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Title: Nonlinear Atom Optics

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). The project objectives were to explore theoretically various aspects of nonlinear atom optics effects in cold-atom waves and traps. During the project a major development occurred: the observation, by as many as a dozen experimental groups, of Bose-Einstein condensation (BEC) in cold-atom traps. This stimulated us to focus our attention on those aspects of nonlinear atom optics relating to BEC, in addition to continuing our work on a nonequilibrium formalism for dealing with the interaction of an electromagnetic field with multi-level atomic systems, allowing for macroscopic coherence effects such as BEC. Studies of several problems in BEC physics have been completed or are near completion, including the suggested use of external electric fields to modify the nature of the interatomic interaction in cold-atom traps; properties of two-phase condensates; and molecular loss processes associated with BEC experiments involving a so-called Feshbach resonance.

Background and Research Objectives:

Magneto-optical traps have made it possible to cool atoms to such low temperatures that their de Broglie wavelengths are large compared with the interatomic separation. This means that macroscopic coherence effects become possible, in the sense that a large number of atoms can occupy a single, superfluid-like quantum state. Cold atoms are expected to be employed in future generations of atomic clocks, in future coherent atomic beam generators ("atom lasers"), possibly in idealized laboratory "quantum computers," and in the study of basic aspects of quantum physics.

During the past three years a major development was made possible with trapped cold-atom systems: the experimental observation of Bose-Einstein condensation in rapid succession by approximately a dozen groups. Loosely speaking, these groups have realized a condensation of a many-atom system into a single, superfluid-like quantum state, an effect first predicted by Einstein in 1923. Although the possibility of observing this phenomenon with cold-atom systems was recognized in our original proposal, the

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explosion of activity that was to occur in the field could hardly have been anticipated.

The objective of this project was to study various aspects of the theory of cold-atom systems, and in particular the nonlinear wave phenomena ("nonlinear atom optics") that could arise when there is macroscopic or many-atom coherence. Bose-Einstein condensation may be viewed in this context as a self-focusing of a many-atom wave function --thus the similarity between the wave equation describing the self-focusing of a laser beam in a nonlinear optical medium and the Gross-Pitaevsky equation describing (approximately) some aspects of Bose-Einstein condensation.

The recent experimental studies stimulated us to focus our efforts on theoretical aspects of BECs while at the same time working to develop on an ongoing basis a general theoretical framework for the study of the many-atom physics of nonlinear atom optics. The former is based on mathematical techniques employed previously in many-body theory by Korenman [1], Hohenberg and Martin [2], and others. The latter efforts were motivated in particular by the experiments of two different groups at MIT: Ketterle et al. [3], who observed a so-called Feshbach resonance effect in BECs, and Kleppner et al. [4], who recently reported the observation of BEC with atomic hydrogen.

Importance to LANL's Science and Technology Base and National R&D Needs

Trapped cold atoms and ions are of interest at LANL in connection with efforts here to produce Bose-Einstein condensation of radioactive species and, separately, to investigate both theoretically and experimentally the possibility of "quantum computation." Nationally there are dozens of experimental groups engaged in basic research in atomic and molecular science using cold-atom traps.

Computational studies of BEC systems have been based to a large extent on numerical solutions of variants of the Gross-Pitaevsky equation alluded to above. While these studies have been useful in explaining some qualitative features of the experimental observations, there are observed effects that thus far are not well understood, and the subject lacks a theoretical foundation that is rigorously based on fundamental many-body physics and is also amenable to quantitative simulations and predictive capabilities. Moreover, beyond a better understanding of Bose-Einstein-condensed systems lies the possibility of identifying interesting basic physics experiments that can be performed with them.

Scientific Approach and Accomplishments

We have developed a nonequilibrium formalism for an electromagnetic field interacting with a multi-level atomic system allowing for the possibility of macroscopic

coherence effects such as Bose-Einstein condensation. This formalism is based on a Green-function or propagator approach introduced many years ago by Schwinger and by Keldysh, and has been used in various forms by others including Korenman [1] and Hohenberg and Martin [2]. We assume at the start, through the assumed form of the commutation relation between quantized field operators, that we are dealing with a bosonic system, i.e., a system of particles obeying Bose as opposed to Fermi statistics. We then proceed to derive equations describing the evolution in time of the quantized field operators for the bosons interacting with themselves and with an applied (possibly also quantized) electromagnetic field. The bosons are assumed to have internal degrees of freedom (quantum states) in addition to translational motion.

The equations for the field operators are more general than a Gross-Pitaevsky-type equation in that equations of the latter form emerge as the lowest-order approximation, an approximation that in other contexts is called the "gapless" approximation [2]. We then introduce "conserving" approximations, the simplest being the so-called Hartree approximation, another being the "Hartree with Exchange" approximation.

Approximations beyond the simplest (gapless) one allow us to study corrections to the Gross-Pitaevsky-type equations arising from the quantized nature of the field variables (operators). Unfortunately these equations are more complicated than a Gross-Pitaevsky equation, whose numerical solution is already a nontrivial exercise. With the advent of experimental reports of Bose-Einstein condensation, we temporarily set aside our anticipated numerical studies of these equations in order to devote our attention to some of the fascinating physics made possible by the experiments. However, we note that the formalism we have developed should find applications in various areas of interest at LANL, including plasmas interacting with electromagnetic fields. Along these lines we note also that a nonequilibrium formalism for the plasma case was discussed many years ago by DuBois [5].

One of the most intriguing features of Bose-Einstein-condensed atomic systems is that it is possible to control and possibly even manipulate the interatomic interactions. We have suggested, for instance, that it should be possible to change the dependence of the dipole-dipole interaction on the interatomic separation by applying either a static or time-varying electric field [6]. In particular, the usual van der Waals interaction varying as the inverse sixth power of the separation can be modified to have an inverse-cube dependence on separation when an electric field is applied. This modification of the dipole-dipole interaction by an applied electric field was recently obtained independently and discussed by Marinescu and You [7], and Taneda and Mori [8] have extended our calculations to include wave-function overlap effects arising at small interatomic separations.

Much more experimental and theoretical work has been done concerning the effects of magnetic fields on Bose-Einstein condensates. The MIT group under Ketterle [3] has reported the observation in atomic sodium condensates of a "Feshbach resonance," a general collisional resonance usually associated with nuclear physics. The Feshbach resonance in these experiments involves an intermediate molecular state having a spin configuration different from that of the atoms forming this state. The variation of an applied magnetic field changes the difference (or "detuning") between the energies of the initial and intermediate states. The effective scattering length characterizing the binary collisions varies with the strength of the magnetic field, allowing it to be "tuned" and thereby opening the possibility for very interesting studies in many-body physics. We have shown [9] that this system is in fact much richer than this; the atom-molecule coupling in the Feshbach resonance can result in a second, molecular condensate coexisting with the atomic condensate. We have suggested that the second condensate might be observable, for instance, as an oscillation in the number of atoms and molecules when the external magnetic field is varied. According to our analysis the properties of a condensate will depend on its history, and in particular whether it is initially above or below resonance as the detuning is slowly varied.

Another fascinating possibility we have uncovered is that of creating a dilute condensate which nevertheless has the liquid-like property of having a self-determined density [10]. In other words, there is the theoretical possibility of creating a very dilute but liquid-like state of matter that is suggested by our study of the density dependence of the many-body ground-state energy.

We have investigated several aspects of two-phase condensates [11-13]. Their population dynamics indicate that the system has two distinct stationary states, depending on the relative phase of the atomic and molecular condensates. As noted above, the particular state the system finds itself in depends on its history. Work still in progress is investigating the possibility that hitherto unexplained molecular loss processes observed in the experiments might be understood via the detuning dependence of the state of the system [14].

We have carried out preliminary calculations of the two-photon absorption spectrum that was measured in the first experimental observation of condensation of atomic hydrogen by Kleppner's group [4]. The calculations thus far have dealt with only one spatial dimension for simplicity, and we are currently extending them to three dimensions.

Several brief research projects were carried out or are still in progress as indirect results of our involvement in this project, and will be given only brief mention here. With Professor Heidi Fearn, who visited LANL for a total of about eight months, in part under

the auspices of the Associated Western Universities, we studied the modification of two-photon frequency down-conversion processes by the presence of mirror surfaces. Our results explained very well the modifications observed by Zeilinger's group at the University of Innsbruck [15]. With Professor Raymond Chiao (University of California at Berkeley) we have been investigating various aspects of what are termed "superluminal" propagation effects in amplifying optical media [16]. Finally, with Professor Larry Spruch and Dr. Martin Schaden (New York University) we have studied theoretically the possibility of a transition frequency shift of a guest atom in a dielectric medium [17].

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