A study of the physics and mathematics behind Bose-Einstein condensation.

3 januari 2007

The physics of Bose-Einstein condensation of dilute atomic gases represents an extremely lively experimental and theoretical branch of modern physics, with at least three Nobel prizes in Physics awarded during the last 10-15 years. A Bose-Einstein condensate is a phase of matter formed by bosons (in this case atoms with integer angular momenta) cooled to temperatures very close to absolute zero (0 kelvins or -273.15 degrees Celsius). Under such supercooled conditions, a large fraction of the atoms collapse into the lowest quantum state, at which point quantum effects become apparent on a macroscopic scale. The transition from a normal gas to a Bose-Einstein condensed systems results in macroscopic phenomema like viscous-free fluid. Quantized vortices can also be formed and recent experiments have verified the intriguing feature that Bose-condensed atoms are “laser-like”. In other words, the matter waves of the atoms are coherent. In recent experiments at MIT one demonstrated a rudimentary “atom laser” that generates a beam of coherent atoms, in analogy to the emission of coherent photons by an optical laser.

The condensates are however extremely fragile. The slightest interaction with the outside world can be enough to warm them past the condensation threshold, forming a normal gas and loosing their interesting properties. It is likely to be some time before any practical applications are developed. Nevertheless, they have proved to be useful in exploring a wide range of questions in fundamental physics, and in the years since the initial discoveries we have seen an explosion in experimental and theoretical activity. Examples include experiments that have demonstrated interference between condensates due to wave-particle duality, the study of superfluidity and quantized vortices, and the slowing of light pulses to very low speeds using electromagnetically induced transparency.

The dynamics of a Bose-Einstein condensate at zero temperature is assumed to be more or less properly described by the Gross-Pitaevskii equation or modified Gross-Pitaevkii equation for denser condensates. The Gross-Pitaevskii equation is a Schrödinger equation with nonlinearities of third order. It is a non-linear partial differential equation. While a description is available when $T = 0$ it is a fact that getting there one must start at some positive $T > 0$. From a practical point of view it is of great importance that this process goes as smoothly, controlled, and predictable as possible in order to open up for possible technical applications. In achieving this a thorough, qualitative, and quantifiable understanding of the phenomena is needed.

It is therefore reasonable to assume any mathematical description of the evolution of such a system, as the temperature drops, to be rich enough and have an intriguing mathematical strtucture well worth of a serios mathematical undertaking.

In a series of well cited papers [5]-[10] Gardiner et.al have developed a quantum kinetic theory designed to describe the behaviour of a dilute quantum Bose gas not only at temperature $T = 0$, but also at $T > 0$. Any theory governing the process of laser cooling must include both quantum mechanics and the thermal effects arising from the finite temperature. The problem with the resulting theory is that the equations are difficult to handle exactly.

In Ref. [12], a combination of the mathematics of the BEC description with that of the quantum kinetic theorey is made, together with the idea of local energy and momentum conservation in order to overcome this situation. The result is an equation governing the coupling of the thermalized condensate band to the Gross-Pitaevskii equation. It is a stochastic Gross-Pitaevskii equation with both additive and multiplicative noise (white in time and correlated in space). Since building a model often involves many approximations it is not clear exactly which properties have survived. Thus, the model requires an analytical/computational investigation. The equation is hitherto not seen in the mathematics community.

The existence of an invariant measure has been theoretically obtained (see [3]) for a significantly simpler (but somewhat similar) equation. We will pursue investigations in this direction. Several functionals of the solution corresponding to physically interesting properties are also important to study. We hope to establish some basic Ito formula. Of course, the natural starting point is a proof of existence and uniqueness of a solution. A result in this direction for a simpler equation is [1].

The experience in the physics part of the team is on the case $T = 0$ and the related numerical methods. The methods are finite element approaches to non-linear partial differential equations and Monte Carlo methods (variational and diffusion Monte Carlo) for quantum mechanical systems at zero temperature. The diffusion Monte Carlo methods yield in principle an exact solution to Schrödinger's equation for many interactiing particles at any density, viz, given a certain Hamiltonian, one obtains the exact solution. The Gross-Pitavaeskii equation is an approximation to the fully interacting cases that works well at the low densities typical for Bose-Einstein condensates. In this density regime, one can approximate the Schrödinger equation for a many-particle system to effective one-particle equations, of which the Gross-Pitavaeskii equation is one possibility.

Comparisons with diffusion Monte Carlo and the Gross-Pitavaeskii equation for Bose-Einstein condensates in many different density regimes show excellent agreement. Monte Carlo methods are, however, extremely time-consuming from a numerical point of view and the Gross-Pitavaeskii equation is the preferred approach. For large systems, even a smallish number such as 100 particles, we may speak of at least two-three orders of magnitude in CPU expenditure. A Bose-Einstein condensate may count millions of atoms, a calculation beyond reach for diffusion Monte Carlo methods.

However, since these methods apply to zero temperature only, we expect that the physics group within CMA will gain insight and experience in the $T > 0$ case. The topic of Bose-Einstein condensate is a hot one and shows good promise of being both scientifically and technologically highly interesting in the foreseeable future. Furthermore, we plan to develop a large code for Monte Carlo calculations at finite T using the path-integral method. As with diffusion Monte carlo methods, this method provides also in principle an exact answer to Schrödinger's equation. The answer serves as a benchmark to our new stochastic Gross-Pitavaeskii equation (SPDE). Path-integral Monte Carlo approaches are again extremely time-consuming. Our path-integral approach will however serve to justify the SPDE approach and provide a theoretical benchmark and justification of the use of the stochastic Gross-Pitavaeskii equation.

The experience of the mathematics part of the team is based on stochastic partial differential equations. The highly non-trivial SPDE associated to Bose-Einstein condensate will ensure that

1) a new important SPDE comes out "on the market",

2) the development of tools suitable for this new class of SPDE will be initiated and hopefully, to some extent, completed,

3) a development of numerical methods will give interesting numerical results where analytical tools are not yet available.

This will certainly provide original input for the stochastic team at CMA as well as open up for opportunities to delve further into this new application. It may also bring about new and original modeling in the finance application.

The article [12] will be the basis for a common investigation and the stochastic Gross-Pitaevskii equation will be the starting point for both mathematical and numerical/computational work aimed at providing a clearer picture of the process of cooling down a Bose gas to condensation.

It is hoped that the theoretical studies will result in publication in journals like "Journals of Mathematical Physics" and that the simulation studies be published in for example "Physical Review".

Referenser

[1] A. De Bouard, A. Debussche. A Stochastic Nonlinear Schrödinger Equation with Multiplicative Noise. *Communications in Mathematical Physics* **205**, 161-181 (1999).

[2] A. De Bouard, A. Debussche. Blow-up for the Stochastic Nonlinear Schrodinger Equation with Multiplicative noise. *Annals of Probability* 2005, **33**, 3, 1078-1110.

[3] A. Debussche, C. Odasso. Ergodicity for the Weakly Damped Stochastic Non-linear Schrodinger Equation. *Journal of Evolution Equations*, **5**, 3, 2005.

[4] C.W. Gardiner, J.R. Angelin, T.I.A. Fudge. The stochastic Gross-Pitaevskii equation. *J. Phys. B: At. Mol. Opt. Phys.* **35**, 1555-1582 (2002).

[5] C.W. Gardiner, P. Zoller. Quantum Kinetic Theory I: A Quantum Kinetic Master Equation for Condensation of a weakly interacting Bose gas without a trapping potential. *Phys. Rev.* A **55**, 2902 (1997).

[6] D. Jaksch, C.W. Gardiner, P. Zoller. Quantum Kinetic Theory II: Simulation of the Quantum Boltzmann master equation. *Phys. Rev.* A **56**, 1 (1997).

[7] C.W. Gardiner, P. Zoller. Quantum Kinetic Theory III: Quantum Kinetic Master Equation for strongly condensated condensated trapped systems. *Phys. Rev.* A **58**, 1 (1998).

[8] D. Jaksch, C.W. Gardiner, K.M. Gheri, P. Zoller. Quantum Kinetic Theory IV: Intensity and amplitude fluctuations of a Bose-Einstein condensate at finite temperature including trap loss. *Phys. Rev.* A **58**, 1450 (1997).

[9] C.W. Gardiner, P. Zoller. Quantum Kinetic Theory V: Quantum kinetic master equation for mutual interaction of condensate and noncondensate. *Phys. Rev.* A **61**, 033601 (2000).

[10] C.W. Gardiner, P. Zoller. Quantum Kinetic Theory VI: The growth of a Bose-Einstein condensate. *Phys. Rev.* A **62**, 033606 (2000).

[11] C.W. Gardiner. *Quantum Noise*, Springer-Verlag, (1991).

[12] C.W. Gardiner, J.R. Anglin, T. I. A Fudge. The stochastic Gross-Pitaevskii equation. *Journal of Physics B: Molecular and Optical Physics*, **35** (2002), 1555-1582.