Bose-Einstein condensation in trapped bosons: A quantum Monte Carlo analysis using OpenCL and GPU programming

The aim of this thesis is to develop diffusion Monte Carlo (DMC) and a Variational Monte Carlo (VMC) programs written in OpenCL, in order to test the potential of Graphical processing units (GPUs) in Monte Carlo studies of both bosonic and fermionic systems.

The thesis will start with existing VMC and DMC codes for bosons and fermions, tailored to run on large supercomputing cluster with thousands of cores. These codes will then be rewritten in OpenCL and tested on different GPUs, in order to see if a considerable speedup can be gained. Such a speedup, if we at least an order of magnitude is gained compared with existing in C++/Fortran codes that run on present supercomputers, will have trememdous consenquences for ab initio studies of quantum mechanical systems. The prices of the GPUs are of the order of few thousands of NOK, compared with large supercomputers which can cost billions of NOK.

The physics cases will deal with Bose-Einstein condensation and studies of the structure of atoms like Neon or Argon. In this way, both bosonic and fermionic systems will be tested.

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., $na_{Rb}^3 \simeq 10^{-6}$ 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. Effects of atoms excited above the condensate have been incorporated within the Popov approximation[8].

The purpose of this master thesis is to go beyond the dilute limit, to test the limits of the above approximations and to explore the properties of the trapped Bose gas as na^3 increases between the dilute limit and the dense limit. The tools to be used are from Variational Monte Carlo (VMC) and Diffusion Monte Carlo methods (DMC) methods.

The aim is to use these methods and evaluate the ground state properties of a trapped, hard sphere Bose gas over a wide range of densities using VMC and DMC 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. The traps we will use are both a spherical symmetric (S) harmonic and an elliptical (E) harmonic trap in three dimensions given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2}m[\omega_{ho}^2(x^2+y^2)+\omega_z^2 z^2] & (E) \end{cases} \tag{1}$$

with

$$H = \sum_i^N \left(\frac{-\hbar^2}{2m}\nabla_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{i<j}^N V_{int}(\mathbf{r}_i, \mathbf{r}_j), \tag{2}$$

as the two-body Hamiltonian of the system. Here ω_{ho}^2 defines the trap potential strength. In the case of the elliptical trap, $V_{ext}(x, y, z)$, $\omega_{ho} = \omega_\perp$ is the trap frequency in the perpendicular or xy plane and ω_z the frequency in the z direction. The mean square vibrational amplitude of a single boson at $T = 0K$ in the trap (1) is $< x^2 >= (\hbar/2m\omega_{ho})$ so that $a_{ho} \equiv (\hbar/m\omega_{ho})^{\frac{1}{2}}$ defines the characteristic length of the trap. The ratio of the frequencies is denoted $\lambda = \omega_z/\omega_\perp$ leading to a ratio of the trap lengths $(a_\perp/a_z) = (\omega_z/\omega_\perp)^{\frac{1}{2}} = \sqrt{\lambda}$.

We represent the inter boson interaction by a pairwise, hard core potential

$$V_{int}(r) = \begin{cases} \infty & r \leq a \\ 0 & r > a \end{cases} \tag{3}$$

where a is the hard core diameter of the bosons. Clearly, $V_{int}(r)$ is zero if the bosons are separated by a distance r greater than a but infinite if they attempt to come within a distance $r \leq a$.

The thesis will use as starting point a recently developed program for bosons by Jon Nilsen, see the reference list. This code is written in C++ and runs efficiently on standard supercomputers.

Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Fall 2010: Develop a VMC and DMC code for boson in OpenCL
- Fall 2010: Develop a VMC and DMC code for fermions in OpenCL. Parallel with this, one needs also a corresponding C++ which can run in parallel on existing supercomputers
- Spring 2011: Extensive benchmarks of codes and writeup of master thesis.

If successful, this thesis will end up in a scientific publication in a journal like Computer Physics Communications.

References

[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, *Science* **269**, 198 (1995).

[2] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).

[3] C.C. Bradley, C.A. Sackett, J.J. Tolett, and R.G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995); C.C. Bradley, C.A. Sackett, and R.G. Hulet, *ibid.* **78**, 985 (1997).

[4] F. Dalfovo, S. Giorgini, L. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999).

[5] N.N. Bogoliubov, *J. Phys. (Moscow)* **11**, 23 (1947).

[6] E.P. Gross, *Nuovo Cimento* **20**, 454 (1961).

[7] L.P. Pitaevskii, *Ah. Eksp. Teor. Fiz.* **40**, 646 (1961) [*Sov. Phys. JETP* **13**, 451 (1961)].

[8] D.A.W. Hutchinson, E. Zaremba, and A. Griffin, *Phys. Rev. Lett.* **78**, 1842 (1997).

[9] J.K. Nilsen, *Comp. Phys. Comm.* **177**, 799 (2007).