the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

SMR 1595 - 13

_____

Joint DEMOCRITOS - ICTP School on

CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

_____

COMPUTER LABORATORY SESSION

PAIR DENSITY MATRIX LABORATORY

*Carlo PIERLEONI and **David M. CEPERLEY

* Univ. di L'Aquila, Italy
** Beckman Institute for Advanced Studies & Technology
University of Illinois at Urbana-Champaign - N.C.S.A.
Il-61801 Urbana, U.S.A.

_____

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

Pair density matrix lab

Carlo Pierleoni & David M. Ceperley

Following the notes on the use of POTGEN SQUARER and FKPIMC, study the specific case of a pair of particles (He4-He4, e-e, e-p, ...). The proposed exercise consists in studying the accuracy of the different levels of approximation for the pair density matrix in a temperature range from the semi-classical limit down to low temperature.

Choose a reasonable temperature grid (according to the thermal wavelength of the particles) and for each temperature in the grid compare: i) the *primitive* approximation ($nsquare = 0$), ii) the pair density matrix in the *end-point* approximation ($norder = 0$), iii) the full pair density matrix at $norder = 1$ and $norder = 2$ ($norder$ corresponds to the sum index n in eq. (4.46) of Rev.Mod.Phys.1995).

1. Copy in your home directory the file
   `/afs/ictp/public/c/cpierleo/PIMC/pdmlab.tgz`.
   Unpack the archive (`tar xvfg pdmlab.tgz`) and go in the directory `PDMLAB`. There are two directories, `NOTES` where you will find this document and a copy of the slides, and `DMD` containing the codes, the documentation (`DMD/doc`) and several input files (`DMD/test`). Compile SQUARER, POTGEN and FKPIMC with the command `make all`.

2. Prepare a file *name.dm* according to the notes (examples are in `DMD/test`).

3. Run POTGEN and get the *name.pot* file. Check whether the accuracy of the grid is OK. Otherwise increase the grid points or/and change the grid type.

4. Run squarer for $norder = 1$ and get the files *name.dmu*, *name.dme*. Look at the file *name.dmo* to check whether the maximum number of partial waves was correct. Check whether the fitting error from the partial wave expansion to the (q,s,z) expansion is acceptable in the physically relevant region of q's, both for the action (second column in *name.dmu*) and for its β derivative (second column in *name.dme*).

5. Plot the various components of the pair action (u_0, u_{10}, u_{11}, etc.) and of its β derivative and check whether they are smooth in the physically relevant region of q's.

6. Repeat steps 4-5 with $norder = 2$ in the SQUARER command.

7. Go through steps 2-6 for any different temperature.

8. Use FKPIMC to check the accuracy of your best approximation to the true pair density matrix. Choose a bunch of significant points (on the diagonal and out diagonal within the effective thermal wavelength of the pair) and run FKPIMC. In the output you will get the difference between the tabulated density matrix and a more accurate estimate from a PIMC calculation.

Example of input files

1. Helium-Helium density matrix

```
UNITS K A
TYPE He4 6.059615
TYPE He4 6.059615
GRID 80 LINEAR .2 8.0
POT HEDF2 6.
DUMP 0 1 2 3 4 5 6 7 8
SQUARER 10.  3 2 50 8
```

2. electron-electron density matrix

```
UNITS H A0
TYPE e 0.5 -1.
TYPE e 0.5 -1.
GRID 80 LOG .01 15.0
POT POWER 10.  0.25 1.  1.
SQUARER 0.1 3 2 15 10
```

3. electron-proton density matrix

```
UNITS H A0
TYPE e 0.5 -1.
TYPE p 2.7231e-4 1.
GRID 80 LOG .001 15.0
POT POWER 10.  0.25 1.  1.
SQUARER 0.1 3 2 15 10
```

4. electron-proton density matrix

```
UNITS H A0
TYPE p 2.7231e-4 1.
TYPE p 2.7231e-4 1.
GRID 200 LINEAR .1 25.0
POT POWER 10.  0.25 1.  1.
SQUARER 0.0033 3 0 15 10
```