

SMR 1595 - 8

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

TAS

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

TAS

TAS is a quantum Monte Carlo code to evaluate properties of simple fermi liquids. Some features:

- Only one component systems in cubic periodic boundary conditions for a fixed V and fixed N
- 2 or 3 dimension (depending on makefile)
- Uses twisted boundary conditions and can average over them.
- Either long-range (Coulomb) or short range potential (helium-helium)
- Quantum crystal or fluid.
- Dynamically changes twist values
- Spin (1/2) or “spinless”.

Program written by D. Ceperley, F-H Zong and C. Lin 1999-2001.

Description of Keywords

Keywords associated with system specification:

- NUMBER #particles[#nppss
number of particles

number of particles in the first spin state. (if zero implies a boson state—no Slater determinant)
- RHO rho, hbs2m, nkact
&nb sp; If RS “line” is present RHO is not needed. RHO is used for a helium calculation.
&nb sp; Hbs2m is $\hbar^2/2$ mass
&nb sp; Nkact is the number of k-shells in the action for Ewald summation.
- RS rs [nkact [cutr
If present this is an electron gas calculation with units of a and Rydbergs.
Rs is the electron density
Nkact are the number of shells of k-vectors used in the action for Ewald summation.
Cutr is the cutoff in real space of all the radial tables (potential, wavefunction g(r))
- HEDF2 [cutr
Helium calculation. Potential is setup in heinit
Cutr is the radial cutoff for all tables including g(r), potential, backflow and threebody.
- THETA ifserial ndim thetax thetay thetaz
Ifserial=0 means a serial run
Ndim is the dimension
Theta (x,y,x) are the twist values
(sets izerophase=1 if all values are zero)

Keywords associated with trial wavefunction:

- EXTRA extra we [c , d , d]
The Jastrow parameters (and an extra term in addition to RPA for the electron gas)
Electron gas $u = \text{extra} \exp(-(\text{we} * r)^2)$
Helium $u = \text{extra} * r^{(-\text{we})} + c * \exp(-d(r-e)^2)$
- c pc pd
If present this is a crystal calculation c and d are the variational parameters.
Orbital is $\exp[-cr^2/(1+d*r)]$

Keywords associated with numerical issues:

- NWALKERS nwalkers
Number of walkers (population) within DMC.
- ETRIAL etrial
Per particle trial energy for DMC

- **TIMER** *nseconds*
Will cause execution to terminate after *nseconds* (current blocks are allowed to finish) user time in seconds.

Keywords associated with initial conditions:

- **READ_COORD** [*file_name*]
Sets the positions of the particles to those in *file_name* ([see format.](#)) extension of *file_name* must be .crd Default *file_name* is id.crd.
- **READ_STATE** [*file_name*]
Sets the internal state (positions, random number seed, ..) to those in filename. Default *file_name* is id.chk. This will supercede all initializations.
- **RESTART**
Begin with last configuration generated by previous run and continue as if job had not concluded. Restarting is appropriate if run has been interrupted before completion or if you want to extend the length of a run. The only changes allowed to id.in are to increase the number of steps or to add more commands "RUN xx" after the last executed step. CHECKPOINT files must have been written for RESTART to be successful. The RESTART command can be placed anywhere in the .in file and it will supercede all other state initializations. The difference between RESTART and READ_STATE is the RESTART will skip steps already performed.
- **SEED** *value*
Random number seed. (integer) See the SPRNG documentation. The default is a random seed constructed from the date and time. If you wish to repeat a run, and you chose the default for the initial run use the number printed on the output listing. To change the generator type, the Makefile must be changed.

Keywords associated with output:

(they will take effect after their occurrence in input)

- **WRITE_COORD** *period*
Writes the particle coordinates onto id.crd with this period. The total number of writes generated by this command will be $nsteps/period$ (each containing natoms lines) $period=0$ will turn off writes (default).
- **WRITE_SCALARS** *period*
Period with which to write scalars for analysis onto the file id.sca. The default is not to write out scalars. This file contains the energy, acceptance ratio and computer time/step.
- **WRITE_SOFK** *period* [*nksofk*]
Period with which to output the structure factor to file id.sk.. Default is not to write out S(k). The pair correlation function is written at the same time onto g(r).
Nksofk is used to set the minimum number of shells of k-values.
- **CHECKPOINT** *period*
Period to spill out coordinates and averages onto file id.chk The checkpoint file is always written at the end of a "RUN" command but if this command is absent, it will be impossible to restart from a partially complete "RUN".
- **DEBUG**
Will cause more printouts on the id.out file.

“DYNAMICAL” Keywords:

These keywords execute in the order in the input file. If RESTART is present, the run will begin in the last CHECKPOINTed state.

nsteps refers to the total number of steps performed.

Tau is the DMC/VMC timestep

Iwarm is the number of blocks to discard in the beginning before taking averages.

- **RUN** VMC *nsteps* tau
- **RUN** DMC *nsteps* tau iwarm
- **RUN** TAVMC *nsteps* tau iwarm *nspb*
Nspb is the number of steps before changing the theta value.
- **SEARCH** tau [*p1* [*p2*
Search parameter space given by parameters *p1* ..*pn*.
Tau controls whether it is a variance or energy minimization.
- **TEST** delta

Test derivatives of the wavefunction.
Delta is the spatial step to compute numerical derivatives.

* For these keywords order is important: they have an effect after their occurrence.

Variable types: string, *integer*, real, KEYWORD, required keyword, required choices.

[Keyword Syntax](#)

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