicists to ensure a meaningful presentation of the data
- The selection of an appropriate color scheme
- The volume rendering of the data to produce a final image

Color Scheme. As previously noted, the product of the numerical simulation is a set of complex-valued data expressed in polar form. Recall that a complex number expressed in polar form has both an angular component and a radial component. For each complex number, the angular component is the phase of the BEC wave function, and the square of the radial component is the BEC wave function's density.

To visualize BEC wave function data, we chose a color scheme that harmonizes effectively with the circular nature of complex numbers expressed in polar form. The HSV (hue, saturation, value) color model offers such a scheme.

The HSV color model expresses hue (the degree of red-, green-, or blueness) in an angular fashion. This angular expression suggests a natural mapping from the phase of the BEC wave function to the hue component of the HSV color model. In particular, a phase of zero maps to red, a phase of $2\pi/3$ maps to green, a phase of $4\pi/3$ maps to blue, and a phase of 2π maps once again to red, thus completing the circle. The remaining phase values are interpolated to the hue component in the expected manner.

The HSV color model expresses saturation in a radial fashion. This suggests a mapping from the BEC wave function's density to the saturation component of the HSV color model. However, such a mapping is not very useful: with a dense emitter volume rendering model (discussed next), high-density regions of the BEC wave function obscure low-density regions. This is unacceptable because the low-density regions are of primary interest.

The HSV color model expresses value (the degree of brightness) in a linear fashion. This is not meant to imply that the human eye perceives brightness in a linear manner. Value is expressed linearly in the sense that it is not expressed in an angular or radial fashion. This allows a mapping from the BEC wave function's density to the value component of the HSV color model. A useful mapping is one that maps low density to high brightness and high density to low brightness. Because vortices correspond to localized suppressions of the BEC wave function, such a mapping exhibits vortex structures because it emphasizes low-density regions and subdues high-density ones.

Volume Rendering. Applying the color scheme just described, we render the BEC wave function data set with a dense emitter volume rendering model.[12] With a dense emitter volume rendering model, each point of the volume emits (and possibly absorbs) light of a particular color. The color scheme determines the color of light that each point emits.

An opacity scheme determines the amount of light that each point absorbs. We obtain the best results with an opacity scheme in which every point absorbs no light—meaning, every point allows light from every other point to pass through itself unimpeded.

Figure 1 displays a volume rendering of BEC wave function data using the Open Visualization Data Explorer (OpenDX) software application package. Twelve vortices appear as bright, column-like, vertical bands. We take some care in rendering this data to prevent uninteresting, low-density, outer regions from obscuring the interesting, low-density, inner vortex structures.

Research Impact

Visualization contributes not only to the exploration of a data set, but to the entire scientific research process as well.

Visualization assists with the programming and validation of the numerical simulation code. In support of NIST's theoretical and experimental research on BECs, visualization exposed errors in early versions of the simulation code and lent confidence to the correctness of the final version of the simulation. In general, a feedback loop exists between data visualization and numerical simulation refinement.

The visualization of the BEC wave function demonstrates at a high conceptual level how the BEC behaves. In particular, the visualization displays the formation and evolution of vortex structures in a rotating BEC. It also suggests why certain observational approaches (such as photography) could fail to detect the vortices in an actual, physical experiment.

The visualization revealed the theoretical existence of vortex structures in rotating BECs, which were confirmed by actual laboratory experiments. A successful outcome stimulates further numerical simulations, further simulation visualizations, and further laboratory experimentation.[13]

Visualization of BECs enhances and accelerates the scientific investigation of this exotic state of matter. Visualization is an integral part of the numerical 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. We expect visualization to play an important role in many of the emerging technologies using BECs, such as superfluid gyroscopes, graviometers, and quantum information devices.

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Certain commercial equipment and software are identified 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.

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