PhD project in Computational Physics for Jon Kristian Nilsen

Vortices in Bose-Einstein Condensates: A Quantum Monte Carlo Analysis

The spectacular demonstration of Bose-Einstein condensation (BEC) in gases of alkali atoms ^{87}Rb, ^{23}Na, ^{7}Li confined in magnetic traps[1, 2, 3] has led to an explosion of interest in confined Bose systems. Of interest is the fraction of condensed atoms, the nature of the condensate, the excitations above the condensate, the atomic density in the trap as a function of Temperature and the critical temperature of BEC, T_c. The extensive progress made up to early 1999 is reviewed by Dalfovo et al.[4].

A key feature of the trapped alkali and atomic hydrogen systems is that they are dilute. The characteristic dimensions of a typical trap for ^{87}Rb is $a_{h0} = (\hbar/m\omega_\perp)^{\frac{1}{2}} = 1 - 2 \times 10^4$ Å (Ref. 1). The interaction between ^{87}Rb atoms can be well represented by its s-wave scattering length, a_{Rb}. This scattering length lies in the range $85 < a_{Rb} < 140a_0$ where $a_0 = 0.5292$ Å is the Bohr radius. The definite value $a_{Rb} = 100a_0$ is usually selected and for calculations the definite ratio of atom size to trap size $a_{Rb}/a_{h0} = 4.33 \times 10^{-3}$ is usually chosen [4]. A typical ^{87}Rb atom density in the trap is $n \simeq 10^{12} - 10^{14}$ atoms/cm^3 giving an inter-atom spacing $\ell \simeq 10^4$ Å. Thus the effective atom size is small compared to both the trap size and the inter-atom spacing, the condition for diluteness (i.e., $na^3_{Rb} \simeq 10^{-6}$ where $n = N/V$ is the number density). In this limit, although the interaction is important, dilute gas approximations such as the Bogoliubov theory[5], valid for small na^3 and large condensate fraction $n_0 = N_0/N$, describe the system well. Also, since most of the atoms are in the condensate (except near T_c), the Gross-Pitaevskii equation[6, 7] for the condensate describes the whole gas well.

Recently however experiments have been performed which go beyond the dilute gas model. These experiments challenge the foundation of the above mean field picture. Ab initio tools like Diffusion Monte Carlo (DMC) and Green's function Monte Carlo (GFMC) methods are therefore to be preferred when one moves to larger densities. DMC and GFMC offer in principle exact solutions of the many-body Schrödinger equation. Furthermore, there has recently been much experimental and theoretical interest in excited states of Bose-Einstein condensates characterized by a quantized circulation, so-called vortices. The existence of these excited condensate states is crucial to studies of the superfluid behavior of trapped atomic condensates

The purpose of this Dr. Scient (PhD) thesis is twofold:

- To develop Diffusion Monte Carlo and GFMC programs for studying systems beyond the dilute limit, both ground state features and excited states. This will allow for in principle exact solutions of Schrödinger's equation for densities beyond the dilute gas limit. The aim is to use these methods and evaluate ground state and excited state properties of a trapped, hard sphere Bose gas over a wide range of densities using DMC and GFMC methods with several trial wave functions. These wave functions are used to study the sensitivity of condensate and non-condensate properties to the hard sphere radius and the number of particles.

  Jon Nilsen has already developed a large parallel Variational Monte Carlo (VMC) code for studying Bose Einstein condensates. In Ref. [8], properties of the ground state and excited states were studied using this program. This paper is part of Jon Nilsen's PhD project.

- The second aim of this thesis project is to study parallel implementations of the DMC and GFMC programs on various machine structures, from local PC clusters to large scale machines available through the NOTUR project, using both distributed and shared memory. The reason for this part is due to the complexity represented by the DMC and GFMC calculations, where tipycally many random walkers are needed in order to get good statistics and to obtain the profiles of the wave functions of the various states. Parallel algorithms are presently the only reasonable way of obtaining statistics of good quality.

  The expertise gained in such studies can also be transferred to other many-body projects, such as the Large-Scale shell model code for nuclear physics studies developed by Torgeir Engeland.

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