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CONTINUUM QUANTUM MONTE CARLO METHODS

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COMPUTER LABORATORY SESSION

CONSTRUCTING AND TESTING THE PAIR ACTION TABLE

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

Constructing and testing the pair action table

- POTGEN: to build the pair potential table
- SQUARER: to compute the pair action and to build the table in terms of (q,s,z) variables
- FKPIMC: to test the pair action table and more in general to estimate matrix elements of two (or more) body density matrix operator.

POTGEN

- INPUT FILE: *qid*.dm

```
UNITS K A
TYPE He4 6.059615
TYPE He4 6.059615
GRID 80 LINEAR .2 8.
POT HEDF2  6.
SQUARER 10. 4 3 3 50 14
```

- OUTPUT FILES:
  - *qid*.dm: few lines are added in this file for tail corrections
  - *qid*.pot: contains the potential table $[r, v(r), rms - error]$

- HINT: be sure that $error \leq 0.01T$ in the relevant range of the grid.

SQUARER

- It computes the pair action: $u(\mathbf{r},\mathbf{r}';\tau) \equiv -\ln\left(\rho(\mathbf{r},\mathbf{r}';\tau)/\rho_0(\mathbf{r},\mathbf{r}';\tau)\right)$
  - Partial waves expansion

$$\rho(\mathbf{r},\mathbf{r}';\tau) = \begin{cases} \frac{1}{2\pi\sqrt{rr'}} \sum_{l=-\infty}^{\infty} \rho_l(r,r';\tau) e^{il\theta} & 2D \\ \frac{1}{4\pi rr'} \sum_{l=0}^{\infty} (2l+1)\rho_l(r,r';\tau) P_l(cos(\theta)) & 3D \end{cases}$$

  - Matrix squaring for each ρ_l:

$$\rho_l(r,r';\tau) = \int_0^{\infty} dr'' \rho_l(r,r'';\tau/2)\rho_l(r'',r';\tau/2)$$

  - Polynomial expansion in $q=(r+r')/2$, $s=|\mathbf{r}-\mathbf{r}'|$, $z=|\mathbf{r}|-|\mathbf{r}'|$

$$u(\mathbf{r},\mathbf{r}';\tau) = \frac{1}{2}\left[u_0(r;\tau)+u_0(r';\tau)\right] + \sum_{k=1}^{n}\sum_{j=0}^{k} u_{kj}(q;\tau) s^{2(k-j)} z^{2k}$$

$(\mathbf{r}=\mathbf{r}_i-\mathbf{r}_j \qquad \mathbf{r}'=\mathbf{r}'_i-\mathbf{r}'_j)$

- INPUT FILES:
  - *qid*.pot
  - *qid*.dm

    `SQUARER temp ndim norder nl nsquare`

    - temp = temperature
    - ndim = spatial dimensionality
    - norder = order of the polynomial expansion
    - nl = cut-off in the partial wave expansion
    - nsquare = number of squarings ($T_{high} = T * 2^{nsquare}$)

- OUTPUT FILES:
  - *qid*.dmu: pair action [$q, rms - error, u_0, u_{10}, u_{11}, u_{20}, u_{21}, u_{22}, \ldots$]
  - *qid*.dme: its temperature derivative [$q, rms-error, u^{\tau}_0, u^{\tau}_{10}, u^{\tau}_{11}, u^{\tau}_{20}, u^{\tau}_{21}, u^{\tau}_{22}, \ldots$]

– *qid*.dmo: standard output

```
 Author: D. Ceperley, University of Illinois. Version  of July23, 1997
 grid nx= 80/ 250  0.2  8.
 spatial dimension= 3
 number of partial waves=  50/ 60
 hbarˆ2(1/m1+1/m2)=  12.11923
 density matrix zeroed at   0.  1.E+90
 order of polynomial fit=  2/ 2
 2d polynomial fit in s and z
 number of derivatives md= 2
 entering initialu
 Beginning matrix squaring nsquare =  8
r  0.20000E+00 rho  0.4916760-175 0.2263450-169
r  0.80000E+01 rho -0.2755357E-08 0.3753826E-03
 partial waves needed = 38/ 50
*****finished isq= 1 temp=   1280.****

.....................................................
.....................................................

 r  0.20000E+00 rho  0.1050187-185 0.2143700-182
 r  0.80000E+01 rho  0.9812816E-05-0.6096106E-03
  mdatam= 1302/ 10000
 order =    0 chimax  0.28187E+00 0.14236E+01
 order =    1 chimax  0.82910E-01 0.61163E+00
 order =    2 chimax  0.13123E-01 0.14876E+00
  partial waves needed = 9/ 50
 *****finished isq= 8 temp=   10.****

  SQUARER completed successfully
```

- HINTS:
  - check that the number of partial waves used never reaches the maximum allowedvalue
  - check that u and u^τ be small at the edge of the grid (for hard core potentials)
  - check the error for the different orders in the polynomial expansion. Acceptable values for the action are less than 1%. The maximum error times the exponentiated action is given in the output. Check also the first column in files *qid*.dmu and *qid*.dme.

FKPIMC

- It computes the pair action by a PIMC calculation of the Feynmann-Kac formula

$$e^{-u(\mathbf{r},\mathbf{r}';\tau)} = \left\langle exp\left[-\int_0^\tau v(\mathbf{q}(t))dt\right]\right\rangle_{RW}$$

$\mathbf{q}(0) = \mathbf{r};\ \mathbf{q}(\tau) = \mathbf{r}'$

$< \ldots >_{RW}$ means an average over brownian bridges from $\mathbf{r}$ to $\mathbf{r}'$

- INPUT FILES:
  - *qid*.pot from POTGEN
  - *qid*.dmu from SQUARER

- fkpimc.in

```
He4                    !  Name of the potential file  (qid.pot)
TYPE He4 6.05961       !  TYPE card only the third parameter lambda is used
GRID 80 LINEAR .1 8.0  !  GRID for the potential used in the qid.dm file
10.0                   !  temperature
2 500 6 64             !  nparts  nsteps   levels   nblocks
2                      !  norder   (n in eq. 4.46 of Rev.Mod.Phys.)
0. 0. 0.               !  x1   y1   z1
0. 0. 0.               !  x1p  y1p  z1p
3.1085 0. 0.           !  x2   y2   z2
3.1085 0. 0.           !  x2p  y2p  z2p
```

- OUTPUT FILE: standard output

```
 Begin Feynman-Kac density matrix computation
 Author: D. Ceperley, University of Illinois. Version  of August 7,1997
 1 CMD:TYPE He4 6.059615
 1 CMD:GRID 80 LINEAR 0.2 8.0
GRID  80  0.2  8.
 temperature=  10.
 number particles= 2
 spatial dimension= 3
 number of terms in the action table= 3
particle    1 initial position     0.00000     0.00000     0.00000
particle    1   final position     0.00000     0.00000     0.00000
particle    2 initial position     3.10850     0.00000     0.00000
particle    2   final position     3.10850     0.00000     0.00000
```

```
  Potential taken from file He4
  finished reading potential
  Density matrix tables in file He4
  finished reading dm tables
  diffusion length=  1.90676926 |R1-R2|=  0.
  V(R1)= -10.0355623 V(R2)= -10.0355623
  number of blocks= 64
  number of levels= 6

  beginning Monte Carlo, nsteps*nblocks= 32000
  level  Action      error
     0 -0.1004E+01  0.0000E+00
     1 -0.6292E+00  0.2556E-02
     2 -0.3809E+00  0.3047E-02
     3 -0.2479E+00  0.3615E-02
     4 -0.1945E+00  0.3472E-02
     5 -0.1779E+00  0.3609E-02
     6 -0.1724E+00  0.3532E-02
extrp  -0.1706E+00  0.3521E-02       ! extrapolation with tau**2
bias               -0.6111E-05
rel.ex              0.5211E+00       ! extrapolation relative to error bar

table  -0.1718E+00                   ! what is in the table qid.dmu
MC-tab              0.1250E-02       ! difference between the table and FK
chi                 0.3550E+00       ! error of the table with respect to FK
```

- HINTS:
  - check the convergence with τ.
  - check **rel.ex** entry. If it is much larger than 1 increase the number of levels
  - check **MC-tab** entry.
  - repeat the calculation for points on the diagonal and out of diagonal within the thermal wavelength.