Jastrow

April 21, 2020

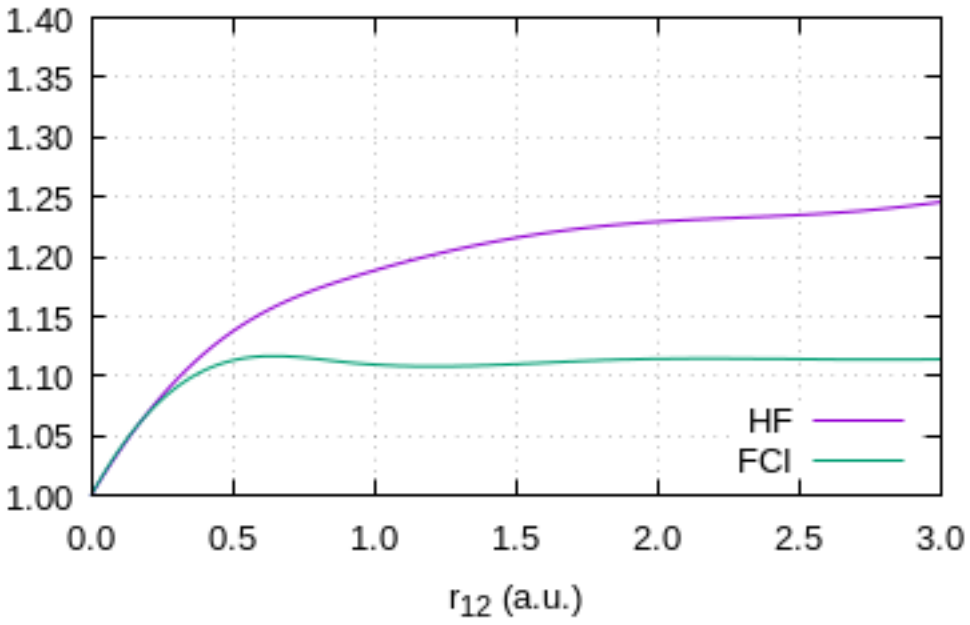
1 Jastrow factors

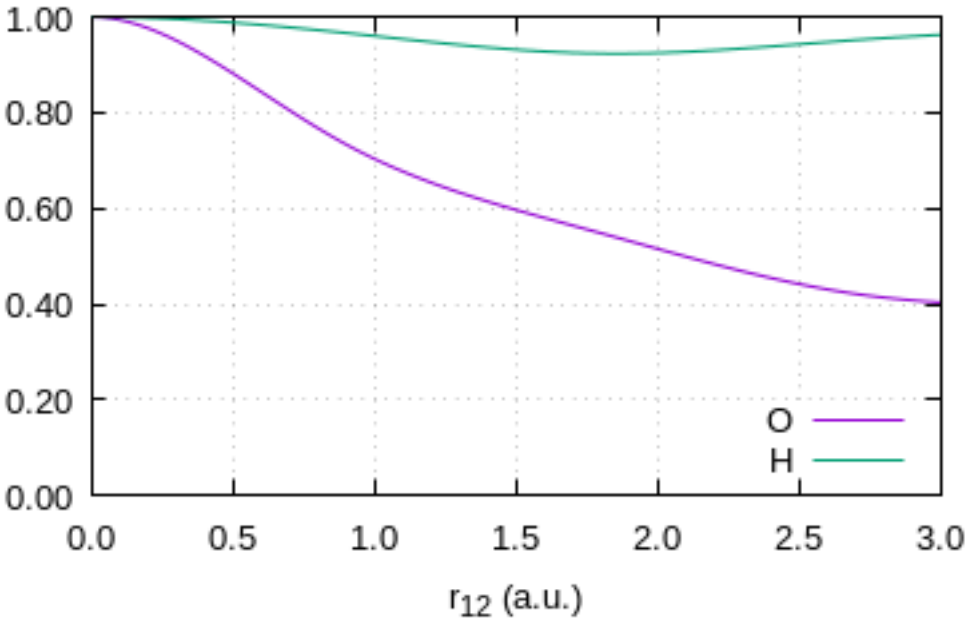
1.1 H2O

[1]:
```
onedet   = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J2.ud_exp.dat"
os = 1.-7.92535494e-01

multidet = "Jastrows/H2O/H2O-cc-pcvTz-multidet.wfj_J2.ud_exp.dat"
ms = 1.-8.59001137e-01

onedet_H = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J1.H_exp.dat"
ohs = 1.-1.03221118e+00
onedet_O = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J1.O_exp.dat"
oos = 1.-1.43887500e+00

#onedet = "~/Anouar/Jastrows/N2H4/N2H4-tr6.wfj_J2.ud_exp.dat"
#os = 1.-8.03464242e-01

!pwd
```

[1]:
```
onedet   = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J2.ud_exp.dat"
os = 1.-7.92535494e-01

multidet = "Jastrows/H2O/H2O-cc-pcvTz-multidet.wfj_J2.ud_exp.dat"
ms = 1.-8.59001137e-01

onedet_H = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J1.H_exp.dat"
ohs = 1.-1.03221118e+00
onedet_O = "Jastrows/H2O/H2O-cc-pcvTz.wfj-1det_J1.O_exp.dat"
oos = 1.-1.43887500e+00

#onedet = "~/Anouar/Jastrows/N2H4/N2H4-tr6.wfj_J2.ud_exp.dat"
#os = 1.-8.03464242e-01

!pwd
/home/scemama/TEX/RSDFT-CIPSI-QMC/Data
unset output
```

[2]:
```
set yrange [1:1.4]
set xrange [0:3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

plot onedet   u 1:($2+os) w l title "HF"\
,    multidet u 1:($2+ms) w l title "FCI"

set yrange [0:1]
plot onedet_O  u 1:($2+oos) w l title "O"\
,    onedet_H  u 1:($2+ohs) w l title "H"
```





[2]:
```
set yrange [1:1.4]
set xrange [0:3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

set output '/tmp/gnuplot-inline-1587464640.145517.692211090260.png'
plot onedet   u 1:($2+os) w l title "HF" ,    multidet u 1:($2+ms) w l title
"FCI"




set yrange [0:1]
set output '/tmp/gnuplot-inline-1587464640.145606.7249194234.png'
plot onedet_O  u 1:($2+oos) w l title "O" ,    onedet_H  u 1:($2+ohs) w l title
"H"
```

[3]:
```
f1(x) = exp(a_1 * x/(1. + b_1*x))
f2(x) = exp(a_2 * x/(1. + b_2*x))
f3(x) = exp(a_3 * x**2+b_3)
f4(x) = exp(a_4 * x**2+b_4)
a_1 = 0.5
a_2 = 0.5
a_3 = 0.5
a_4 = 0.5
b_1 = 1.
b_2 = 1.
b_3 = 1.
b_4 = 1.

fit f1(x) onedet   u 1:($2+os) via b_1
fit f2(x) multidet u 1:($2+ms) via b_2
fit [0:1] f3(x) onedet_O   u 1:($2+oos) via a_3, b_3
fit [0:1] f4(x) onedet_H   u 1:($2+ohs) via a_4, b_4
```

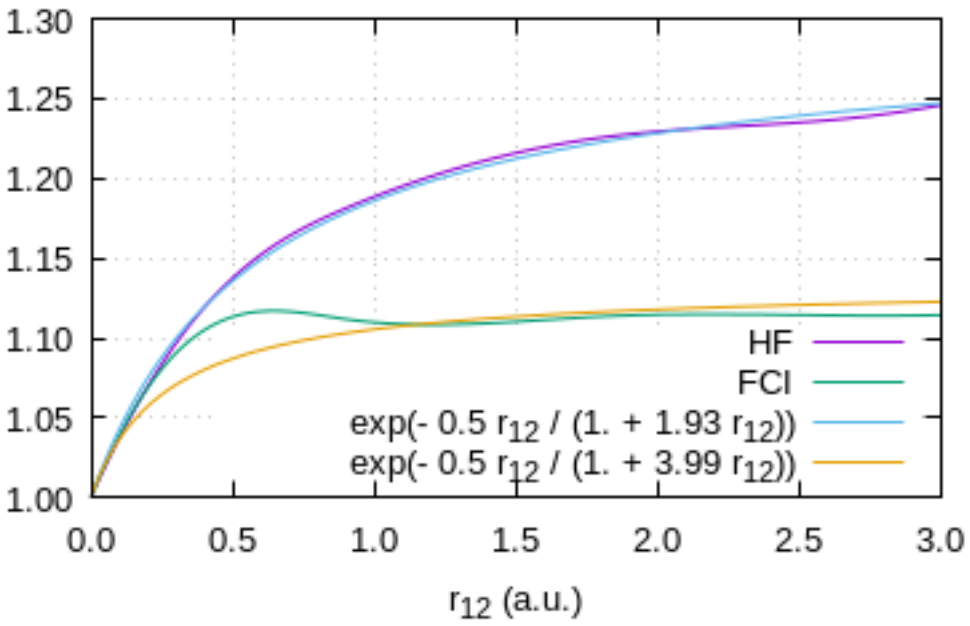
[3]:
```
unset output
 f1(x) = exp(a_1 * x/(1. + b_1*x))
f2(x) = exp(a_2 * x/(1. + b_2*x))
f3(x) = exp(a_3 * x**2+b_3)
f4(x) = exp(a_4 * x**2+b_4)
a_1 = 0.5
a_2 = 0.5
a_3 = 0.5
a_4 = 0.5
b_1 = 1.
b_2 = 1.
b_3 = 1.
b_4 = 1.

fit f1(x) onedet   u 1:($2+os) via b_1
Max. number of data points scaled up to: 3072
iter      chisq       delta/lim  lambda   b_1
   0 5.7947436972e+01   0.00e+00  2.58e-01    1.000000e+00


   1 5.1445429129e+00  -1.03e+06  2.58e-02    1.538628e+00
   2 1.4305276261e-01  -3.50e+06  2.58e-03    1.862386e+00
   3 3.1749513729e-02  -3.51e+05  2.58e-04    1.928474e+00
   4 3.1669788584e-02  -2.52e+02  2.58e-05    1.930350e+00


   * 3.1669788590e-02   1.98e-05  2.58e-04    1.930346e+00
   * 3.1669788590e-02   1.98e-05  2.58e-03    1.930346e+00
```

```
   * 3.1669788590e-02   1.98e-05  2.58e-02    1.930346e+00
   * 3.1669788590e-02   1.98e-05  2.58e-01    1.930346e+00
   * 3.1669788589e-02   1.67e-05  2.58e+00    1.930346e+00


   5 3.1669788530e-02  -1.69e-04  2.58e-01    1.930347e+00
iter      chisq       delta/lim  lambda   b_1

After 5 iterations the fit converged.
final sum of squares of residuals : 0.0316698
rel. change during last iteration : -1.69165e-09

degrees of freedom    (FIT_NDF)                        : 2999
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.00324963
variance of residuals (reduced chisquare) = WSSR/ndf   : 1.05601e-05

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
b_1             = 1.93035          +/- 0.0006837    (0.03542%)
fit f2(x) multidet u 1:($2+ms) via b_2
Max. number of data points scaled up to: 3072
iter      chisq       delta/lim  lambda   b_2
   0 1.6351844388e+02   0.00e+00  2.58e-01    1.000000e+00


   1 2.8331475972e+01  -4.77e+05  2.58e-02    1.903108e+00
   2 3.2508405969e+00  -7.72e+05  2.58e-03    2.993388e+00
   3 4.4711074925e-01  -6.27e+05  2.58e-04    3.771719e+00
   4 3.5779184535e-01  -2.50e+04  2.58e-05    3.979382e+00
   5 3.5770183297e-01  -2.52e+01  2.58e-06    3.986616e+00


   6 3.5770182428e-01  -2.43e-03  2.58e-07    3.986505e+00
iter      chisq       delta/lim  lambda   b_2

After 6 iterations the fit converged.
final sum of squares of residuals : 0.357702
rel. change during last iteration : -2.42953e-08

degrees of freedom    (FIT_NDF)                        : 2999
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.0109212
variance of residuals (reduced chisquare) = WSSR/ndf   : 0.000119274

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
b_2             = 3.9865           +/- 0.008324     (0.2088%)
fit [0:1] f3(x) onedet_0   u 1:($2+oos) via a_3, b_3
```

```
iter      chisq       delta/lim  lambda   a_3           b_3
   0 5.9977169495e+03   0.00e+00  2.41e+00    5.000000e-01   1.000000e+00
   1 5.3596427313e+02  -1.02e+06  2.41e-01    2.883807e-01   3.494757e-01
   2 2.5513945129e+01  -2.00e+06  2.41e-02   -5.571542e-02   3.008984e-02
   3 4.3942069520e-01  -5.71e+06  2.41e-03   -3.233185e-01  -1.938040e-02
   4 1.3950695794e-01  -2.15e+05  2.41e-04   -3.784304e-01  -1.599114e-02
   5 1.3930187120e-01  -1.47e+02  2.41e-05   -3.801893e-01  -1.569610e-02
   6 1.3930184761e-01  -1.69e-02  2.41e-06   -3.802119e-01  -1.569005e-02
iter      chisq       delta/lim  lambda   a_3           b_3

After 6 iterations the fit converged.
final sum of squares of residuals : 0.139302
rel. change during last iteration : -1.69332e-07

degrees of freedom    (FIT_NDF)                        : 998
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.0118144
variance of residuals (reduced chisquare) = WSSR/ndf   : 0.000139581

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
a_3             = -0.380212        +/- 0.001559     (0.41%)
b_3             = -0.0156901       +/- 0.0005992    (3.819%)

correlation matrix of the fit parameters:
                a_3    b_3
a_3             1.000
b_3            -0.704  1.000
fit [0:1] f4(x) onedet_H   u 1:($2+ohs) via a_4, b_4
iter      chisq       delta/lim  lambda   a_4           b_4
   0 5.3856009833e+03   0.00e+00  2.41e+00    5.000000e-01   1.000000e+00
   1 4.3790957890e+02  -1.13e+06  2.41e-01    3.455453e-01   3.625475e-01
   2 1.5298404788e+01  -2.76e+06  2.41e-02    1.187994e-01   5.316664e-02
   3 7.1643957948e-02  -2.13e+07  2.41e-03   -2.301630e-02  -5.474022e-04
   4 4.7733373771e-04  -1.49e+07  2.41e-04   -4.157329e-02  -9.283341e-04



   5 4.7373176545e-04  -7.60e+02  2.41e-05   -4.173964e-02  -9.101041e-04
   6 4.7373176473e-04  -1.53e-04  2.41e-06   -4.173975e-02  -9.100709e-04
iter      chisq       delta/lim  lambda   a_4           b_4

After 6 iterations the fit converged.
final sum of squares of residuals : 0.000473732
rel. change during last iteration : -1.52553e-09

degrees of freedom    (FIT_NDF)                        : 998
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.000688971
variance of residuals (reduced chisquare) = WSSR/ndf   : 4.74681e-07
```

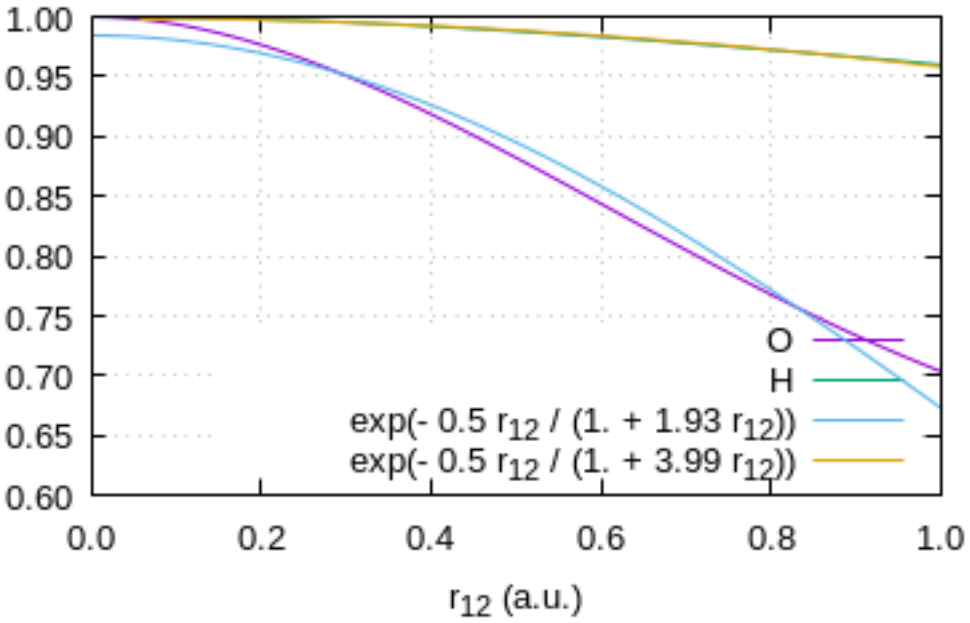
```
Final set of parameters            Asymptotic Standard Error
=======================            ==========================
a_4             = -0.0417397       +/- 7.482e-05    (0.1792%)
b_4             = -0.000910071     +/- 3.289e-05    (3.614%)

correlation matrix of the fit parameters:
                a_4    b_4
a_4             1.000
b_4            -0.740  1.000
unset output
```

[4]:
```
set xrange [0:3]
set yrange [1.:1.3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

plot onedet   u 1:($2+os) w l title "HF"\
,    multidet u 1:($2+ms) w l title "FCI"\
,    f1(x) title "exp(- 0.5 r_{12} / (1. + 1.93 r_{12}))"\
,    f2(x) title "exp(- 0.5 r_{12} / (1. + 3.99 r_{12}))"
```



[4]:
```
set xrange [0:3]
set yrange [1.:1.3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

set output '/tmp/gnuplot-inline-1587464644.6269653.290848243961.png'
plot onedet   u 1:($2+os) w l title "HF" ,    multidet u 1:($2+ms) w l title
"FCI" ,    f1(x) title "exp(- 0.5 r_{12} / (1. + 1.93 r_{12}))" ,    f2(x) title
"exp(- 0.5 r_{12} / (1. + 3.99 r_{12}))"


unset output
```

[5]:
```
set xrange [0:1]
set yrange [0.6:1.]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

plot onedet_O   u 1:($2+oos) w l title "O"\
,    onedet_H   u 1:($2+ohs) w l title "H"\
,    f3(x) title "exp(- 0.5 r_{12} / (1. + 1.93 r_{12}))"\
,    f4(x) title "exp(- 0.5 r_{12} / (1. + 3.99 r_{12}))"
```



[5]:
```
set xrange [0:1]
set yrange [0.6:1.]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

set output '/tmp/gnuplot-inline-1587464645.4823086.669140871663.png'
plot onedet_O   u 1:($2+oos) w l title "O" ,    onedet_H   u 1:($2+ohs) w l
title "H" ,    f3(x) title "exp(- 0.5 r_{12} / (1. + 1.93 r_{12}))" ,    f4(x)
title "exp(- 0.5 r_{12} / (1. + 3.99 r_{12}))"


unset output
```

[6]:
```
#set term pdf font "Times,15pt"
#set output "jastrow_h2o.pdf"
```

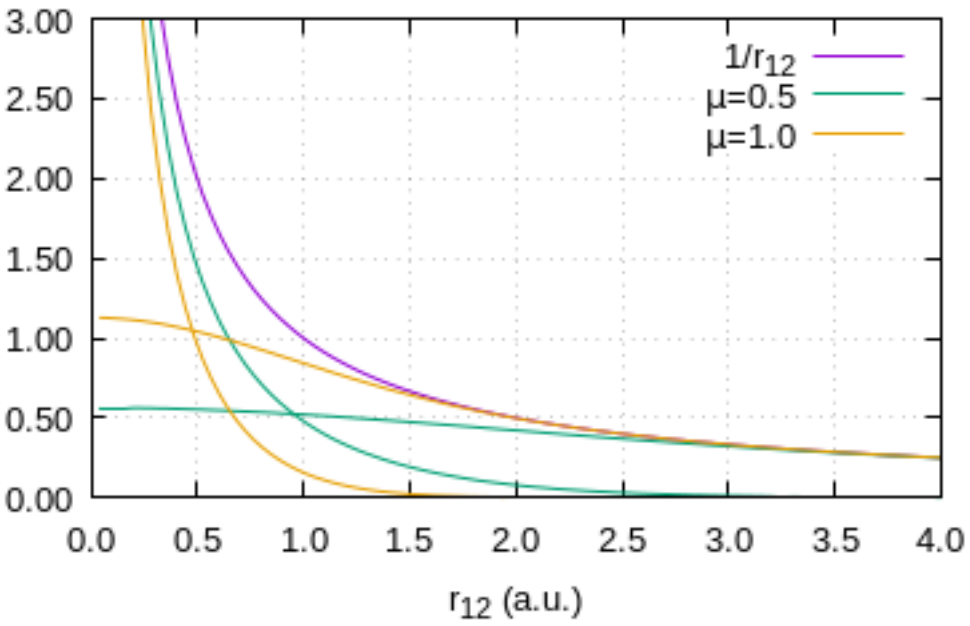
[6]:
```
#set term pdf font "Times,15pt"
#set output "jastrow_h2o.pdf"
unset output
```

1.2 Range-separated Coulomb operator

[7]:
```
w(x) = 1./x
w_lr(mu,x) = erf(mu*x)/x
w_sr(mu,x) = w(x) - w_lr(mu,x)
```

[7]:
```
w(x) = 1./x
w_lr(mu,x) = erf(mu*x)/x
w_sr(mu,x) = w(x) - w_lr(mu,x)
unset output
```

[8]:
```
set xrange [0:4]
set yrange [0:3]
set key top right
plot w(x)        title '1/r_{12}',\
     w_lr(0.5,x) title '{/Symbol m}=0.5' ls 2,\
     w_sr(0.5,x) notitle ls 2, \
     w_lr(1.0,x) title '{/Symbol m}=1.0' ls 4,\
     w_sr(1.0,x) notitle ls 4
```



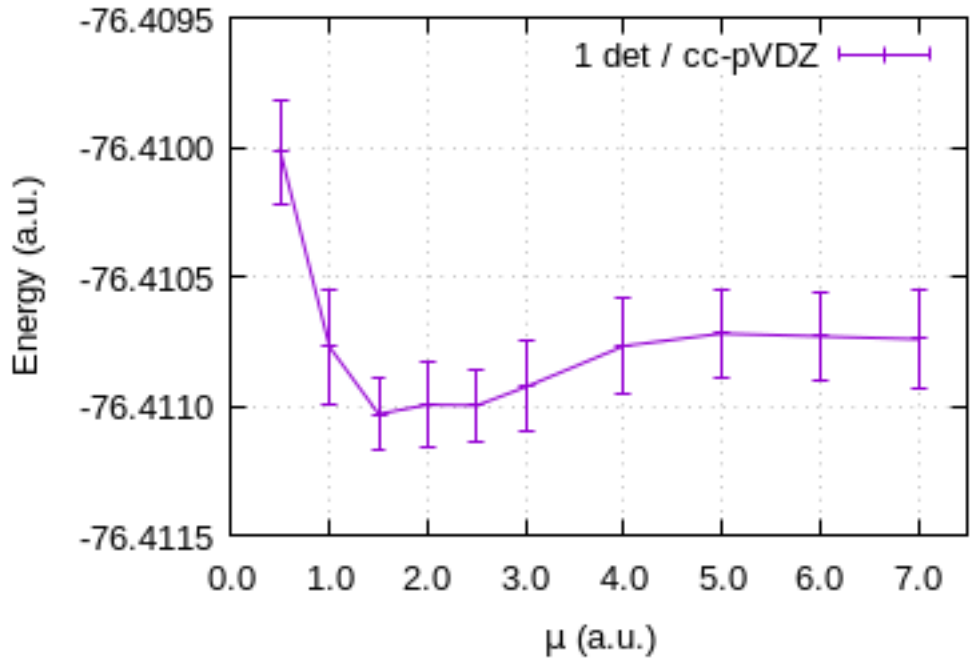
[8]:
```
set xrange [0:4]
set yrange [0:3]
set key top right
set output '/tmp/gnuplot-inline-1587464664.164814.164661607519.png'
```

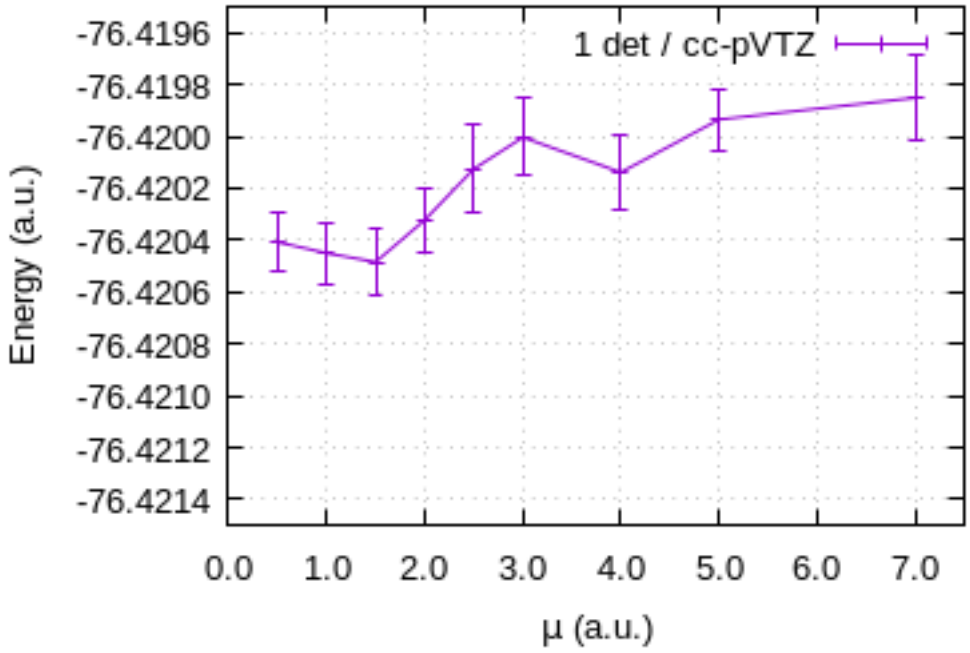
```
plot w(x)        title '1/r_{12}',      w_lr(0.5,x) title '{/Symbol m}=0.5' ls
2,      w_sr(0.5,x) notitle ls 2,       w_lr(1.0,x) title '{/Symbol m}=1.0' ls
4,      w_sr(1.0,x) notitle ls 4
unset output
```

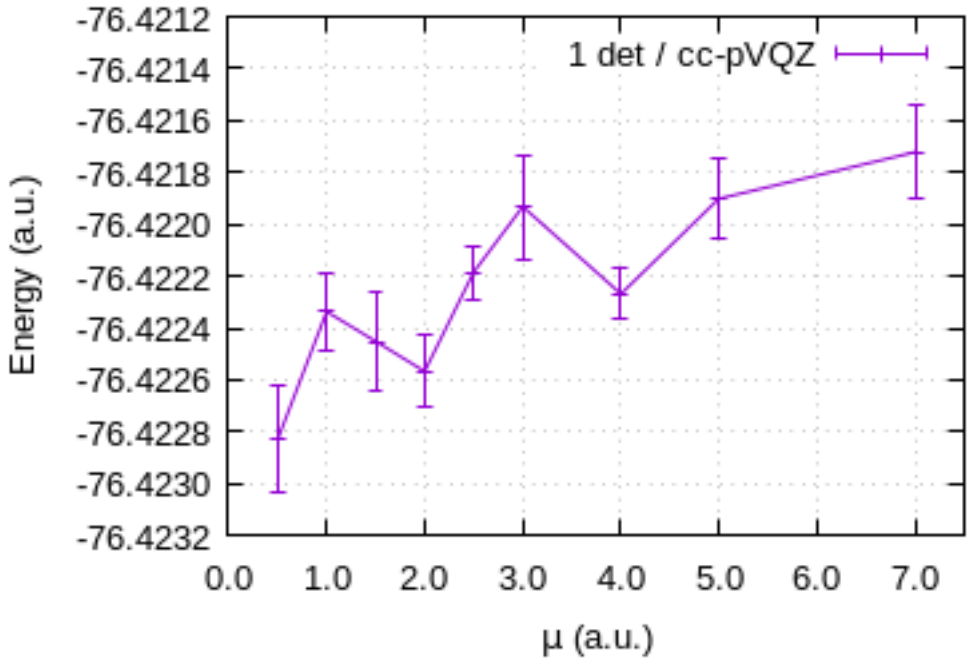
1.3 DMC Energies

1.3.1 Single-determinant

[10]:
```
data = "Jastrows/data_dmc"
set key top right
set xrange [0:7.5]
set xlabel "{/Symbol m} (a.u.)"
set ylabel "Energy (a.u.)"
set format y "%.4f"
set yrange [-76.4115:-76.4095]
plot data index 0 u 1:5:6 w errorlines title "1 det / cc-pVDZ"
set yrange [-76.4215:-76.4195]
plot data index 1 u 1:5:6 w errorlines title "1 det / cc-pVTZ"
set yrange [-76.4232:-76.4212]
plot data index 2 u 1:5:6 w errorlines title "1 det / cc-pVQZ"
```





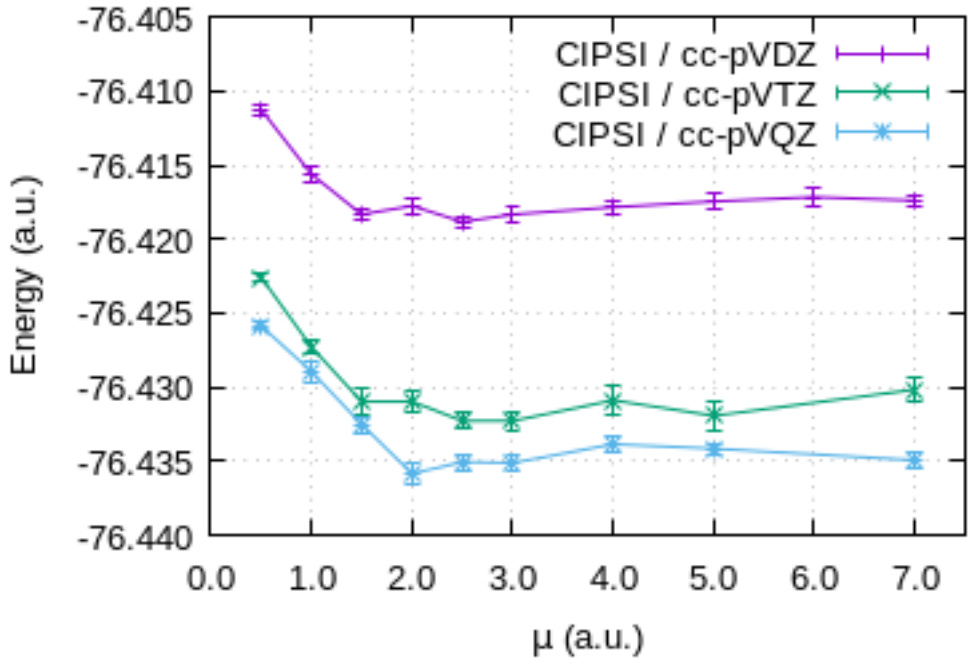


[10]:
```
data = "Jastrows/data_dmc"
set key top right
set xrange [0:7.5]
```

```
set xlabel "{/Symbol m} (a.u.)"
set ylabel "Energy (a.u.)"
set format y "%.4f"
set yrange [-76.4115:-76.4095]
set output '/tmp/gnuplot-inline-1587464672.3021863.691199111999.png'
plot data index 0 u 1:5:6 w errorlines title "1 det / cc-pVDZ"
set yrange [-76.4215:-76.4195]
set output '/tmp/gnuplot-inline-1587464672.302258.883689911885.png'
plot data index 1 u 1:5:6 w errorlines title "1 det / cc-pVTZ"
set yrange [-76.4232:-76.4212]
set output '/tmp/gnuplot-inline-1587464672.3023045.89529610025.png'
plot data index 2 u 1:5:6 w errorlines title "1 det / cc-pVQZ"
unset output
```

1.3.2 Multi-determinant

[11]:
```
data = "Jastrows/data_dmc"
set key top right
set xrange [0:7.5]
set xlabel "{/Symbol m} (a.u.)"
set ylabel "Energy (a.u.)"
set format y "%.3f"
set yrange [-76.44:-76.405]
plot data index 0 u 1:7:8 w errorlines title "CIPSI / cc-pVDZ", \
data index 1 u 1:7:8 w errorlines title "CIPSI / cc-pVTZ", \
data index 2 u 1:7:8 w errorlines title "CIPSI / cc-pVQZ"
```



[11]:
```
data = "Jastrows/data_dmc"
set key top right
set xrange [0:7.5]
set xlabel "{/Symbol m} (a.u.)"
set ylabel "Energy (a.u.)"
set format y "%.3f"
set yrange [-76.44:-76.405]
set output '/tmp/gnuplot-inline-1587464684.3126948.332194534957.png'
plot data index 0 u 1:7:8 w errorlines title "CIPSI / cc-pVDZ",  data index 1 u
1:7:8 w errorlines title "CIPSI / cc-pVTZ",  data index 2 u 1:7:8 w errorlines
title "CIPSI / cc-pVQZ"
unset output
```

1.4 Fit μ

$\Psi(r_1, \ldots, r_N)$ is a CI trial wave function:

$$|\Psi\rangle = \sum_{I \in \mathcal{B}} c_I |I\rangle$$

When running a FN-DMC calculation, the fixed-node wave function can be written as

$\Phi(r_1, \ldots, r_N) = \Psi(r_1, \ldots, r_N) \times w(r_1, \ldots, r_N)$, where w is a positive function, such that

$$E = \min_w \frac{\langle w\Psi | H | \Psi \rangle}{\langle w\Psi | \Psi \rangle}$$

We want to find the change in the potential that would model the effect of the FN-DMC. This corresponds to removing some short-range potential:

$$\frac{\langle w\Psi | V_{ee} | w\Psi \rangle}{\langle w\Psi | w\Psi \rangle} = \frac{\langle \Psi | V_{ee} - \delta V_{ee} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

where

$$V_{ee} = \frac{1}{r_{12}}$$

and

$$\delta V_{ee} = \alpha \left(\frac{1}{r_{12}} - \frac{\mathrm{erf}(\mu r_{12})}{r_{12}} \right).$$

$$\frac{\langle w\Psi | V_{ee} | w\Psi \rangle}{\langle w\Psi | w\Psi \rangle} = \frac{\langle \Psi | V_{ee} | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \alpha \frac{\langle \Psi | V_{ee} | \Psi \rangle}{\langle \Psi | \Psi \rangle} + \alpha \frac{\langle \Psi | V_{ee}^{lr} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\frac{\langle \Psi | w^2 V_{ee} | \Psi \rangle}{\langle w\Psi | w\Psi \rangle} = (1 - \alpha) \langle \Psi | V_{ee} | \Psi \rangle + \alpha \langle \Psi | V_{ee}^{lr} | \Psi \rangle$$

$$w^2 = \left[(1 - \alpha) + \alpha \, \mathrm{erf}(\mu \, r_{12}) \right] \langle w\Psi | w\Psi \rangle$$

To find the parameter μ, we minimize

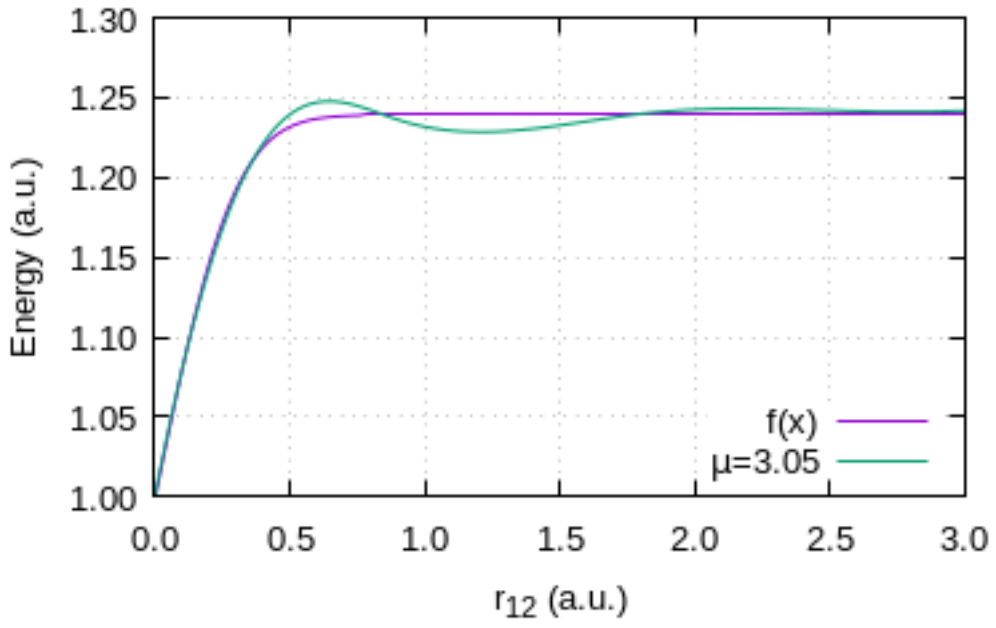
$$\int \left| a \, \mathrm{erf}(\mu \, r_{12}) + b - w(r_{12})^2 \right|^2 \mathrm{d}r_{12}$$

[12]:
```
set yrange [1:1.3]
set xrange [0:3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

f(x) = (a * (erf(mu*x)) +b)
mu = 2.
b=1.
a = 1.
fit f(x) multidet u 1:( ($2+ms)**2 ) via a, b, mu
```

[12]:
```
set yrange [1:1.3]
set xrange [0:3]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

f(x) = (a * (erf(mu*x)) +b)
mu = 2.
b=1.
a = 1.
fit f(x) multidet u 1:( ($2+ms)**2 ) via a, b, mu
Max. number of data points scaled up to: 3072
iter      chisq       delta/lim  lambda   a             b             mu
   0 1.4844650639e+03   0.00e+00  7.96e-01    1.000000e+00   1.000000e+00
2.000000e+00


   1 6.1263778783e-01  -2.42e+08  7.96e-02    2.358053e-01   1.001813e+00
2.187483e+00
   2 1.0286041895e-01  -4.96e+05  7.96e-03    2.362049e-01   1.001768e+00
2.898819e+00
   3 8.8809271871e-02  -1.58e+04  7.96e-04    2.419347e-01   9.971019e-01
3.071483e+00


   4 8.8738434949e-02  -7.98e+01  7.96e-05    2.413214e-01   9.977999e-01
3.052213e+00
   5 8.8736855066e-02  -1.78e+00  7.96e-06    2.414138e-01   9.977008e-01
3.054867e+00
   * 8.8736862980e-02   8.92e-03  7.96e-05    2.414014e-01   9.977142e-01
3.054509e+00


   * 8.8736862980e-02   8.92e-03  7.96e-04    2.414014e-01   9.977142e-01
3.054509e+00
   * 8.8736862980e-02   8.92e-03  7.96e-03    2.414014e-01   9.977142e-01
3.054509e+00
   * 8.8736862977e-02   8.91e-03  7.96e-02    2.414014e-01   9.977142e-01
3.054509e+00
   * 8.8736862692e-02   8.59e-03  7.96e-01    2.414015e-01   9.977141e-01
3.054511e+00


   6 8.8736851827e-02  -3.65e-03  7.96e-02    2.414067e-01   9.977084e-01
3.054660e+00
```

```
iter      chisq       delta/lim  lambda   a             b             mu

After 6 iterations the fit converged.
final sum of squares of residuals : 0.0887369
rel. change during last iteration : -3.65015e-08

degrees of freedom    (FIT_NDF)                        : 2997
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.00544137
variance of residuals (reduced chisquare) = WSSR/ndf   : 2.96086e-05

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
a                 = 0.241407       +/- 0.0006833    (0.283%)
b                 = 0.997708       +/- 0.0006832    (0.06848%)
mu                = 3.05466        +/- 0.01162      (0.3804%)

correlation matrix of the fit parameters:
                a      b      mu
a               1.000
b              -0.987  1.000
mu              0.590 -0.636  1.000
unset output
```

[13]:
```
plot f(x), multidet u 1:( ($2+ms)**2) title "{/Symbol m}=3.05" w l
```



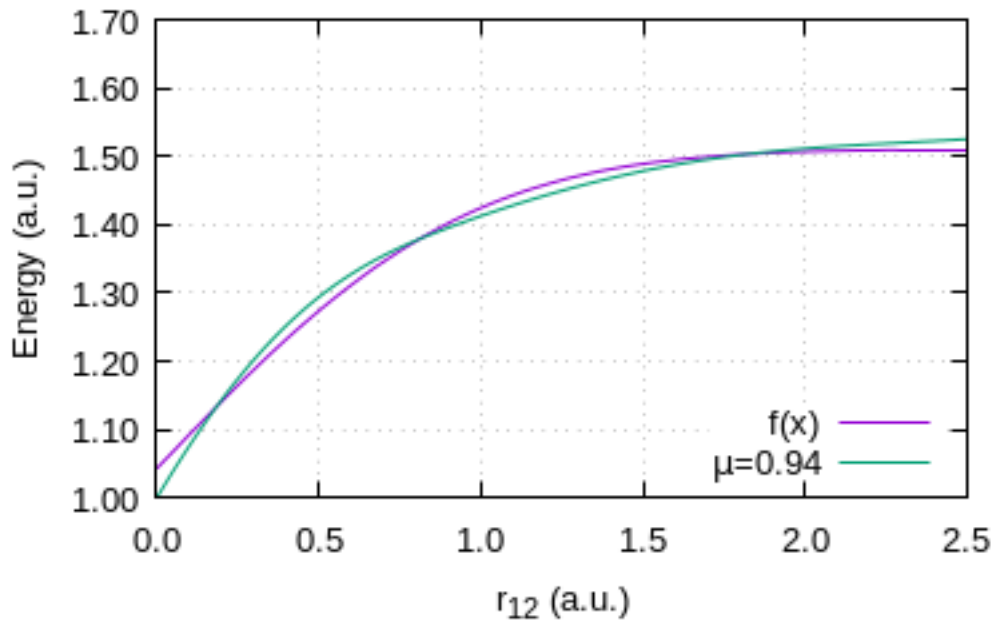
[13]:
```
set output '/tmp/gnuplot-inline-1587464703.6283643.751356038540.png'
plot f(x), multidet u 1:( ($2+ms)**2) title "{/Symbol m}=3.05" w l
```

[14]:
```
set yrange [1:1.7]
set xrange [0:2.5]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

f(x) = (a * (erf(mu*x)) +b)
mu = 2.
b=1.
a = 1.
fit f(x) onedet   u 1:( ($2+os)**2) via a, b, mu
```

[14]:
```
unset output
 set yrange [1:1.7]
set xrange [0:2.5]
set grid
set xlabel "r_{12} (a.u.)"
set format y "%.2f"
set format x "%.1f"
set key bottom right

f(x) = (a * (erf(mu*x)) +b)
mu = 2.
b=1.
a = 1.
fit f(x) onedet   u 1:( ($2+os)**2) via a, b, mu
Max. number of data points scaled up to: 3072
iter      chisq       delta/lim  lambda   a             b             mu
   0 6.3210450983e+02   0.00e+00  7.92e-01    1.000000e+00   1.000000e+00
2.000000e+00


   1 3.7399726680e+00  -1.68e+07  7.92e-02    4.372151e-01   1.042051e+00
1.438663e+00
   2 1.0886112747e+00  -2.44e+05  7.92e-03    4.564069e-01   1.038516e+00
9.132499e-01
   3 4.1264008258e-01  -1.64e+05  7.92e-04    4.670442e-01   1.043923e+00
9.352905e-01
```

```
   4 4.1237511508e-01  -6.43e+01  7.92e-05    4.674657e-01   1.043147e+00
9.390785e-01
   5 4.1236761417e-01  -1.82e+00  7.92e-06    4.675227e-01   1.043020e+00
9.397870e-01
   * 4.1236765338e-01   9.51e-03  7.92e-05    4.675328e-01   1.042997e+00
9.399192e-01


   * 4.1236765338e-01   9.51e-03  7.92e-04    4.675328e-01   1.042997e+00
9.399192e-01
   * 4.1236765338e-01   9.51e-03  7.92e-03    4.675328e-01   1.042997e+00
9.399192e-01


   * 4.1236765338e-01   9.51e-03  7.92e-02    4.675328e-01   1.042997e+00
9.399192e-01
   * 4.1236765335e-01   9.50e-03  7.92e-01    4.675328e-01   1.042997e+00
9.399192e-01
   * 4.1236765043e-01   8.79e-03  7.92e+00    4.675326e-01   1.042997e+00
9.399178e-01
   6 4.1236757813e-01  -8.74e-03  7.92e-01    4.675248e-01   1.043011e+00
9.398501e-01
iter      chisq       delta/lim  lambda   a             b             mu

After 6 iterations the fit converged.
final sum of squares of residuals : 0.412368
rel. change during last iteration : -8.74041e-08

degrees of freedom    (FIT_NDF)                        : 2497
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.0128509
variance of residuals (reduced chisquare) = WSSR/ndf   : 0.000165145

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
a               = 0.467525         +/- 0.0009255    (0.198%)
b               = 1.04301          +/- 0.0009232    (0.08851%)
mu              = 0.93985          +/- 0.003224     (0.3431%)

correlation matrix of the fit parameters:
                a      b      mu
a               1.000
b              -0.873  1.000
mu              0.269 -0.620  1.000
unset output
```

[15]:
```
plot f(x), onedet   u 1:( ($2+os)**2 ) title "{/Symbol m}=0.94" w l
```



[15]:
```
set output '/tmp/gnuplot-inline-1587464715.1665385.128003803699.png'
plot f(x), onedet   u 1:( ($2+os)**2 ) title "{/Symbol m}=0.94" w l
unset output
```

[ ]: