Monte-Carlo Methods in Optical Model Analysis of Antiprotonic Atoms

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OUTLINE

- Why Monte Carlo methods? the case of kaonic atoms
- Resonance near threshold and the need for additional input beyond single-nucleon amplitudes
- A short guide to MC methods and some results
- Aniprotonic atoms: similarities and differences
- Paris 2009 amplitudes: earlier results
- Paris 2009 amplitudes: MC results
- Summary and outlook

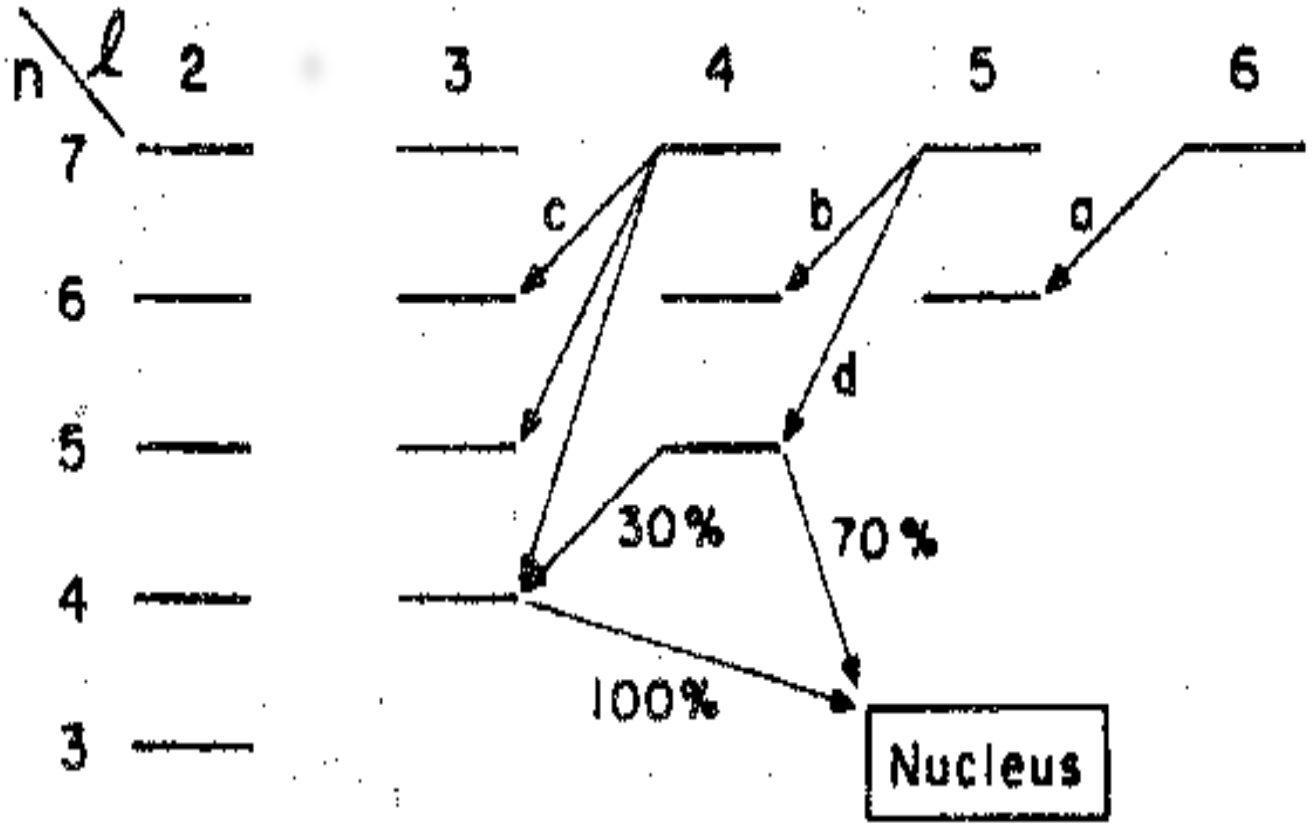
Introduction and background

Close to 300 observables of strong-interaction effects in pionic, kaonic and antiprotonic atoms enabled extensive analyses in terms of hadron-nucleus optical potentials.

Phenomenological potentials have been gradually replaced by more theoretically-based approaches.

In the last decade potentials built on hadron-nucleon scattering amplitudes showed a need for additional input and revealed possible difficulties with conventional analyses.

Schematics of exotic-atom energy levels



Following NPA231 (1974) 477

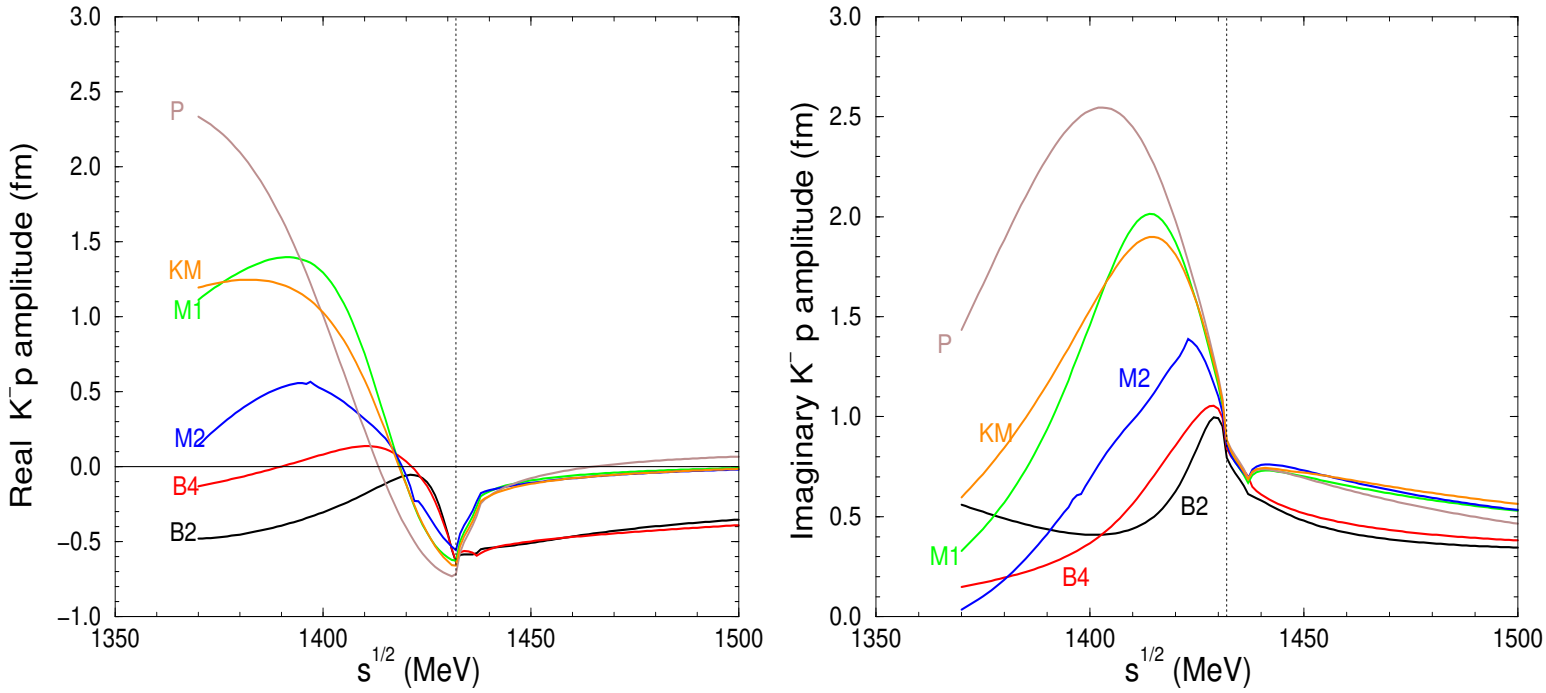
Kaonic atoms experiments

- Results from CERN, Argonne, Rutherford Lab., BNL
- Use weighted averages
- Good accuracies for shifts and widths
- Reasonable accuracies for yields (= upper level widths)

Measured strong interaction level shifts and width, measured relative yields of upper to lower level transitions.

Phenomenological optical potentials produced fits to experiments with χ^2 of 130 for 65 data points, with 3 adjustable parameters.

Six chiral $K^- N$ models constrained by fits to near-threshold data, including the SIDDHARTA result for K^-H at threshold



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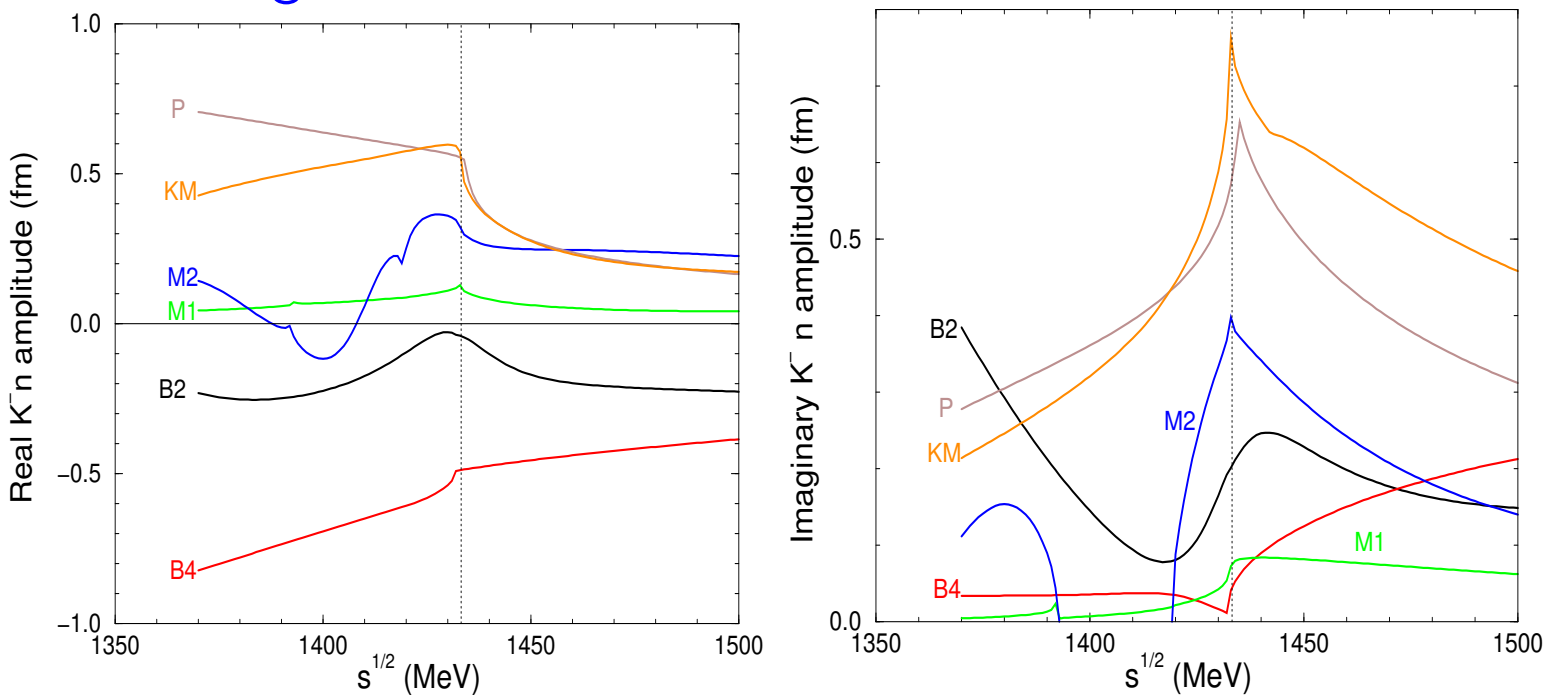


Reminder of 'in-medium kinematics'

Adopt the Mandelstam variable $s = (E_{K^-} + E_N)^2 - (\vec{p}_{K^-} + \vec{p}_N)^2$ as the argument transforming free-space to in-medium $K^- N$ amplitudes.

In the hadronic atom c.m. frame the average of $(\vec{p}_{K^-} + \vec{p}_N)^2$ is

the average of $\vec{p}_N^{\,2} + \frac{A-2}{A}\vec{p}_{K^-}^{\,2}$, with A the atomic mass.

Both the energies and the momenta cause $\sqrt{s}$ to be below $M_N + m_K$.

Reminder of 'in-medium kinematics'

Adopt the Mandelstam variable $s = (E_{K^-} + E_N)^2 - (\vec{p}_{K^-} + \vec{p}_N)^2$ as the argument transforming free-space to in-medium $K^- N$ amplitudes.
$\delta\sqrt{s} = \sqrt{s} - E_{\rm th}$, $E_{\rm th} = m_{K^-} + m_N$, then to first order in $B/E_{\rm th}$ one gets

$$\delta\sqrt{s} = -B_N \rho/\bar{\rho} - \beta_N [T_N (\rho/\bar{\rho})^{2/3} + B_{K^-} \rho/\rho_0] + \beta_{K^-} [{\rm Re}\ V_{K^-} + V_c (\rho/\rho_0)^{1/3}],$$

$\beta_N = m_N/(m_N + m_{K^-})$, $\beta_{K^-} = m_{K^-}/(m_N + m_{K^-})$, $\rho_0 = 0.17$ fm^{-3}.
Average binding energy $B_N = 8.5$ MeV, T_N=23 MeV (Fermi gas model).
The specific ρ/ρ_0 and $\rho/\bar{\rho}$ forms ensure that $\delta\sqrt{s} \to 0$ when $\rho \to 0$

Solving by iterations, $\sqrt{s}$ and hence amplitudes become functions of ρ, essentially *averaging over subthreshold energies.*

Accepting 'Minimal Substitution' (MS), $V_c(r)$ is subtracted from $\delta\sqrt{s}$, (as supported by analyses of pion-nucleus experiments).

For attractive potentials the energy $\sqrt{s}$ is below threshold within the nuclear medium.

In addition there are corrections due to Pauli correlations.

The algorithm performs averaging over subthreshold energies.

PLB 702 (2011) 402; PRC 84 (2011) 045206; NPA 899 (2013) 60; EPJ Web of Conferences 81 (2014) 01018; NPA 959 (2017) 66; (partial list).

The Pauli-corrected single-nucleon potential is,
T. Waas, M. Rho, W. Weise, NPA 617 (1997) 449 (WRW)

$$2\mu_K V_{K^-}^{(1)}(\rho) = -4\pi \left[\frac{(2\tilde{f}_{K^-p} - \tilde{f}_{K^-n})\,\frac{1}{2}\rho_p}{1 + \frac{1}{4}\xi_k(\rho)\tilde{f}_0\rho(r)} + \frac{\tilde{f}_{K^-n}(\frac{1}{2}\rho_p + \rho_n)}{1 + \frac{1}{4}\xi_k(\rho)\tilde{f}_1\rho(r)} \right],$$

$\tilde{f}_{K^-N}(\rho)$ are related kinematically to the in-medium K^-N c.m. amplitudes $f_{K^-N}(\rho)$ by $\tilde{f}_{K^-N}(\rho) = (1 + \frac{A-1}{A}\frac{\mu_K}{m_N})f_{K^-N}(\rho)$. The Pauli correlation factor $\xi_k(\rho)$ is defined by

$$\xi_k(\rho) = \frac{9\pi}{k_F^2}\left(4\int_0^\infty \frac{dr}{r}\,\exp(\mathrm{i}kr)\,j_1^2(k_F r)\right),$$

with $k = [(E_{K^-} - i\Gamma/2)^2 - m_k^2]^{1/2}$ and where Γ is the width of the particular kaonic atom state. $k_F = (3\pi^2\rho/2)^{1/3}$.
With $q = -ik/k_F$ the above integral (x4) is

$$4I_k(\rho) = 1 - \frac{q^2}{6} + \frac{q^2}{4}(2 + \frac{q^2}{6})\,\ln(1 + \frac{4}{q^2}) - \frac{4}{3}q\,(\frac{\pi}{2} - \mathrm{arctg}(q/2)),$$

χ^2 for 65 kaonic atoms data points from optical potentials based only on single-nucleon amplitudes.

model	B2	B4	M1	M2	P	KM
$\chi^2(65)$	1174	2358	2544	3548	2300	1806

χ^2 for 18 high quality data points (P, S, Cl, Cu, Ag, Pb)

model	B2	B4	M1	M2	P	KM
$\chi^2(18)$	364	733	949	1232	480	449

Not fits!

Good fits to the data are obtained by adding to the combined single-nucleon amplitudes an empirical amplitude $B_0(\rho/\rho_0)^\alpha$ and varying the 3 parameters ReB_0, ImB_0 and α.
For example, based on the KM amplitudes,
$\chi^2(65)$=119.4,
Re$B_0 = -0.60 \pm 1.96$ fm,
Im$B_0 = 2.39 \pm 4.34$ fm,
$\alpha = 1.46 \pm 1.85$.

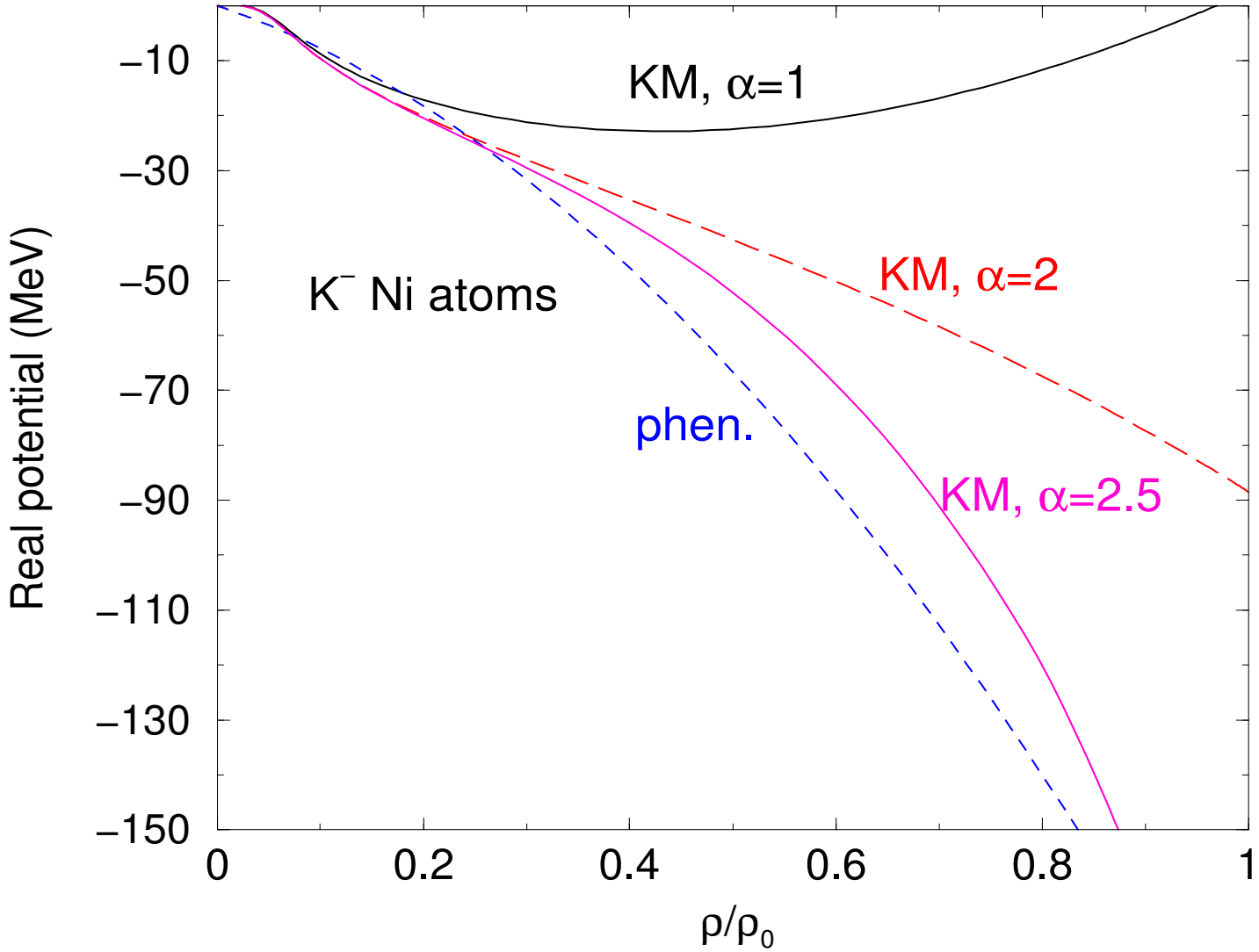
????

Fits to 65 kaonic atoms data points when single-nucleon amplitudes are supplemented by a $B_0(\rho/\rho_0)^\alpha$ amplitude with fixed α compatible with its best-fit value. B in units of fm.

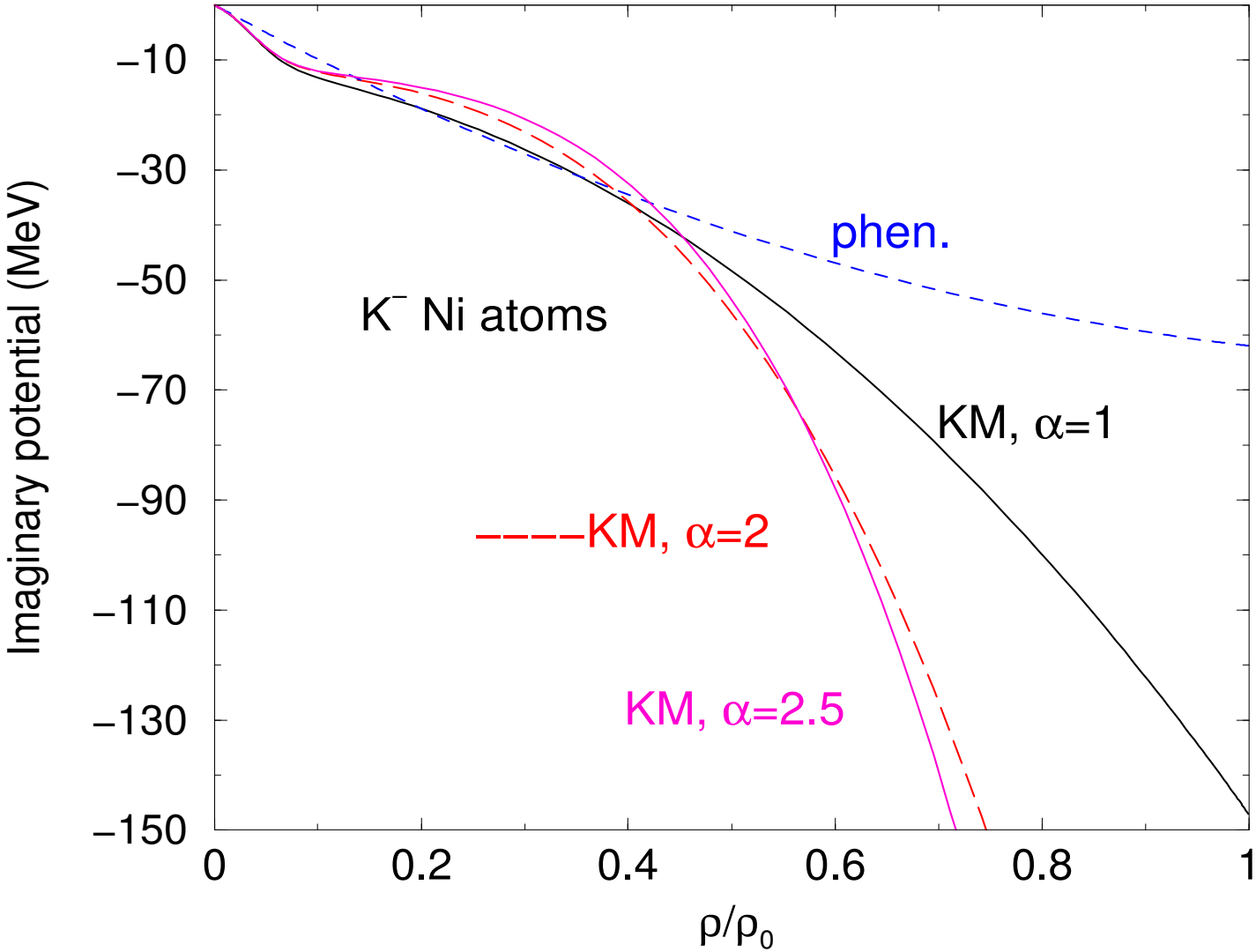
model	B2	B4	M1	M2	P	KM
α	0.3	0.3	0.3	1.0	1.0	1.0
ReB_0	2.4±0.2	3.1±0.1	0.3±0.1	2.1±0.2	−1.3±0.2	−0.9±0.2
ImB_0	0.8±0.1	0.8±0.1	0.8±0.1	1.2±0.2	1.5±0.2	1.4±0.2
$\chi^2(65)$	111	105	121	109	125	123

Is it necessary to go subthreshold?
Example for KM, when $\delta\sqrt{s}$=0:
$\alpha = 1.0$, Re$B_0 = -1.8 \pm 0.1$, Im$B_0 = -1.1 \pm 0.1$, $\chi^2(65)$ =139

Negative ImB_0 and/or significantly larger χ^2 obtained for all six models when taken on threshold.
Similar problems when ignoring Pauli correlations.



Arbitrary model-dependence above 25% of central density



Arbitrary model-dependence above 50% of central density.
Well-defined below 50% of central density.

Reducing uncertainties of optical potentials

The phenomenological multinucleon amplitude $B_0(\rho/\rho_0)^\alpha$ is a source of uncertainties due to correlations between the exponent α and B_0. χ^2 searches on three parameters lead to meaningless results. So far we had to grid on α and fit only two parameters, ReB_0 and ImB_0.

A way out is by replacing the error-matrix approach by Monte-Carlo techniques.

In the Monte-Carlo method we assume many repetitions, $\mathrm{i} = 1, ...\mathrm{N}$ of ALL the experiments, where every individual result (shift, width, or yield, $\mathrm{k} = 1, ...65$) is moved randomly assuming Gaussian distribution. A random Gaussian shift $f_{\mathrm{k}}^{\mathrm{i}}$ in units of standard deviation multiply each "experimental" (1σ) error, to provide a 'new result', with its old original uncertainty:

$$expr(\mathrm{k}) \pm \Delta(\mathrm{k}) \rightarrow [expr(\mathrm{k}) + f_{\mathrm{k}}^{\mathrm{i}}\Delta(\mathrm{k})] \pm \Delta(\mathrm{k})$$

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$$expr(\mathrm{k}) \pm \Delta(\mathrm{k}) \rightarrow [expr(\mathrm{k}) + f_{\mathrm{k}}^{\mathrm{i}}\Delta(\mathrm{k})] \pm \Delta(\mathrm{k})$$

Then new χ^2 fits are made, varying all three parameters that again lead to meaningless results.

Repeating the process typically 200 to 500 times produces distributions of α, ReB_0 and ImB_0 with amazingly well-defined average values and small uncertainties.

For a Gaussian $\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$ and for two [0,1] random numbers z_1 and z_2 we get a random

$$\frac{x-\mu}{\sigma} = f = \sqrt{-2logz_1}cos(2\pi z_2).$$

For N repetitions of χ^2 fits we get parameters α_i, β_i etc.

Numerically,

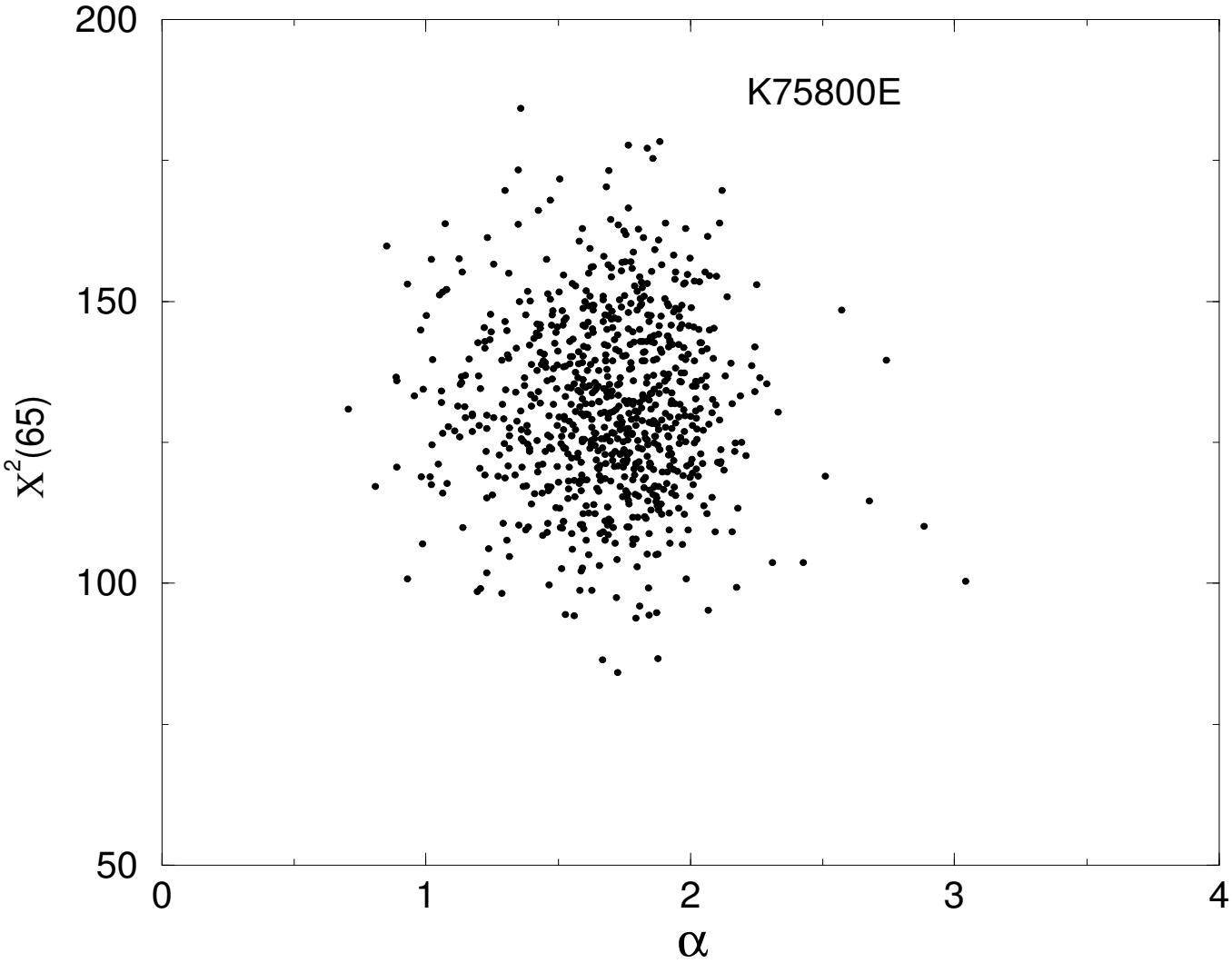
$\sigma_\alpha^2 = \frac{N}{N-1}\Sigma_i(\alpha_i - \bar{\alpha})^2, \qquad \bar{\alpha} = \frac{1}{N}\Sigma_i(\alpha_i),$

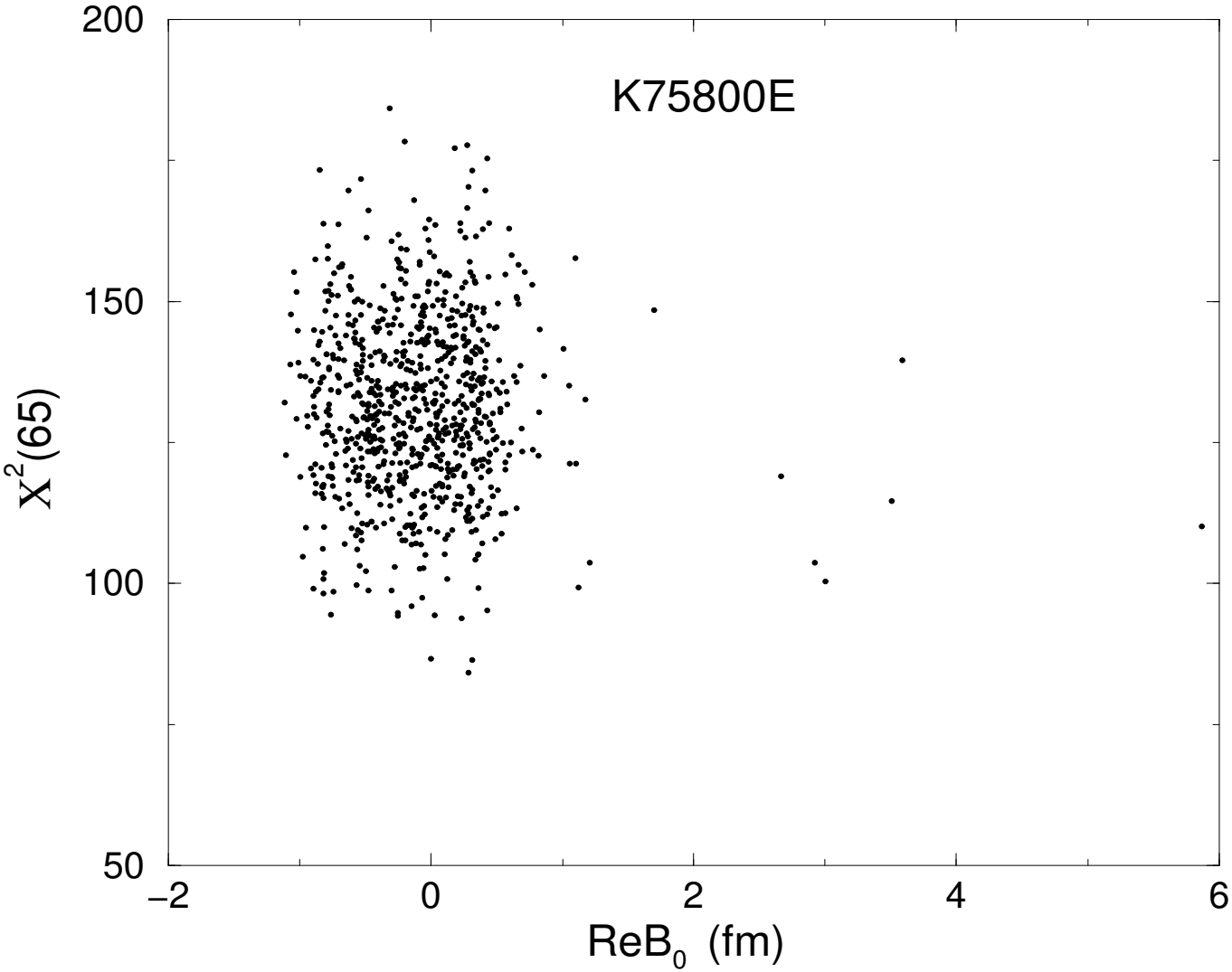
$\sigma_{\alpha\beta} = \frac{1}{N}\Sigma_i(\alpha_i - \bar{\alpha})(\beta_i - \bar{\beta})$

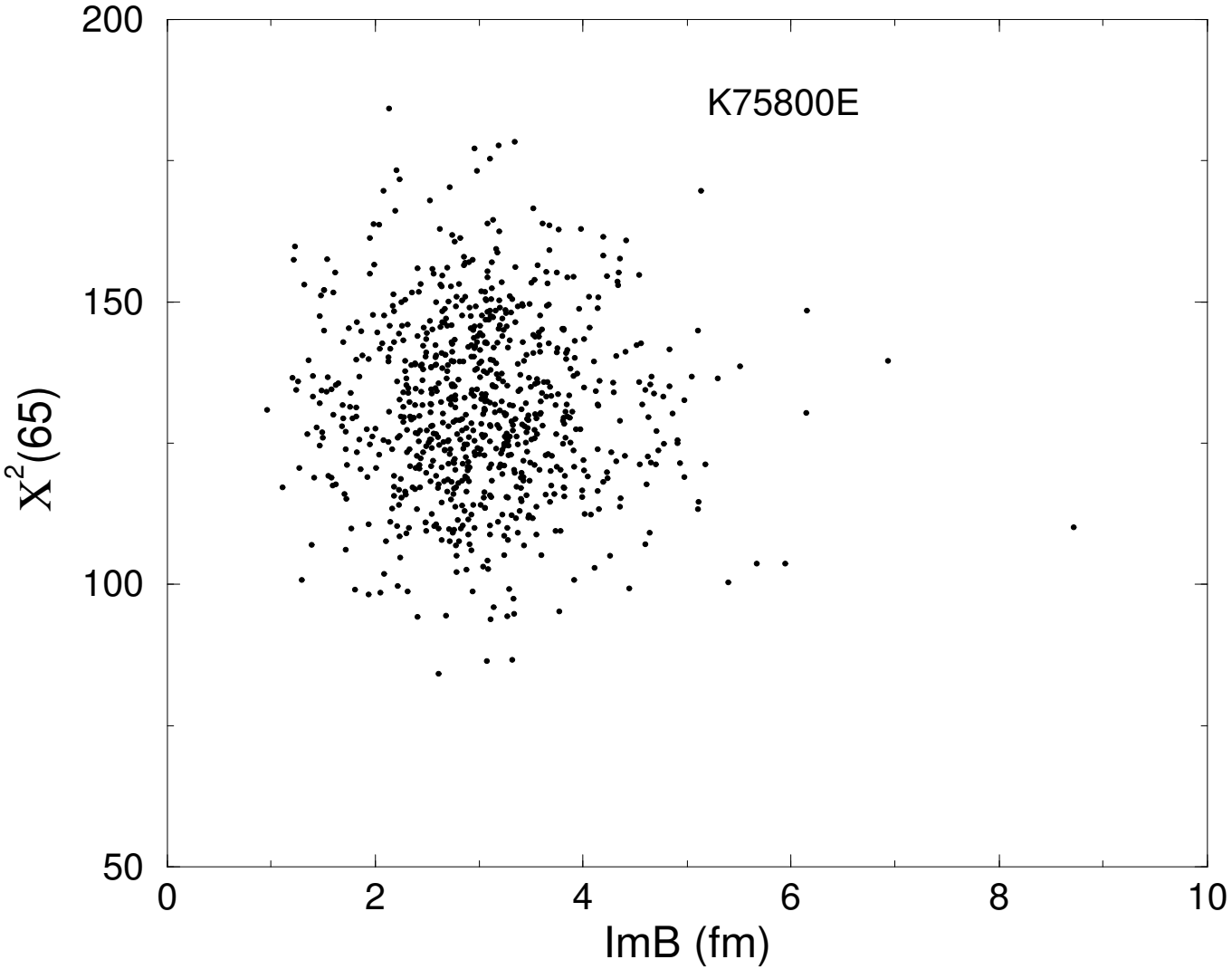
and correlations

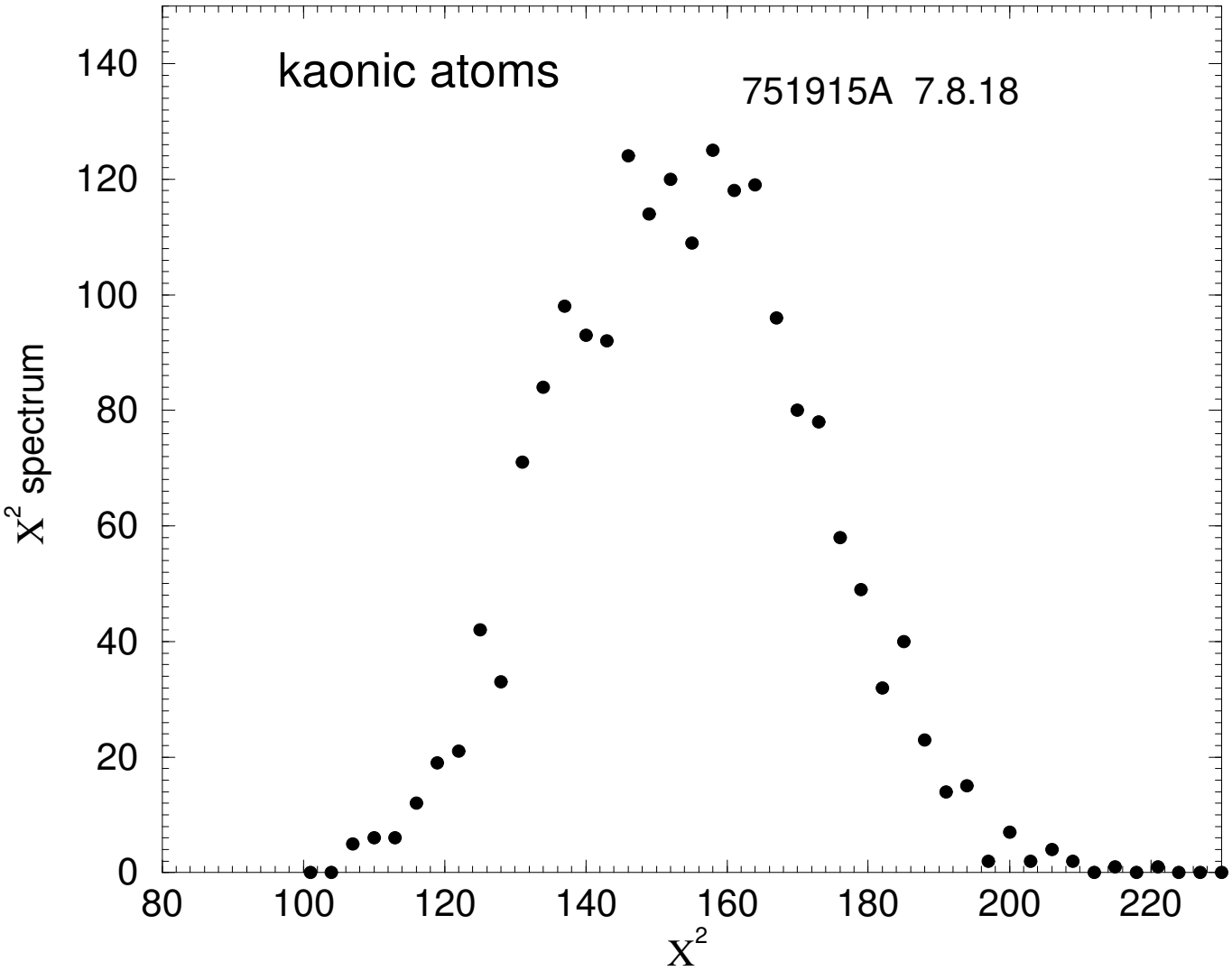
$C_{\alpha\beta} = \frac{\sigma_{\alpha\beta}}{\sigma_\alpha\sigma_\beta}.$

In principle similar results are available from regular χ^2 minimisation.


K75800E
200
150
100
50
0
1
2
3
4
$X^2(65)$
α


K75800E
200
150
100
50
–2
0
2
4
6
X²(65)
ReB₀ (fm)


K75800E
200
150
100
50
0
2
4
6
8
10
X²(65)
ImB (fm)

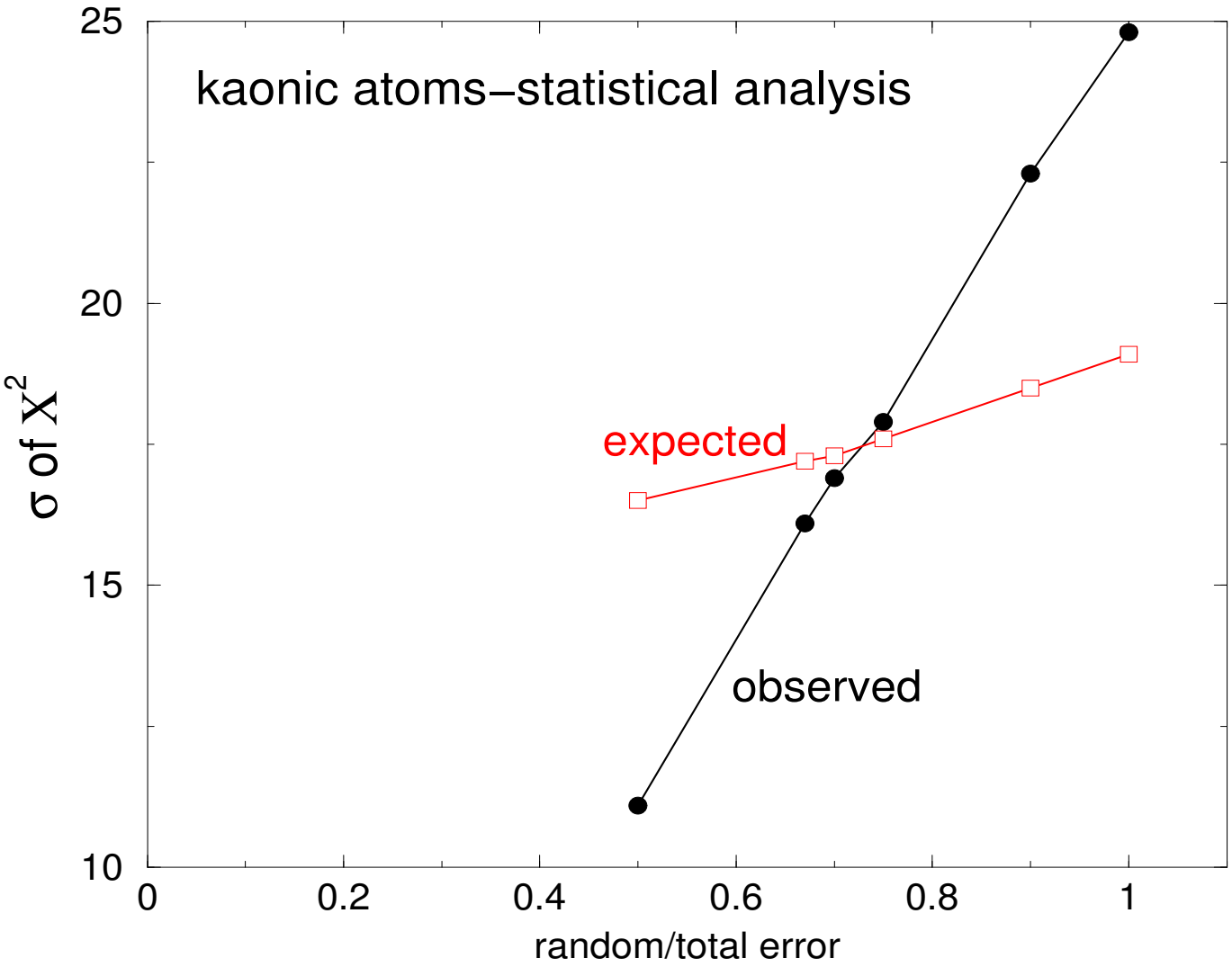


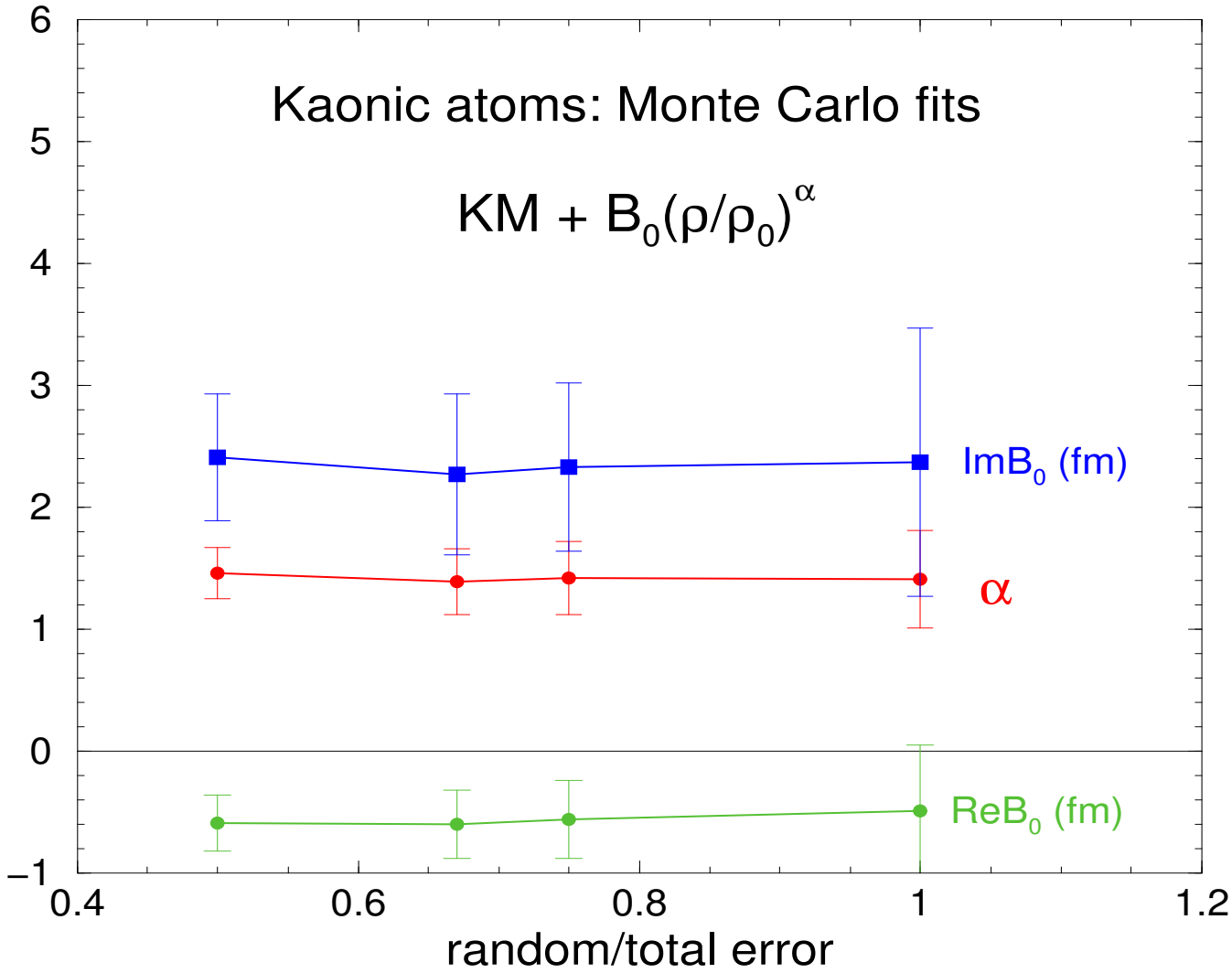
Passing the 'upper and lower 16% test' for a Gaussian.

With 65-3=62 degrees of freedom we can test whether the hundreds of χ^2 values follow the expected relation of

$$var(\chi^2) = 2(\chi^2)_{ave}.$$

From some of the experimental papers we note that the quoted errors contain, in several examples, non-statistical contributions of up to 30%. Therefore we check the effects of limiting the above f factor to a fraction of the quoted experimental error.


kaonic atoms–statistical analysis
expected
observed
σ of X^2
random/total error
25
20
15
10
0
0.2
0.4
0.6
0.8
1


Kaonic atoms: Monte Carlo fits
KM + $B_0(\rho/\rho_0)^\alpha$
ImB_0 (fm)
α
ReB_0 (fm)
6
5
4
3
2
1
0
−1
0.4
0.6
0.8
1
1.2
random/total error

Good fits to the data are obtained by adding to the combined single-nucleon amplitudes an empirical amplitude $B_0(\rho/\rho_0)^\alpha$ and varying the 3 parameters ReB_0, ImB_0 and α.
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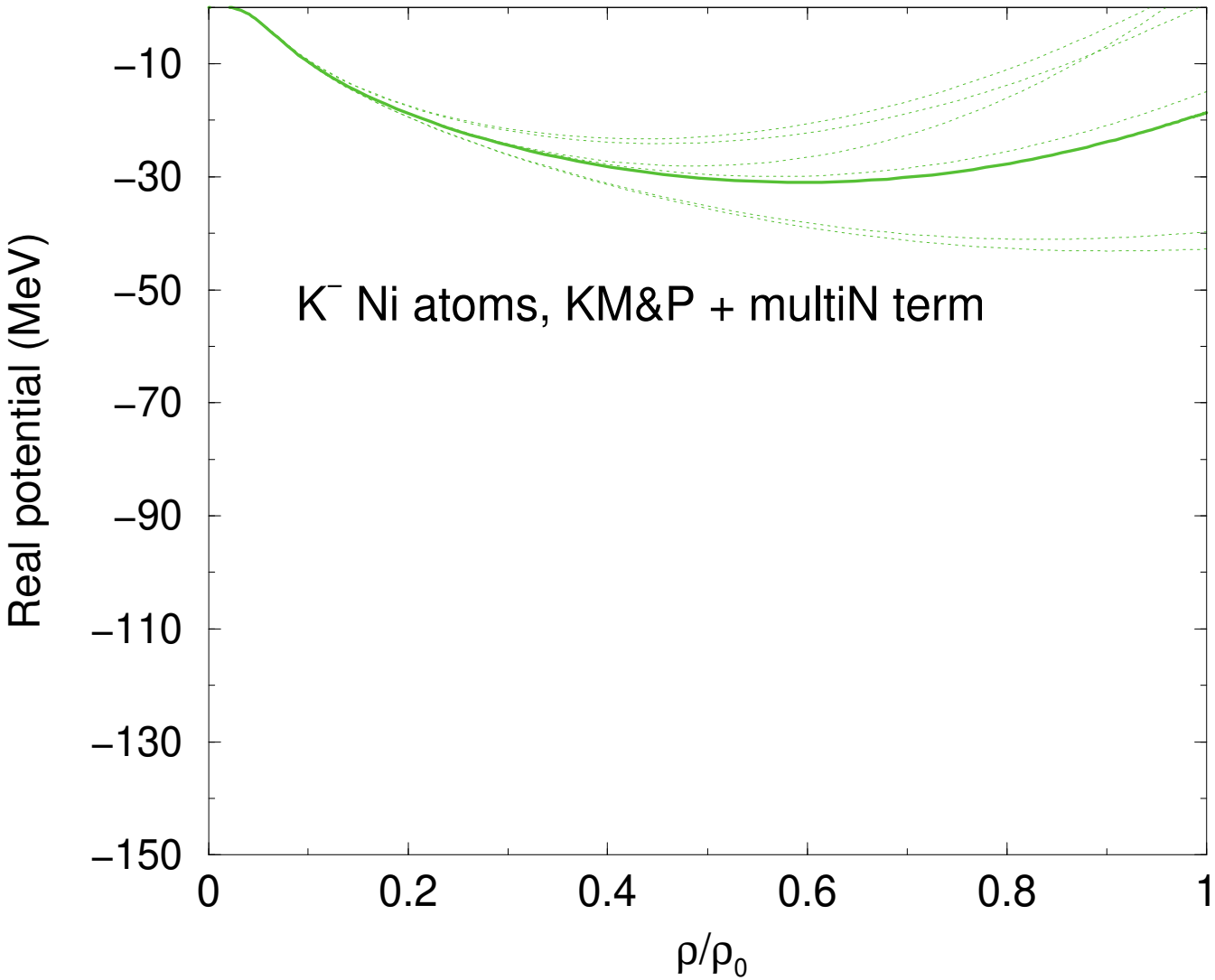
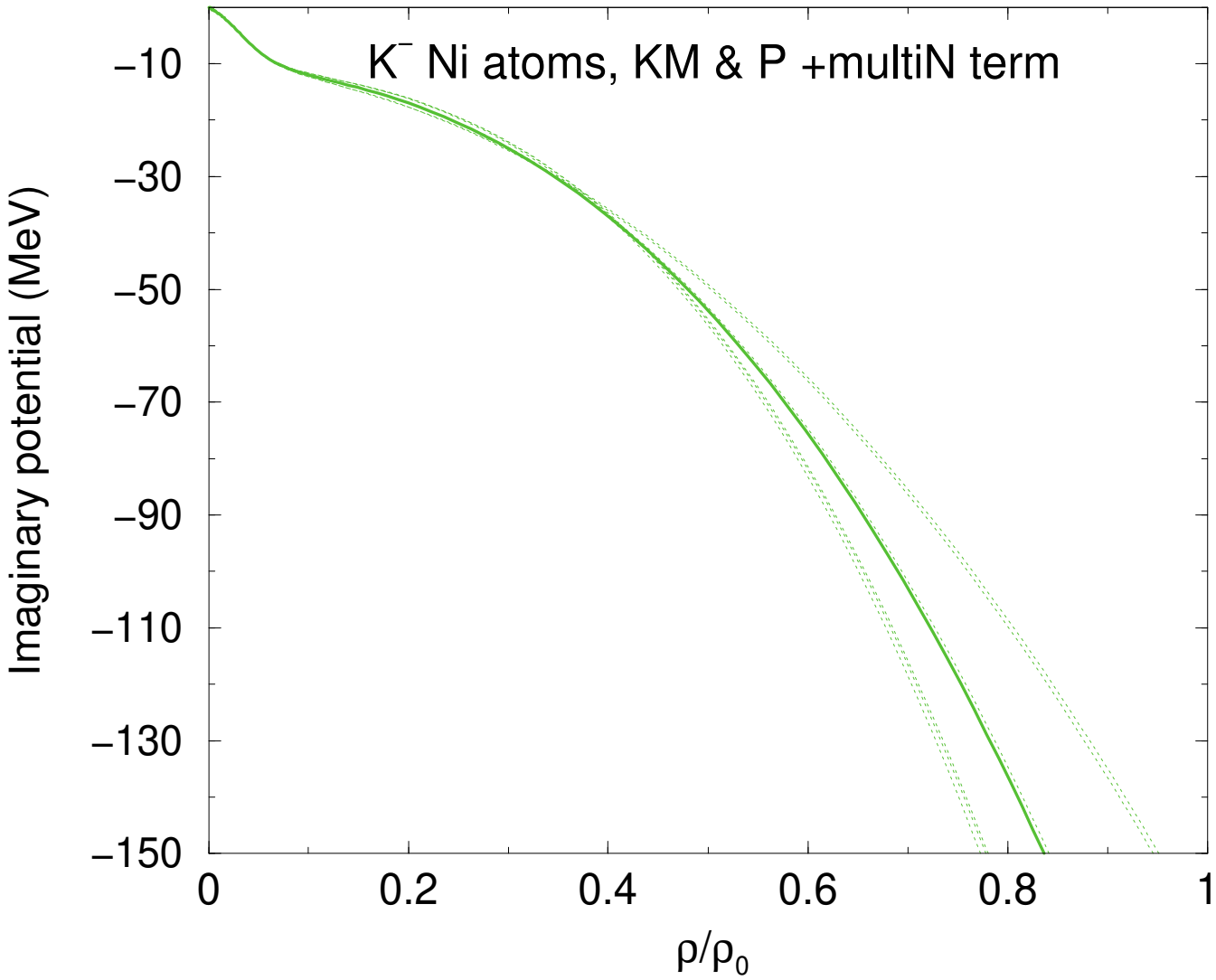
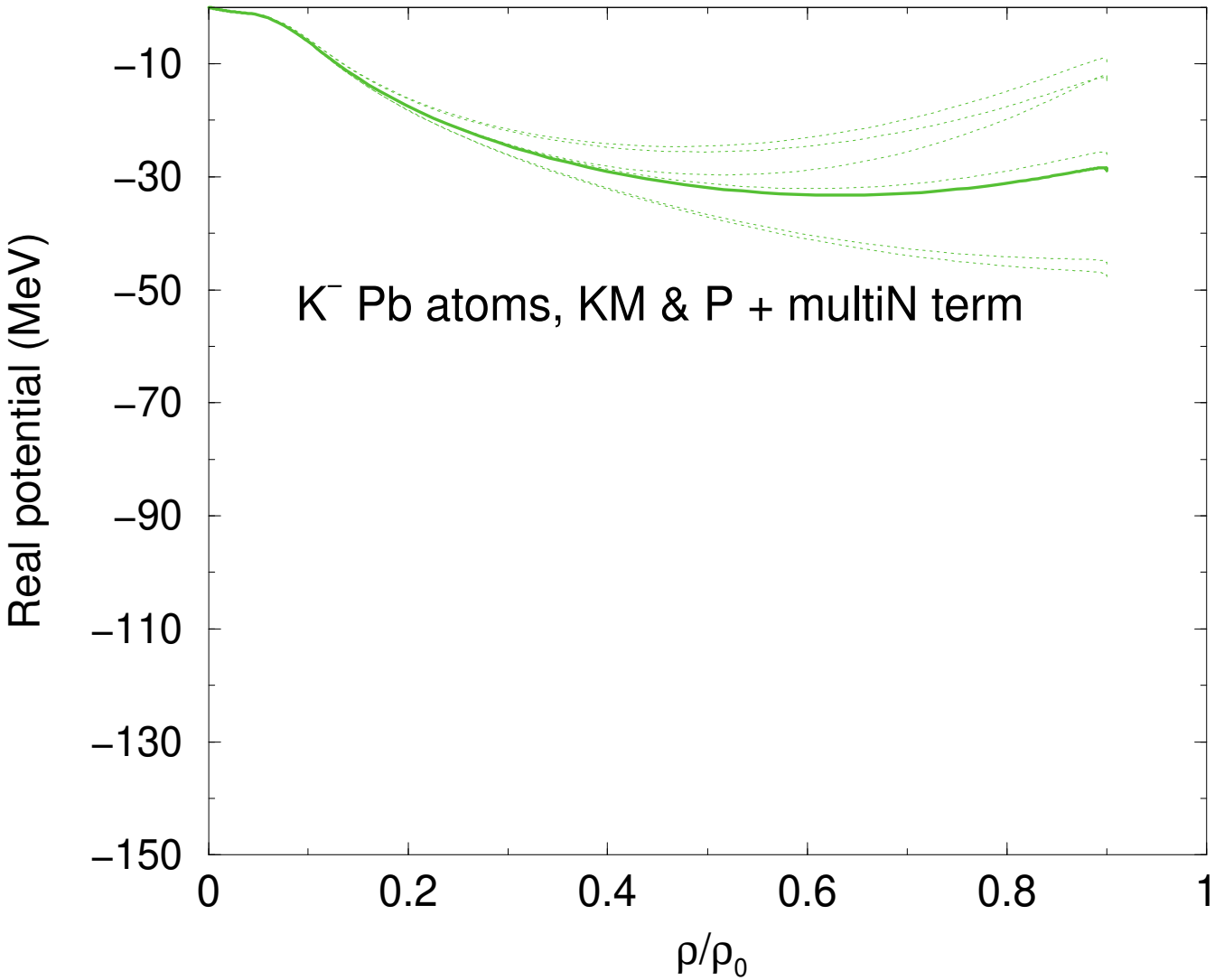
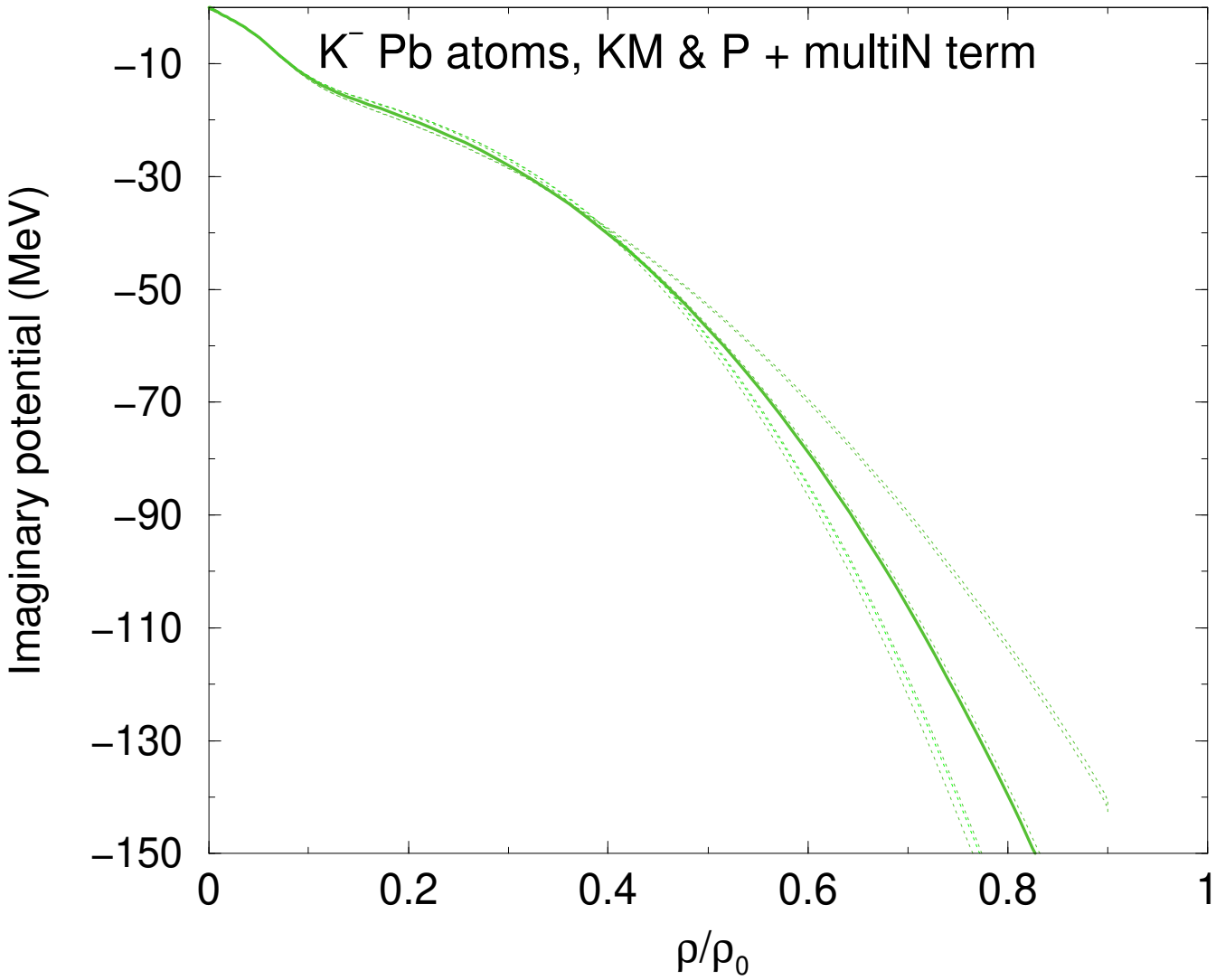
Im$B_0 = 2.39 \pm 4.34$ fm,
$\alpha = 1.46 \pm 1.85$.
From the Monte-Carlo technique we get
$\chi^2(65)$=119.4, (this is NOT χ^2_{ave})
Re$B_0 = -0.55 \pm 0.33$ fm,
Im$B_0 = 2.39 \pm 0.72$ fm,
$\alpha = 1.44 \pm 0.31$.

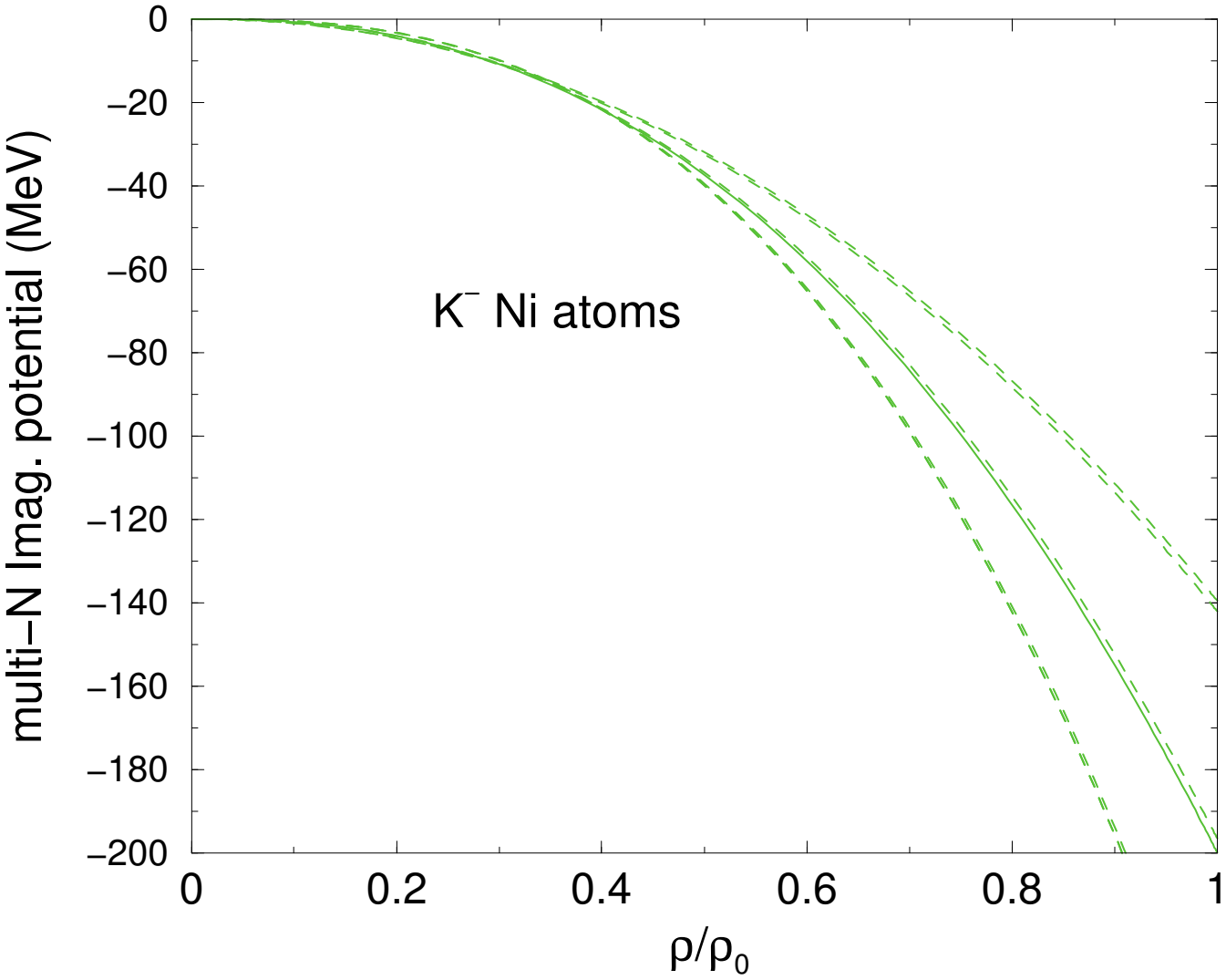
Now it makes sense to look at the potentials.


Real potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0
K⁻ Ni atoms, KM&P + multiN term


K⁻ Ni atoms, KM & P +multiN term
Imaginary potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0

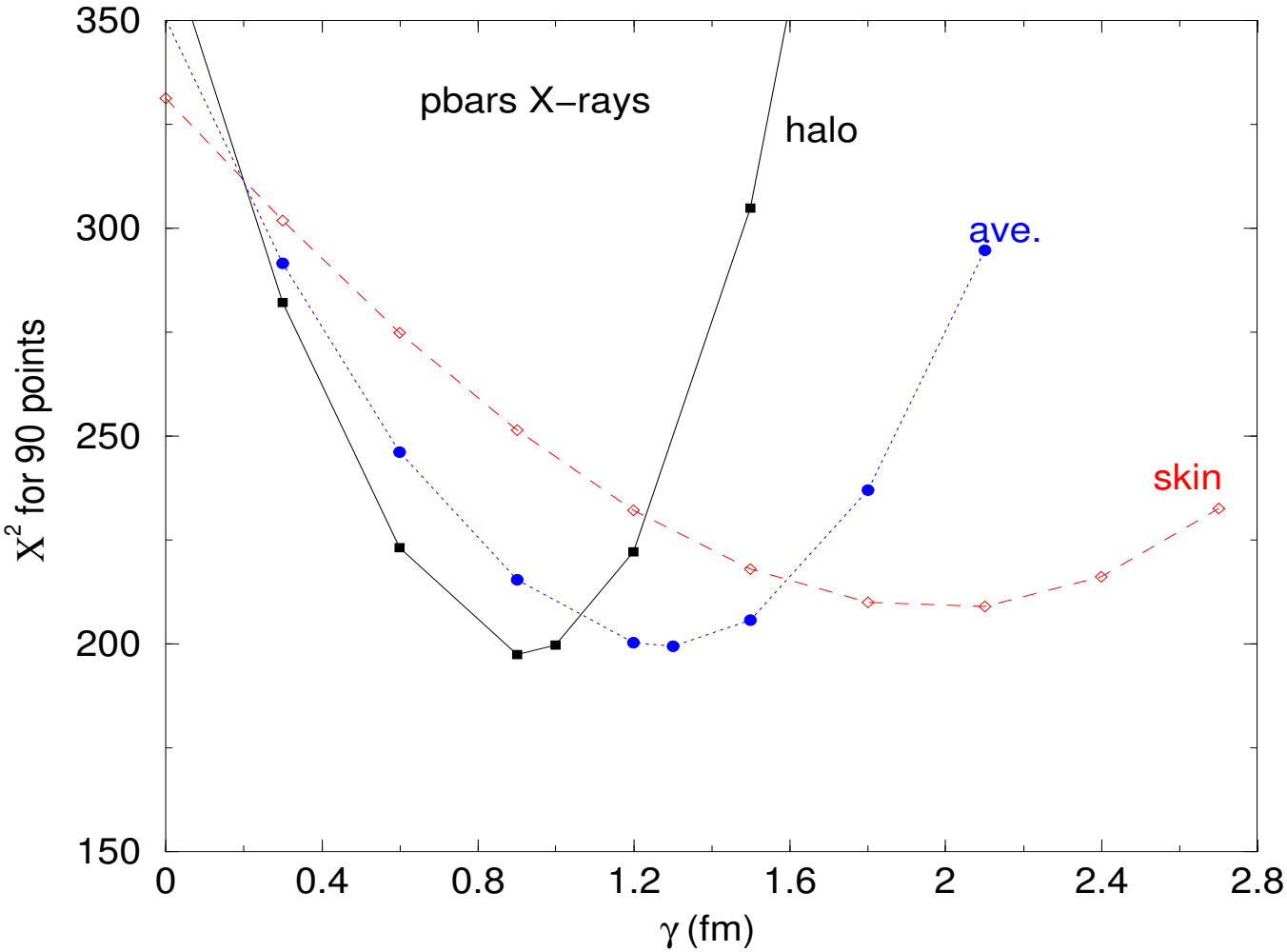

Real potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0
K⁻ Pb atoms, KM & P + multiN term


K⁻ Pb atoms, KM & P + multiN term
Imaginary potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0

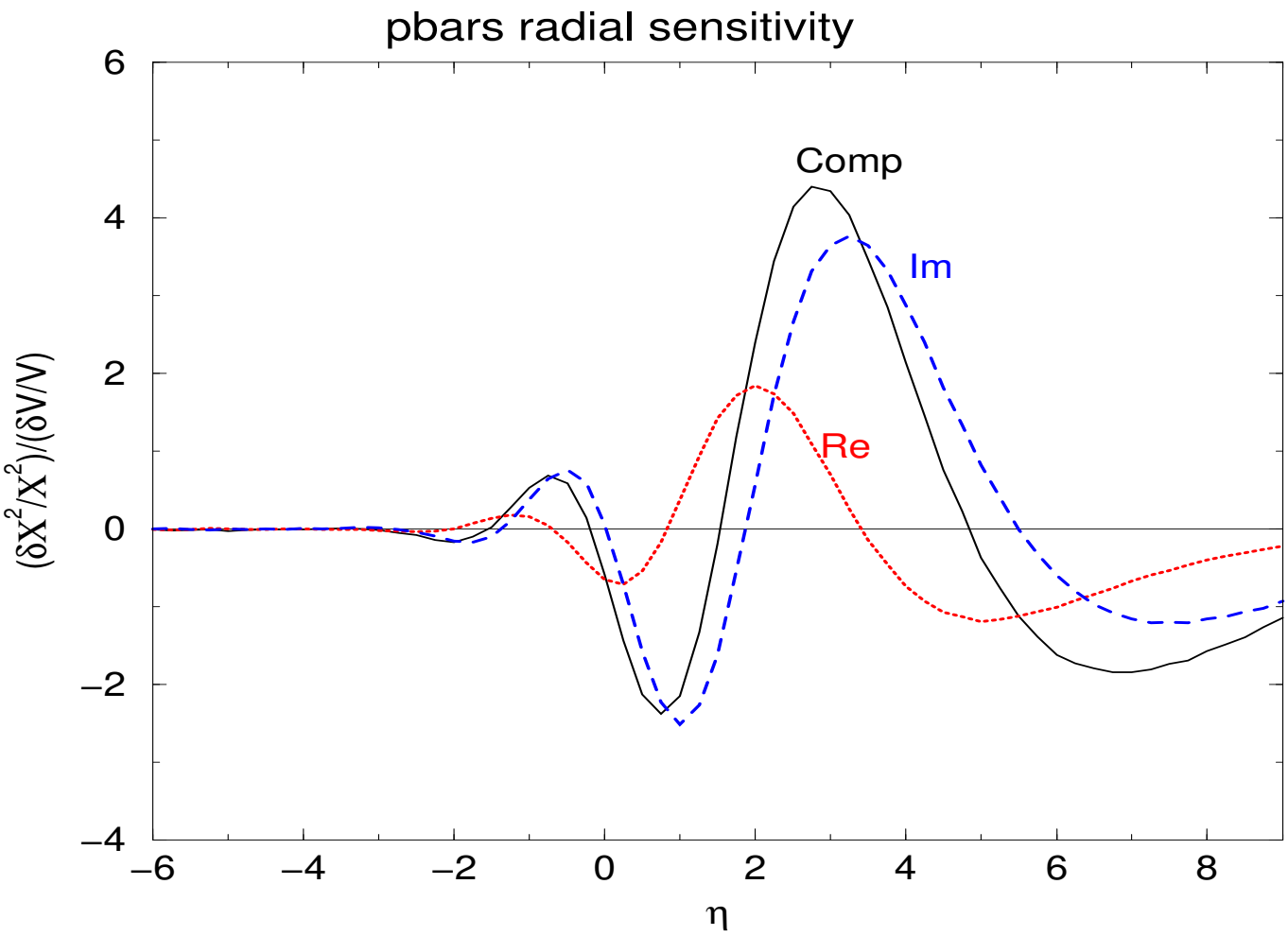

multi–N Imag. potential (MeV)
0
–20
–40
–60
–80
–100
–120
–140
–160
–180
–200
K⁻ Ni atoms
0
0.2
0.4
0.6
0.8
1
ρ/ρ0

Antiprotonic Atoms

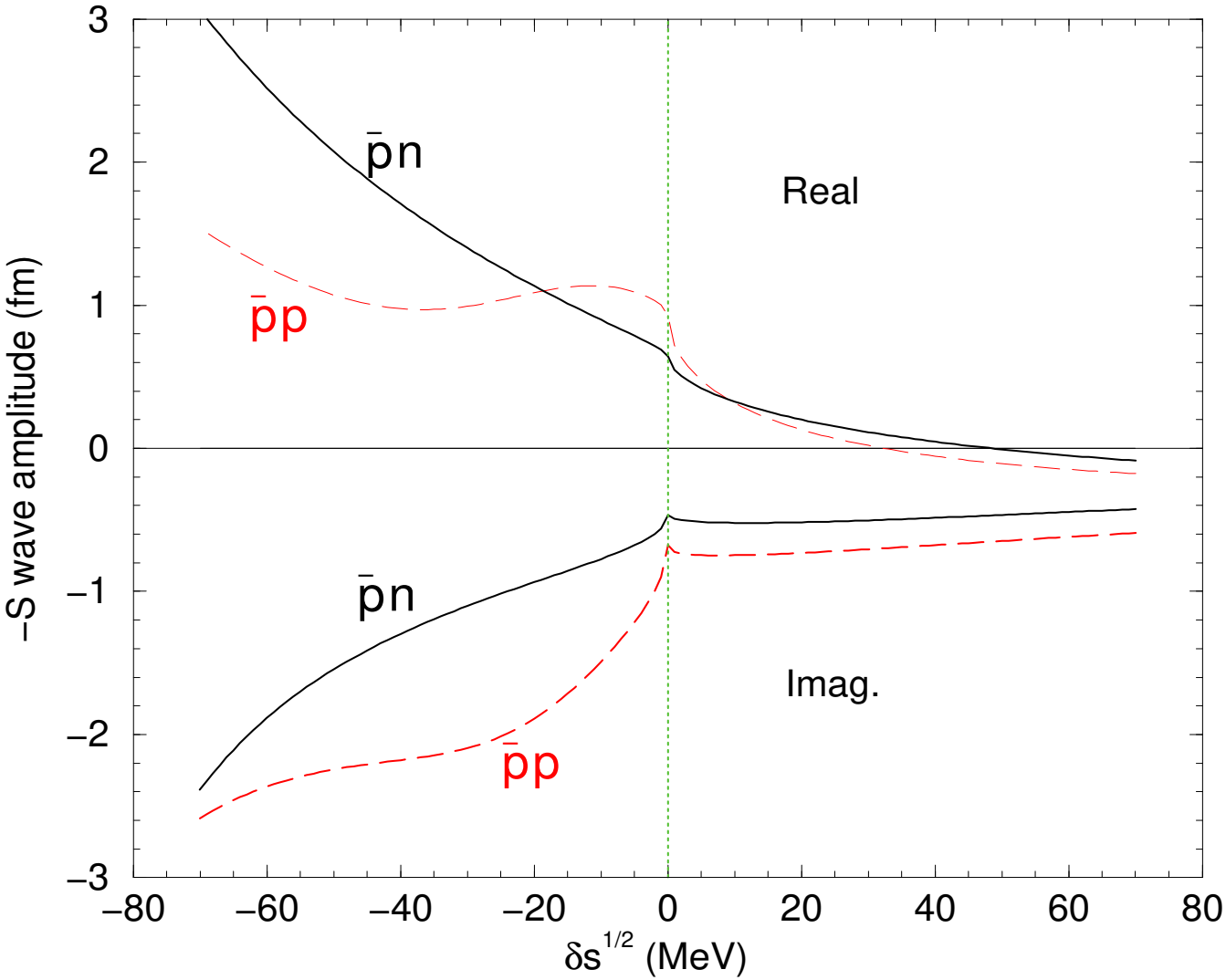
- Good experimental results throughout the Periodic Table. (PS209)
- Stronger absorption than in Kaonic atoms.
- For purely phenomenological potential χ^2=200 for 90 points, with 3 fit parameters.
- *s*-and *p*-wave amplitudes available across threshold, e.g. Paris 2009.



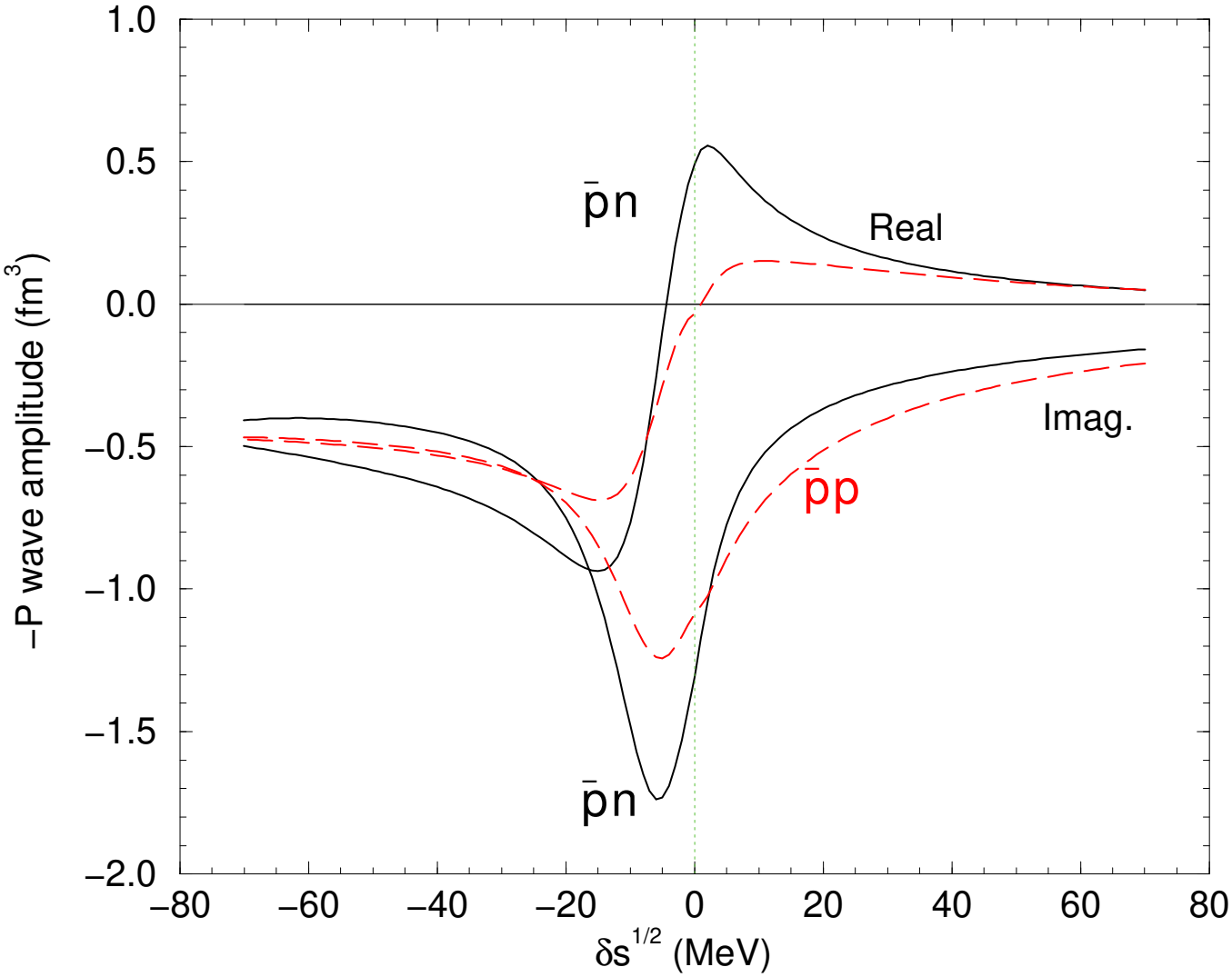
Global fit of a '$t\rho$' potential $(b_0 + \mathrm{i}b_1)\rho$ for ρ folded with a finite-range Gaussian with rms radius of 1.1 fm. Neutron 'skin' is parametrized as $r_n - r_p = \gamma \frac{N-Z}{A} + \delta$



$\eta = (r - R_{1/2})/a$, sensitivity near 5% of central density and less.



Antiproton-nucleon *s*-wave scattering amplitudes around threshold from the Paris 2009 potential. Negative values represent attraction and absorption.



Antiproton-nucleon *p*-wave scattering amplitudes around threshold from the Paris 2009 potential. Negative values represent attraction and absorption.

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T. Waas, M. Rho, W. Weise, NPA 617 (1997) 449 (WRW)

$$2\mu_{\bar{p}} V_{\bar{p}}(\rho) = -4\pi \left[\frac{(2\tilde{f}_{\bar{p}p} - \tilde{f}_{\bar{p}n})\,\frac{1}{2}\rho_p}{1 + \frac{1}{4}\xi_k(\rho)\tilde{f}_0\rho(r)} + \frac{\tilde{f}_{\bar{p}n}(\frac{1}{2}\rho_p + \rho_n)}{1 + \frac{1}{4}\xi_k(\rho)\tilde{f}_1\rho(r)} \right],$$

$\tilde{f}_{\bar{p}N}(\rho)$ are related kinematically to the in-medium $\bar{p}N$ c.m. amplitudes $f_{\bar{p}N}(\rho)$ by $\tilde{f}_{\bar{p}N}(\rho) = (1 + \frac{A-1}{A}\frac{\mu_{\bar{p}}}{m_N})f_{\bar{p}N}(\rho)$. The Pauli correlation factor $\xi_k(\rho)$ is defined by

$$\xi_k(\rho) = \frac{9\pi}{k_F^2}\left(4\int_0^\infty \frac{dr}{r}\,\exp(\mathrm{i}kr)\,j_1^2(k_F r)\right),$$

with $k = [(E_{\bar{p}} - i\Gamma/2)^2 - m_{\bar{p}}^2]^{1/2}$ and where Γ is the width of the particular antiprotonic atom state. $k_F = (3\pi^2\rho/2)^{1/3}$.
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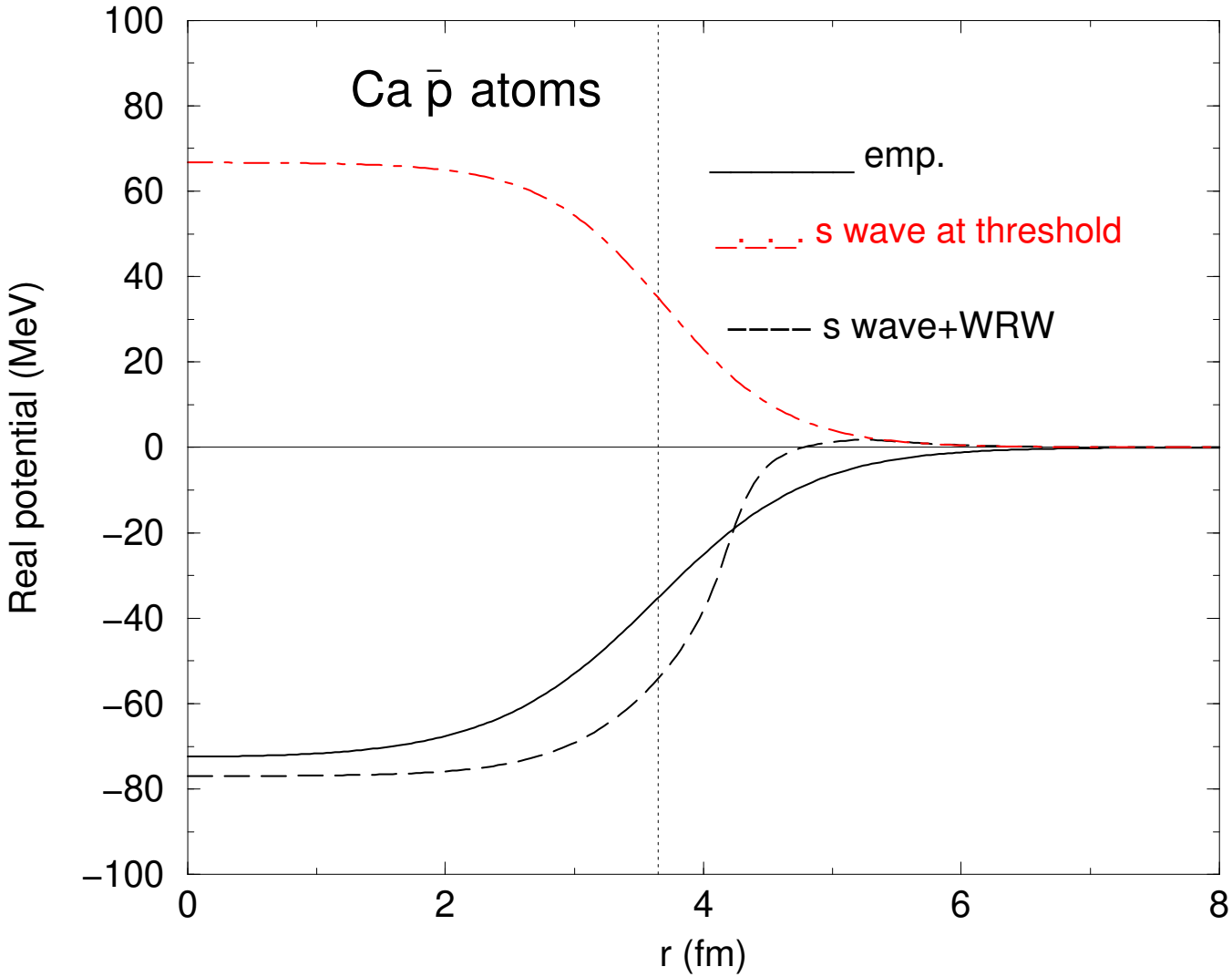
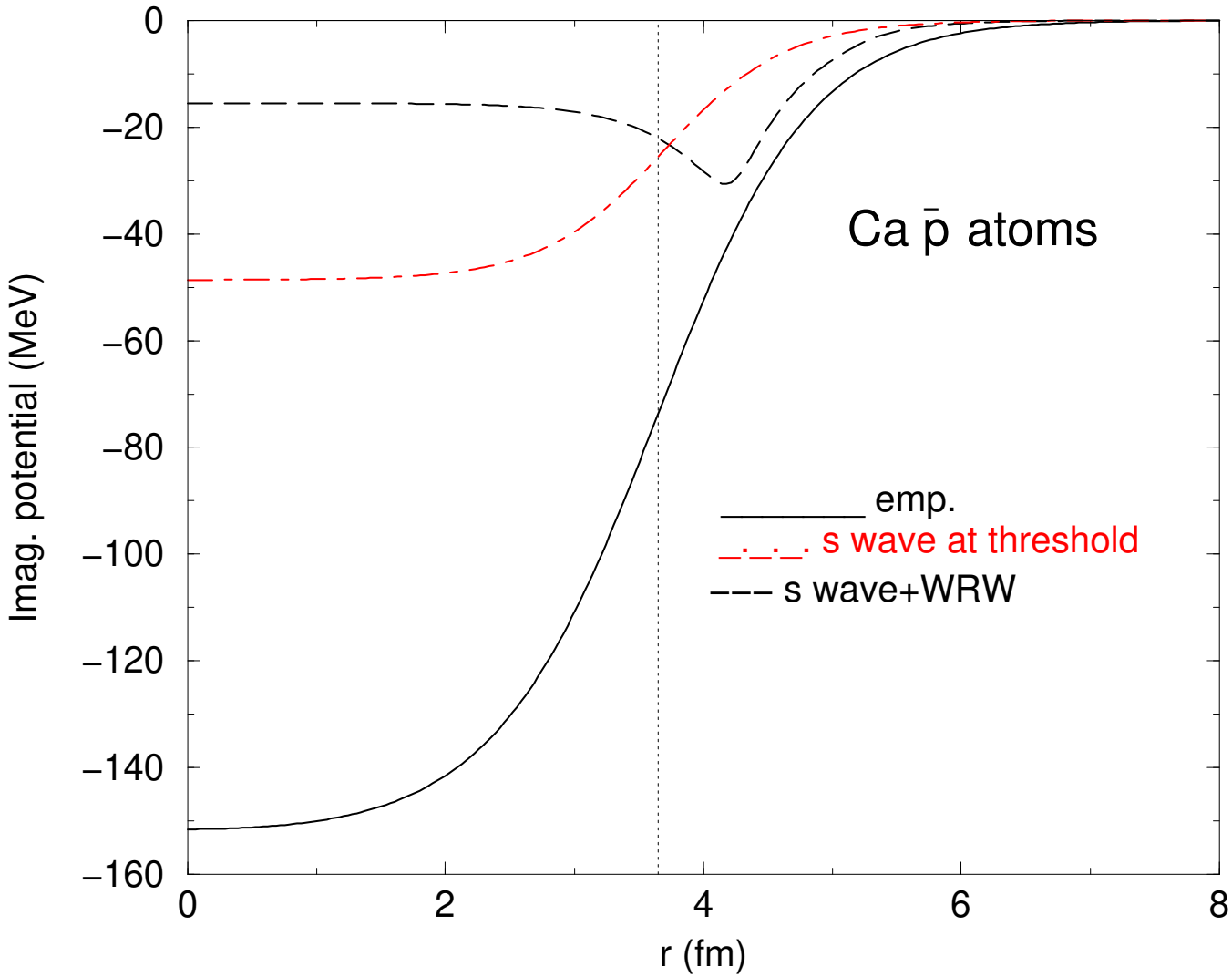
From E.F., A. Gal, B. Loiseau, S. Wycech, NPA 943 (101) (2017).

Comparisons between calculation and experiment for $\bar{p}$ atoms, using various options of S-wave and P-wave potentials. The symbol '09 means that $\bar{p}N$ amplitudes were used with 'in medium kinematics'. When indicated, these were multiplied by a scaling factor given in parentheses. When units of fm^3 are listed, the corresponding parameter was empirical.

	S-wave	Real P-wave	Imag. P-wave	$\chi^2(90)$
1	emp.	-	-	199
2	-	1.9±0.1 fm^3	2.8±0.1 fm^3	206
3	'09	'09	'09	2304
4	'09	2.9±0.1 fm^3	1.8±0.1 fm^3	203
5	'09	'09×(−10.0±0.9)	'09×(3.1±0.2)	571
6	'09	2.9±0.1 fm^3	'09×(1.3±0.1)	218


Ca p̄ atoms
emp.
s wave at threshold
s wave+WRW
Real potential (MeV)
r (fm)
100
80
60
40
20
0
−20
−40
−60
−80
−100
0
2
4
6
8

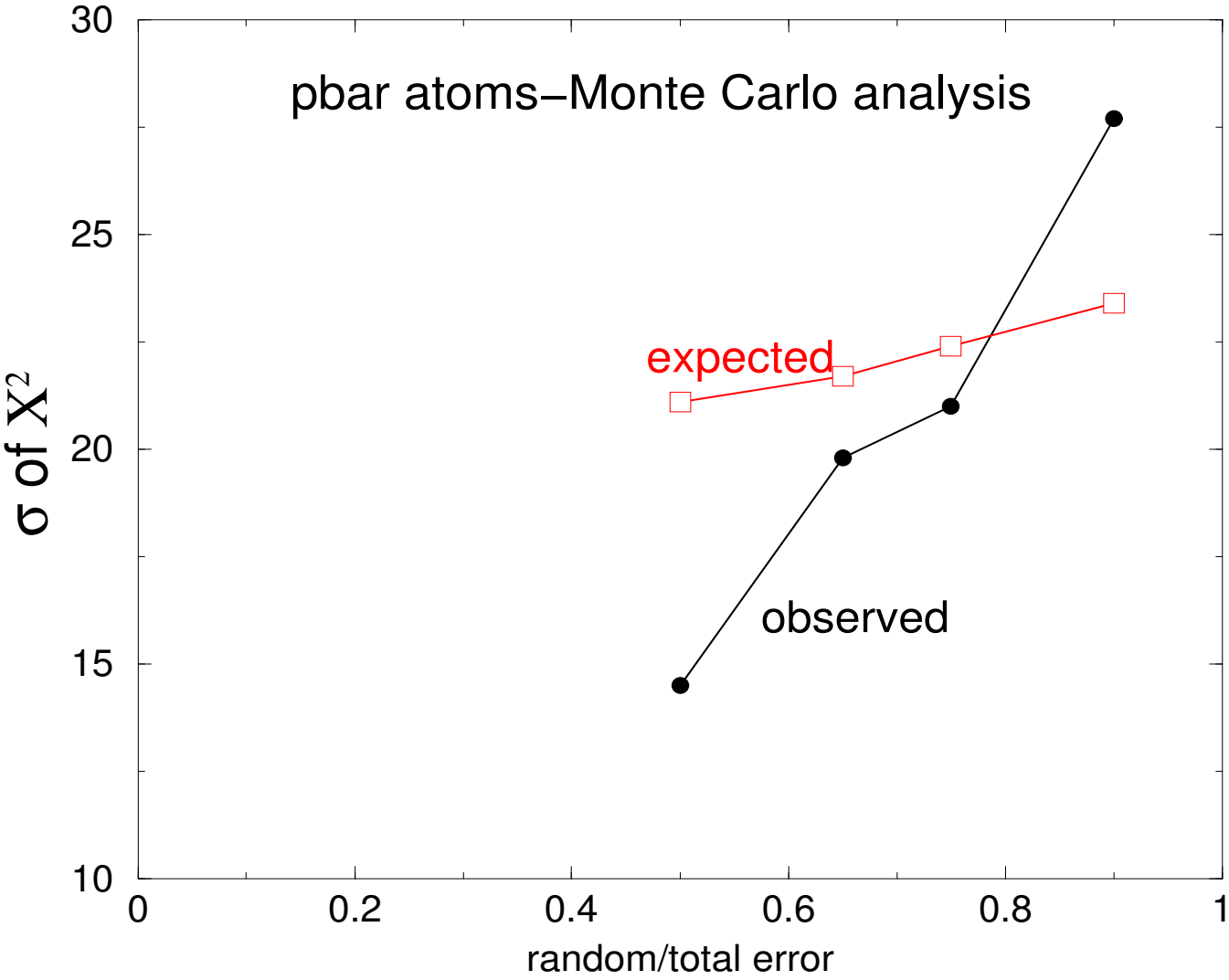

0
−20
−40
−60
−80
−100
−120
−140
−160
0
2
4
6
8
Imag. potential (MeV)
r (fm)
Ca p̄ atoms
emp.
s wave at threshold
s wave+WRW

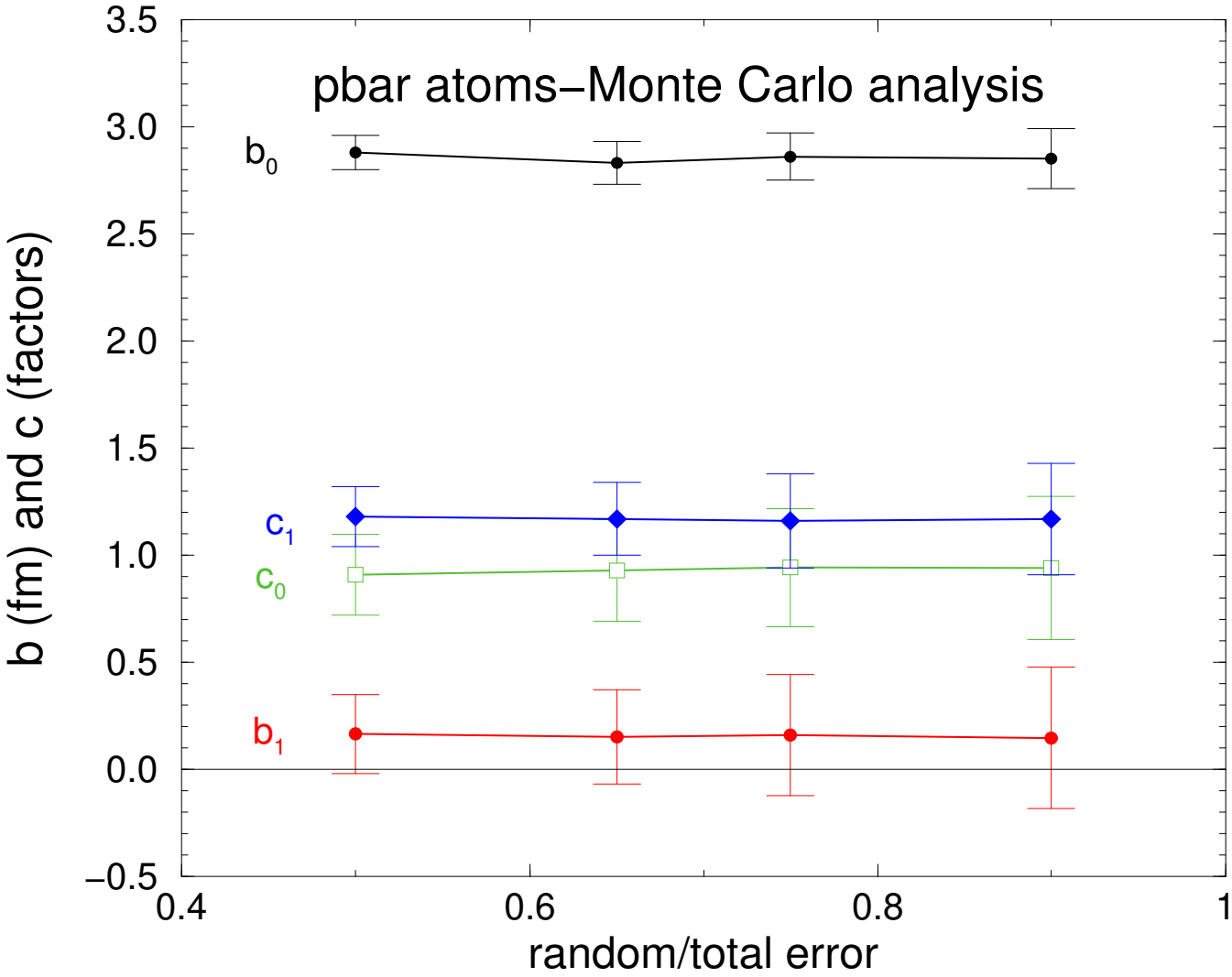
For an optical potential built on the Paris amplitudes the χ^2 for 90 points is 2300 to 3200, depending on details.

Try adding scattering amplitude b_0 + i b_1 to the s-wave amplitude and rescale the real and imaginary p-wave amplidues by c_0 and c_1, respectively.

A conventional fit achieves $\chi^2(90)$=201.0,
b_0=2.85±0.24 fm, b_1=0.14±0.51 fm
c_0=0.95±0.55, c_1=1.18±0.40

b_1 almost 0 ?, c_0 and c_1 almost 1 ?
Need Monte Carlo fits!


pbar atoms–Monte Carlo analysis
expected
observed
σ of X²
random/total error
30
25
20
15
10
0
0.2
0.4
0.6
0.8
1


pbar atoms–Monte Carlo analysis
b (fm) and c (factors)
random/total error
b0
c1
c0
b1
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
–0.5
0.4
0.6
0.8
1

A conventional fit achieves $\chi^2(90)$=201.0,
b_0=2.85±0.24 fm, b_1=0.14±0.51 fm
c_0=0.95±0.55, c_1=1.18±0.40

Monte Carlo results, $\chi^2(90) = 201.1$
b_0=2.86±0.11 fm, b_1=0.16±0.18 fm
c_0=0.94±0.28, c_1=1.16±0.22

In addition no evidence for a non-linear dependence on density,
$(\rho/\rho_0)^\alpha, \alpha = 0.01 \pm 0.09$

Eigenvectors from the covariant matrix

Single fit

b_0	b_1	c_0	c_1
0.849437E+00	0.221790E+00	-0.133396E+00	-0.459861E+00
-0.361218E+00	0.379792E+00	0.555787E+00	-0.645275E+00
0.324327E+00	0.365376E+00	0.644267E+00	0.588415E+00
-0.206860E+00	0.820407E+00	-0.508159E+00	0.160982E+00

Monte Carlo fit

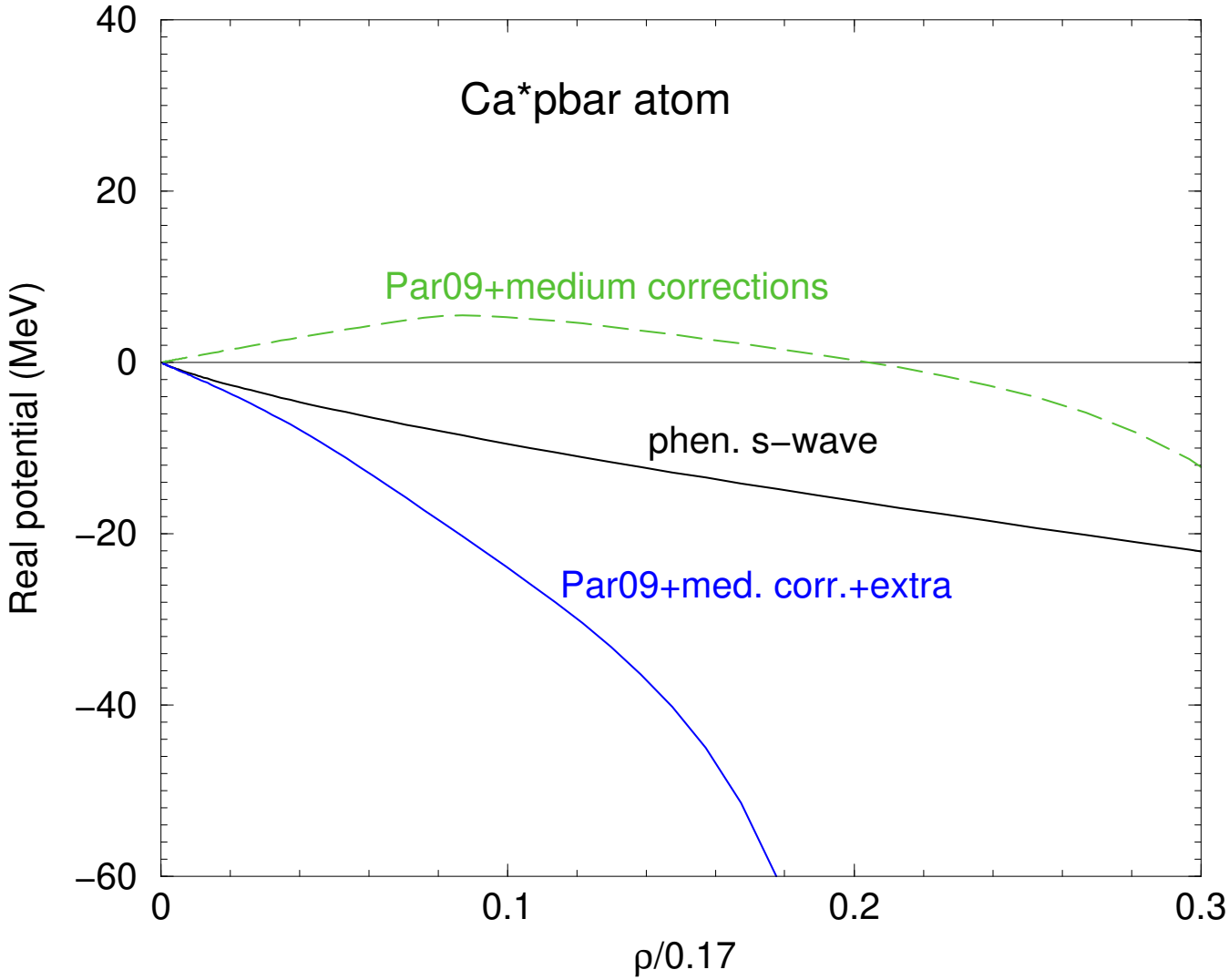
b_0	b_1	c_0	c_1
0.991048E+00	-0.544676E-01	-0.121697E+00	-0.692262E-02
-0.425983E-01	0.655316E+00	-0.660869E+00	0.363316E+00
0.125795E+00	0.601945E+00	0.739425E+00	0.274023E+00
-0.136266E-01	-0.453052E+00	0.411514E-01	0.890430E+00

Including an 'angle transformation' term, a conventional fit achieves $\chi^2(90)$=199.4,
b_0=2.326±0.18 fm, b_1=0.22±0.74 fm
c_0=0.905±0.66, c_1=1.10±0.62

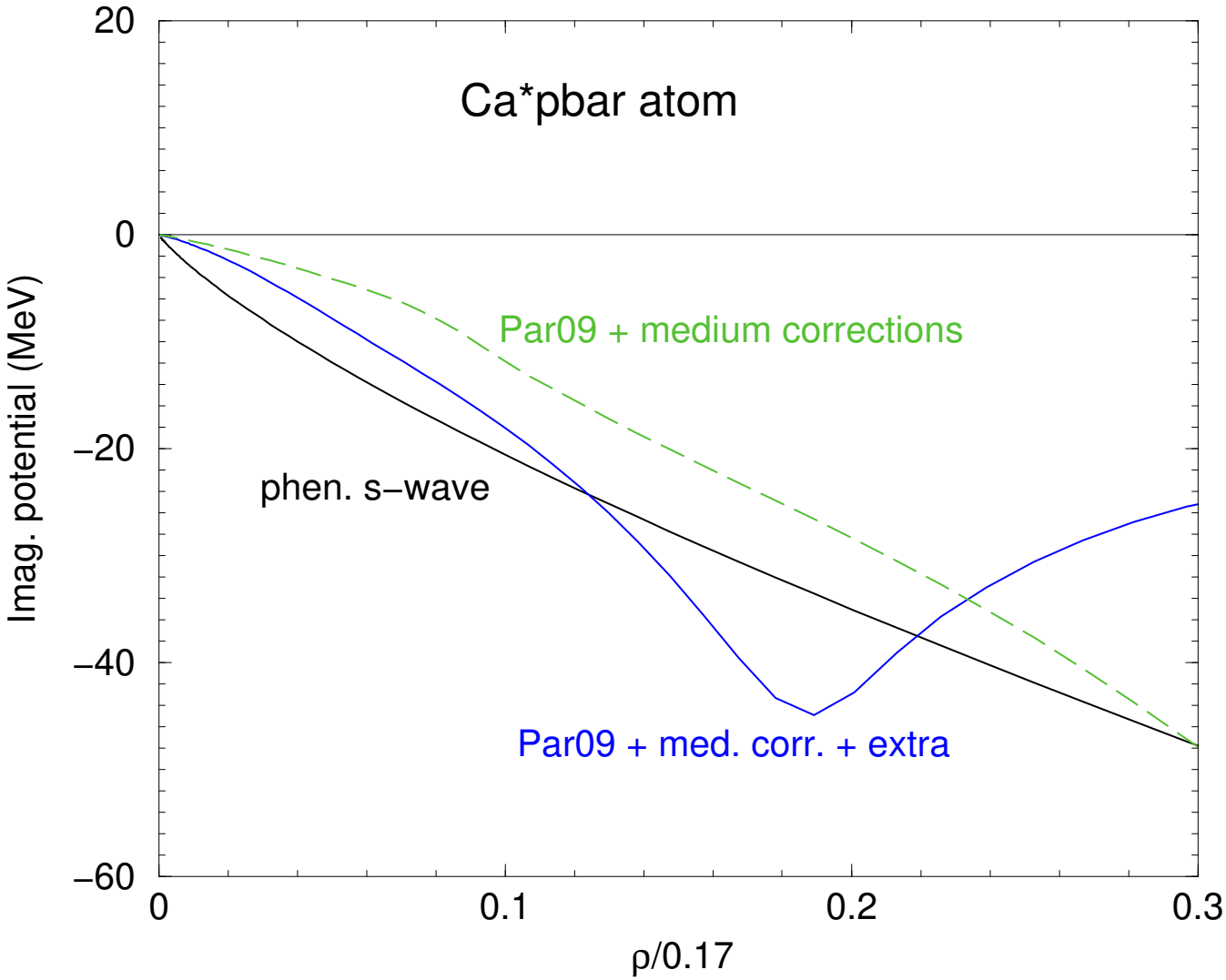
Monte Carlo results, $\chi^2(90) = 199.4$
b_0=2.314±0.12 fm, b_1=0.24±0.29 fm
c_0=0.93±0.23, c_1=1.08±0.23
With eigenvectors

b_0	b_1	c_0	c_1
0.982697E+00	-0.976823E-01	-0.145523E+00	-0.598997E-01
-0.815286E-02	0.734660E+00	-0.640365E+00	0.223920E+00
0.179122E+00	0.437305E+00	0.690784E+00	0.547263E+00
-0.464276E-01	-0.509408E+00	-0.302611E+00	0.804223E+00

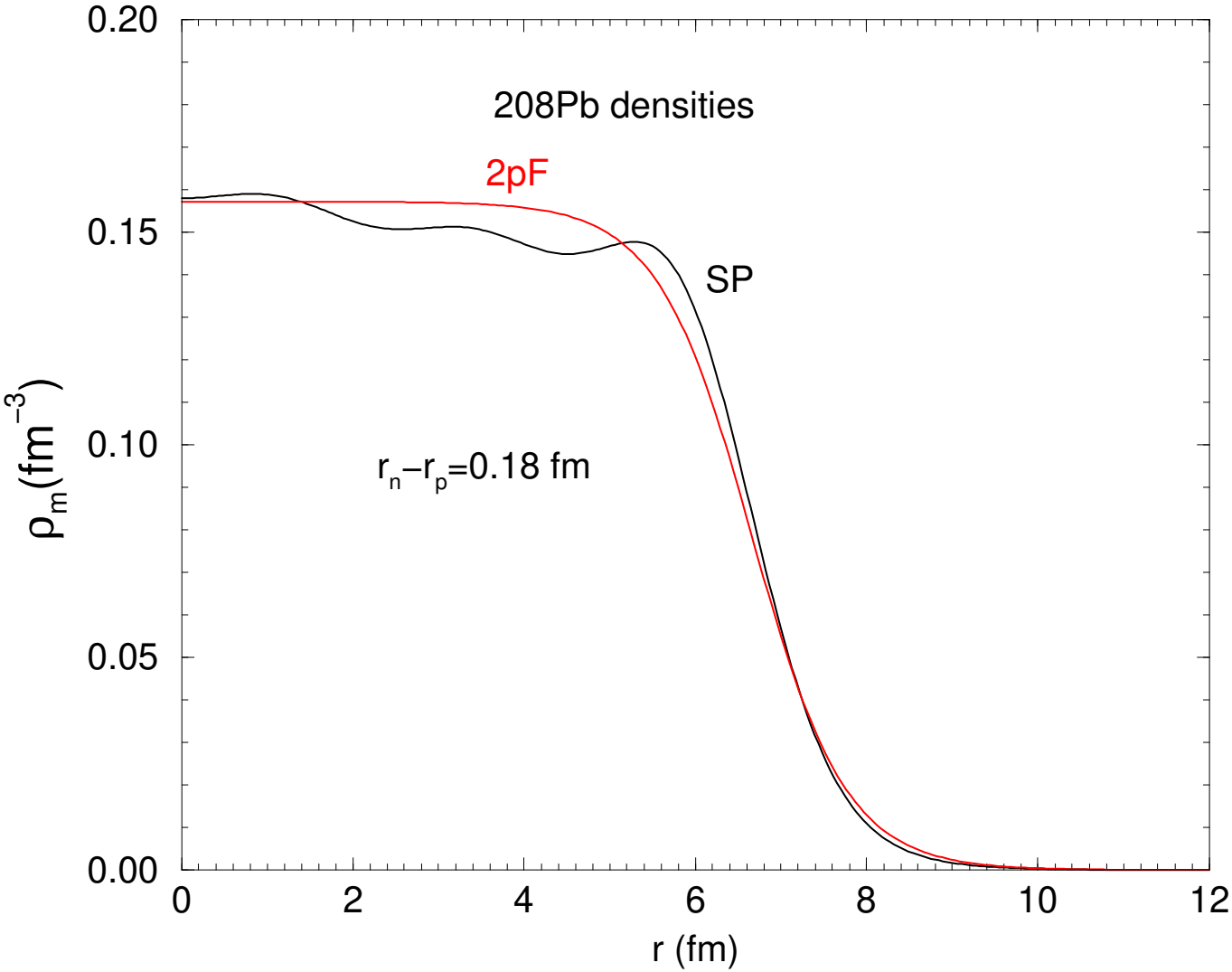
b_0 and c_1 emerge as the more relevant parameters. Indeed varying only b_0 and c_1 (with b_1=0, $c_0 = 1.$), we get
χ^2=200.7, b_0=2.207±0.11 fm, c_1=1.176±0.067.

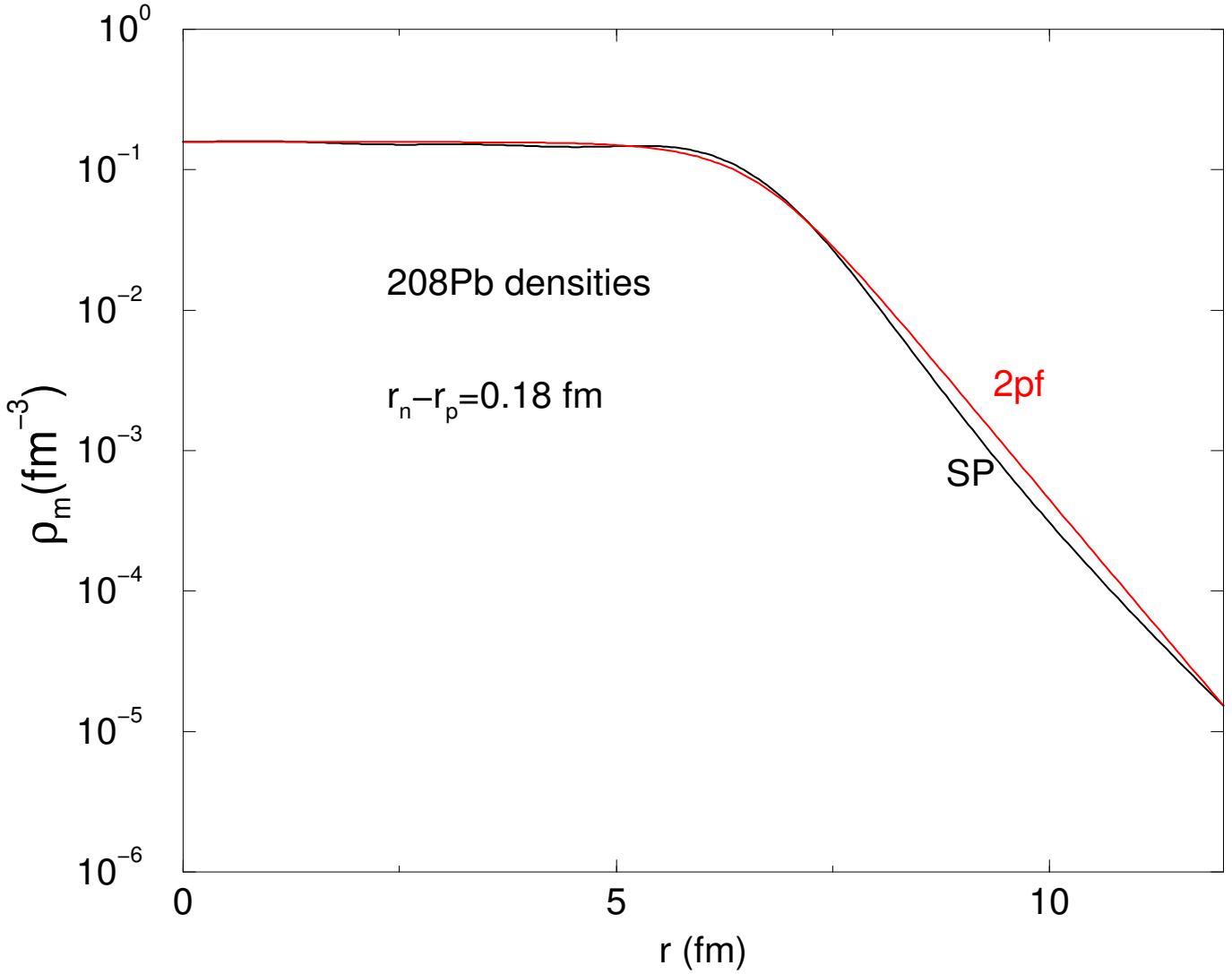


Medium corrections=in medium kinematics + Pauli (WRW).



Medium corrections=in medium kinematics + Pauli (WRW).

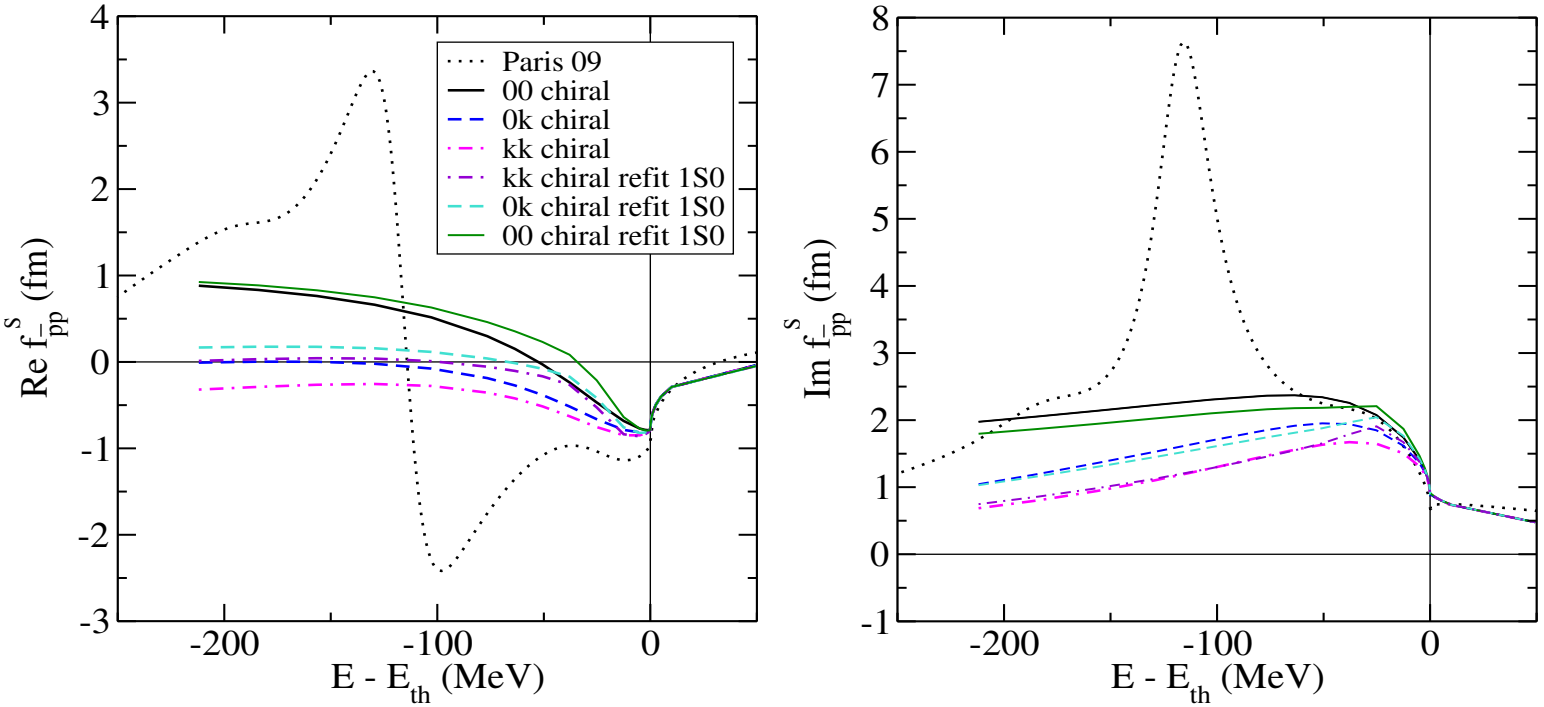

208Pb densities
2pF
SP
$r_n - r_p$=0.18 fm
ρ_m(fm^{-3})
r (fm)
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12


208Pb densities
$r_n - r_p$=0.18 fm
2pf
SP
ρ_m(fm^{-3})
r (fm)
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
5
10

Concluding remarks

- Based on hadron-nucleon scattering amplitudes, Monte Carlo methods in optical model analyses of hadronic atom data achieve significantly improved accuracies compared to conventional methods.
- Antiprotonic atoms are sensitive to very small (5%) densities.
- No evidence for 'multinucleon' terms, i.e. non-linear in density.
- The Paris 2009 pbar-nucleon amplitudes may need some enhancement of the real s-wave part and the imaginary p-wave part.
- Repeating analyses with more 'microscopic' densities. e.g. RMF ones, could be useful.

Two talks tomorrow:
(i) Johann Haidenbauer
(ii) Jaroslava Hrtánková



Thank you for your attention!