

SMR 1595 - 21

**Joint DEMOCRITOS - ICTP School on
CONTINUUM QUANTUM MONTE CARLO METHODS
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COMPUTER LABORATORY SESSION

UPI - LAB

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These are preliminary lecture notes, intended only for distribution to participants.

UPI lab

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The aim of today’s lab is to get some experience on the use of UPI code and to better understand several issues of PIMC such as i) choice of the optimal a priori probability for moving the paths ($T(s_i \rightarrow s_j)$), ii) choice of the time slice τ , iii) sampling permutations. We will consider as a practical example a system of 32 atoms of ${}^4\text{He}$ at $\rho = 0.02179\text{\AA}^{-3}$ which has the superfluid phase below $T = 2.15\text{K}$. We will provide a density matrix file slightly different from what you have produced yesterday with squarer. It contains tables for the density matrix and the β derivative at several temperatures. They are used by UPI in the bisection algorithm. Also the format is quite different.

Here are the directions to compile the executable, to get the density matrix tables and to set up a run:

1. Copy the tar file with the command
`cp /afs/ictp/public/c/cpierleo/PIMC/upilab.tgz .`
2. Unpack the tar file `tar xvfz upilab.tgz` and go in the directory UPILAB. There are three directories:
 - **NOTES** contains this document and a copy of the slides,
 - **UPI** contains the upi code (UPI/pimc), several useful libraries (UPI/fnlib, UPI/forlib), machine dependent files for several different architectures (UPI/*rtl), density matrix related codes (UPI/sqdir), analysis tools (UPI/analysis), setup codes (UPI/setup)
 - **WORK** contains a density matrix directory (WORK/DMDIR) and a working directory for any different system studied
3. Go into the directory UPILAB/UPI/ and install and compile the UPI code by the command `make`
4. Go into the directory UPILAB/UPI/setup/ and compile the setup code OCSET:
`make ocset`
5. Go into a working directory in UPILAB/WORK
6. link the density matrix file into the actual directory `ln -s ../DMDIR/He4.nd.dm .`
7. Run `ocset (./ocset)` and fill the fields interactively for any different run you want to performe (see the presentation).

8. In case you want to change the some compilation options for the upi code, go in UPI-LAB/UPI, issue the command `make clean`, edit the file `machconfig` and change the option for your present architecture. Then recompile upi by the command `make`.

Part 1) of the lab consists in fixing a relatively high temperature and running the code with several different settings. The aim is to understand the relative importance of the different kind of moves such as bisection reconstruction of paths and displace moves. We will work at fixed T and ρ . In this part of the lab we will use the driver OMOVE only (no permutation are attempted)!

1. Fix the number of slices and the bisection level in order to have a reasonable acceptance (in file `qid.acc`).
2. Run two simulations of many short blocks (few hundreds blocks of 20 steps) without and with DISPLACE.
3. Compare the results obtained for several quantities using the package DATASPORK. In particular check the correlation time of various quantities.
4. Repeat the study with twice as many time slices keeping the same bisection level
5. Increase the bisection level in such a way to move the same imaginary time interval as in point 2 and compare the correlation times
6. Change the level of bisection and check how the correlation time changes
7. Repeat point 2 with the keyword FREESAMP in the `qid.sy` file (free particle sampling) and compare the efficiency.

Part 2) of the lab consists in running several simulatons at a given temperature for an increasing number of time slices. Since the optimal value of the time slice mainly depends on the density one can make the convergence study at relatively high temperature, and once τ is chosen, lower the temperature by increasing the number of time slices at fixed τ . For ${}^4\text{He}$ at this density, I suggest to study the convergence at $T = 5\text{K}$ running with M between 4 and 32 and looking at the convergence of several quantities. In particular look at the total energy and try to get an idea of the optimal choice of τ . Compare the thermodynamic and the virial estimators for the kinetic energy and note the behaviour of the error with M .

Part 3) of the lab consists in exploring the sampling of permutations for superfluid ${}^4\text{He}$. Choose here $\tau = 40\text{K}^{-1}$ which should be close to what you have found in part 2. Make several runs for decreasing temperature and check the acceptance of the various levels of bisection and for the different number of movers. Check the cycle probability with temperature. Look at various properties of the system as the superfluid density (Winding number in `qid.out`) and the effective mass (`qid.em`).