Monte-Carlo Methods in Optical Model Analysis of Kaonic Atoms

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OUTLINE

- A quick survey of conventional optical model analyses
- Resonance near threshold and the need for additional input beyond single-nucleon amplitudes
- A short guide to MC methods and some results
- Beyond the single nucleon absorption
- New results: The Barcelona 2N potentials
- Summary and outlook

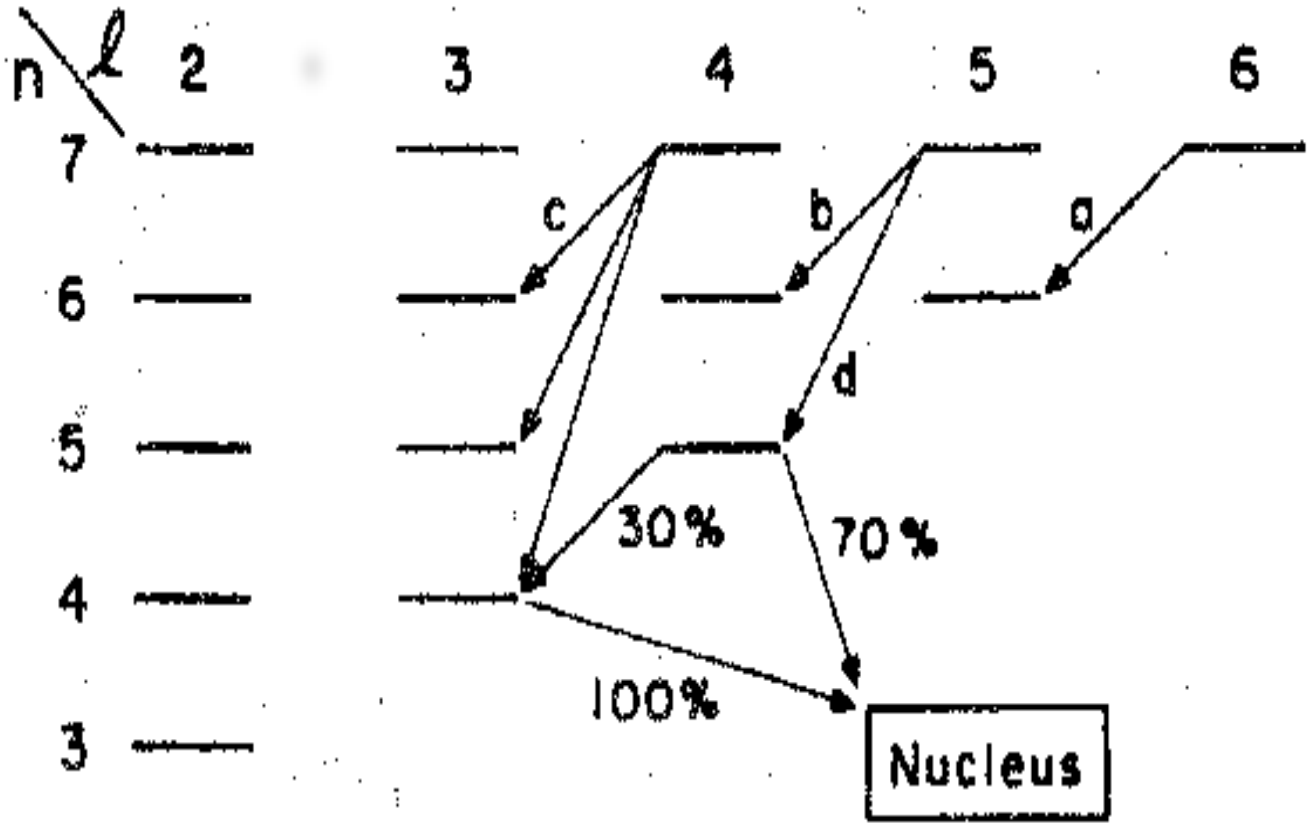
Introduction and background

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 relative yields (= upper level widths)

Puzzles with early data for H and He removed by new precision experiments at KEK and Frascati between 1997 and 2007.

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

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

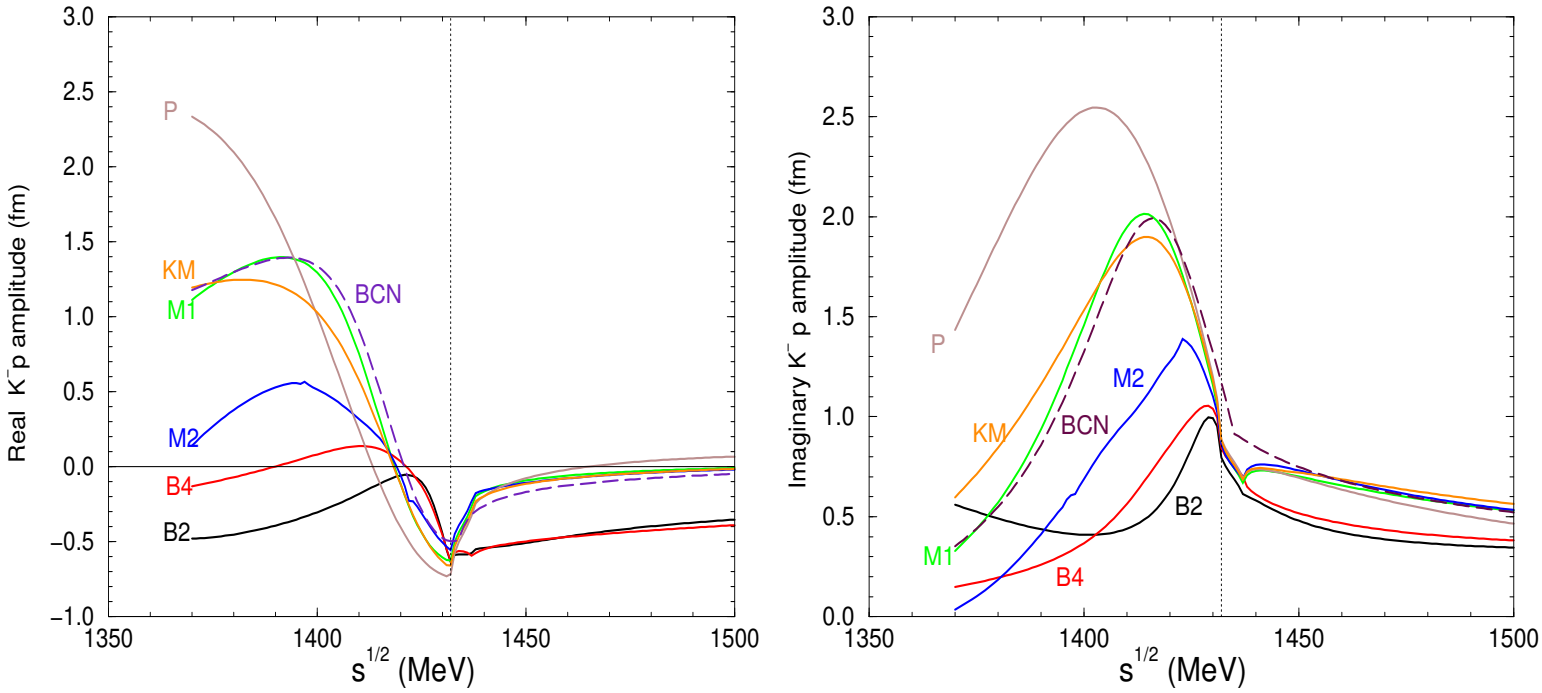
Early attempts to use 'chiral' amplitudes

Ramos & Oset, NPA 671 (2000) 481
Baca et al., NPA 673 (2000) 335
Cieply et al.,NPA 696 (2001) 173

- Poor agreement with data ($\chi^2(65)$=300)
- Reduced χ^2 to 200 with typical 50% rescaling
- χ^2=130 by adding a $t\rho$ term with NEGATIVE absorption

Something is missing!

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



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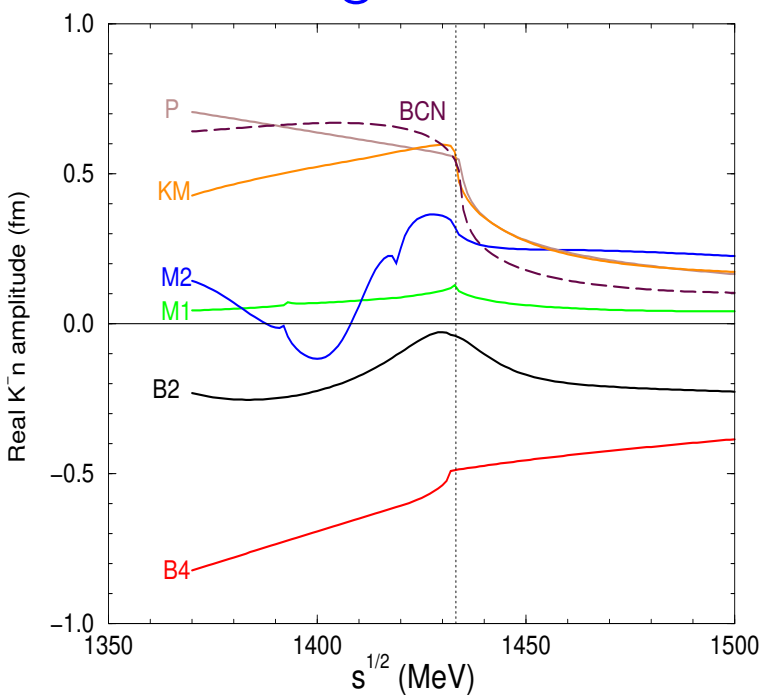
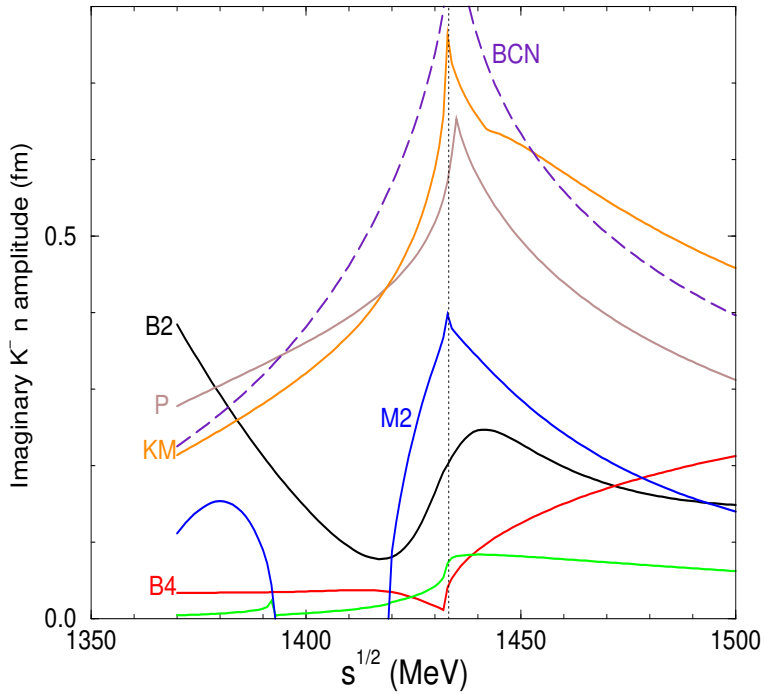




Reminder of 'in-medium kinematics'

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 nuclear mass number.

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,
$\alpha = 1.46 \pm 1.85$.

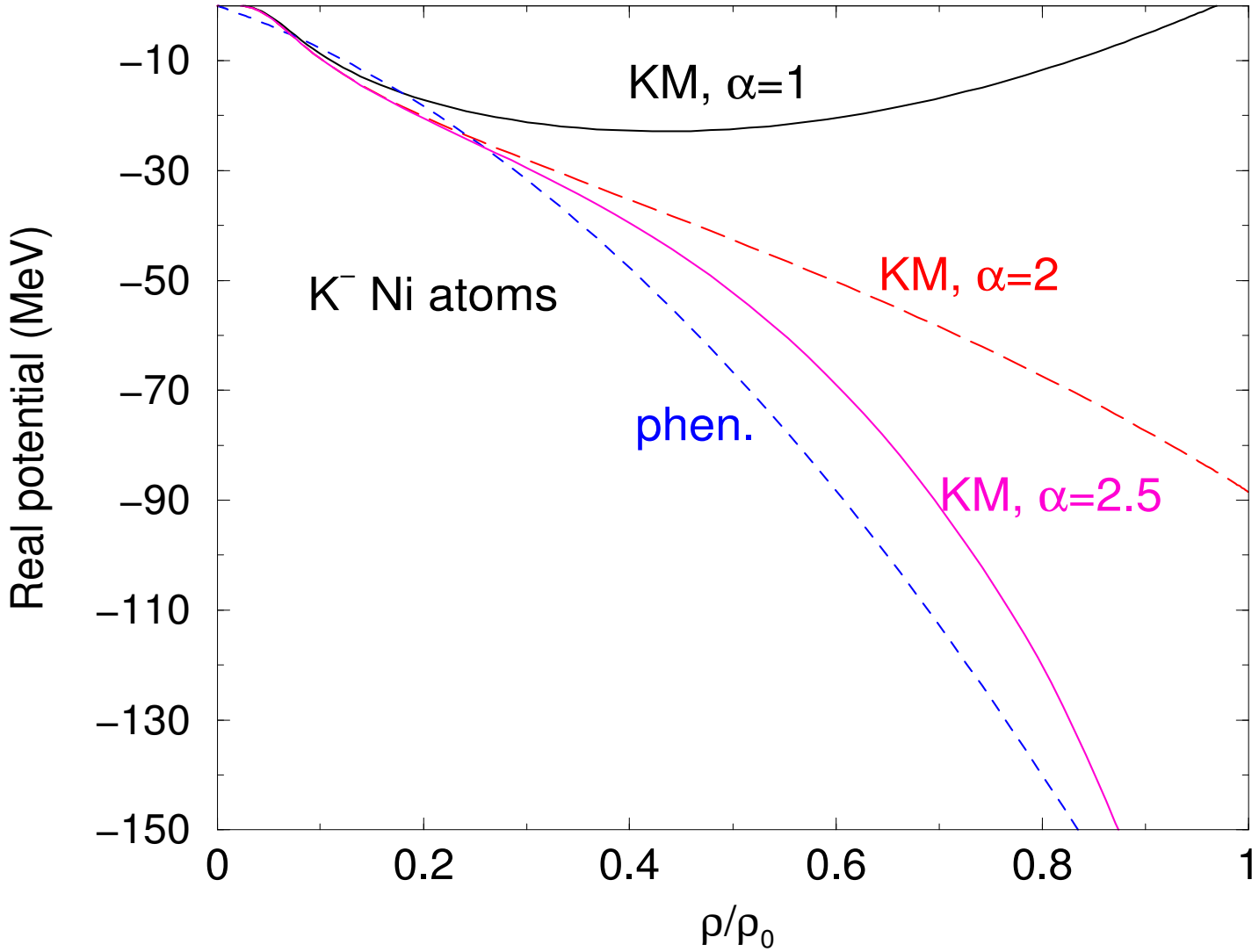
????

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.

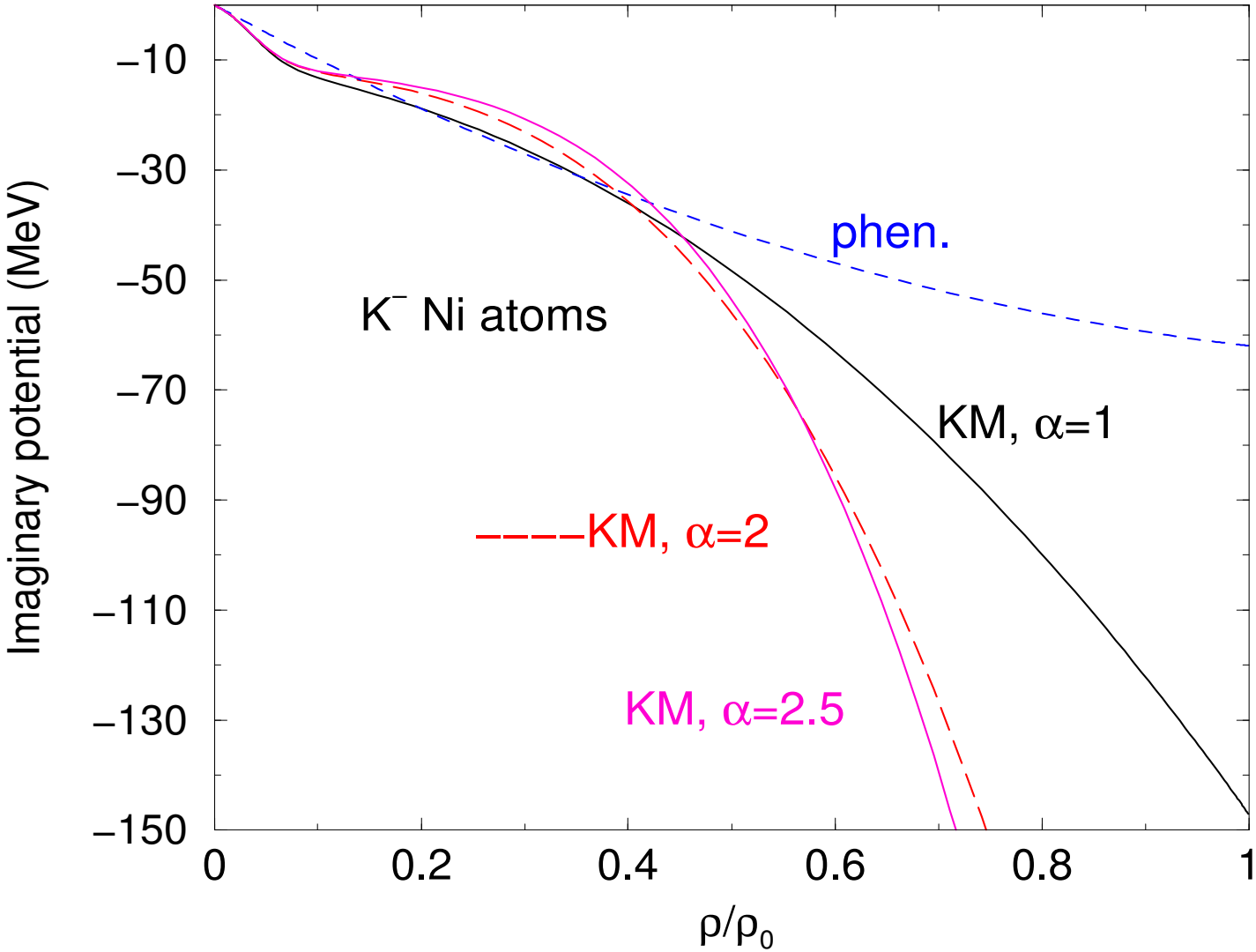
model	BCN	M1	M2	P	KM
α	1.0	0.3	1.0	1.0	1.0
ReB_0	-1.3 ± 0.3	0.3 ± 0.1	2.1 ± 0.2	-1.3 ± 0.2	-0.9 ± 0.2
ImB_0	1.9 ± 0.3	0.8 ± 0.1	1.2 ± 0.2	1.5 ± 0.2	1.4 ± 0.2
$\chi^2(65)$	129	121	109	125	123

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 seven 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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Then new χ^2 fits are made, varying all three parameters that again lead to large uncertainties.

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,

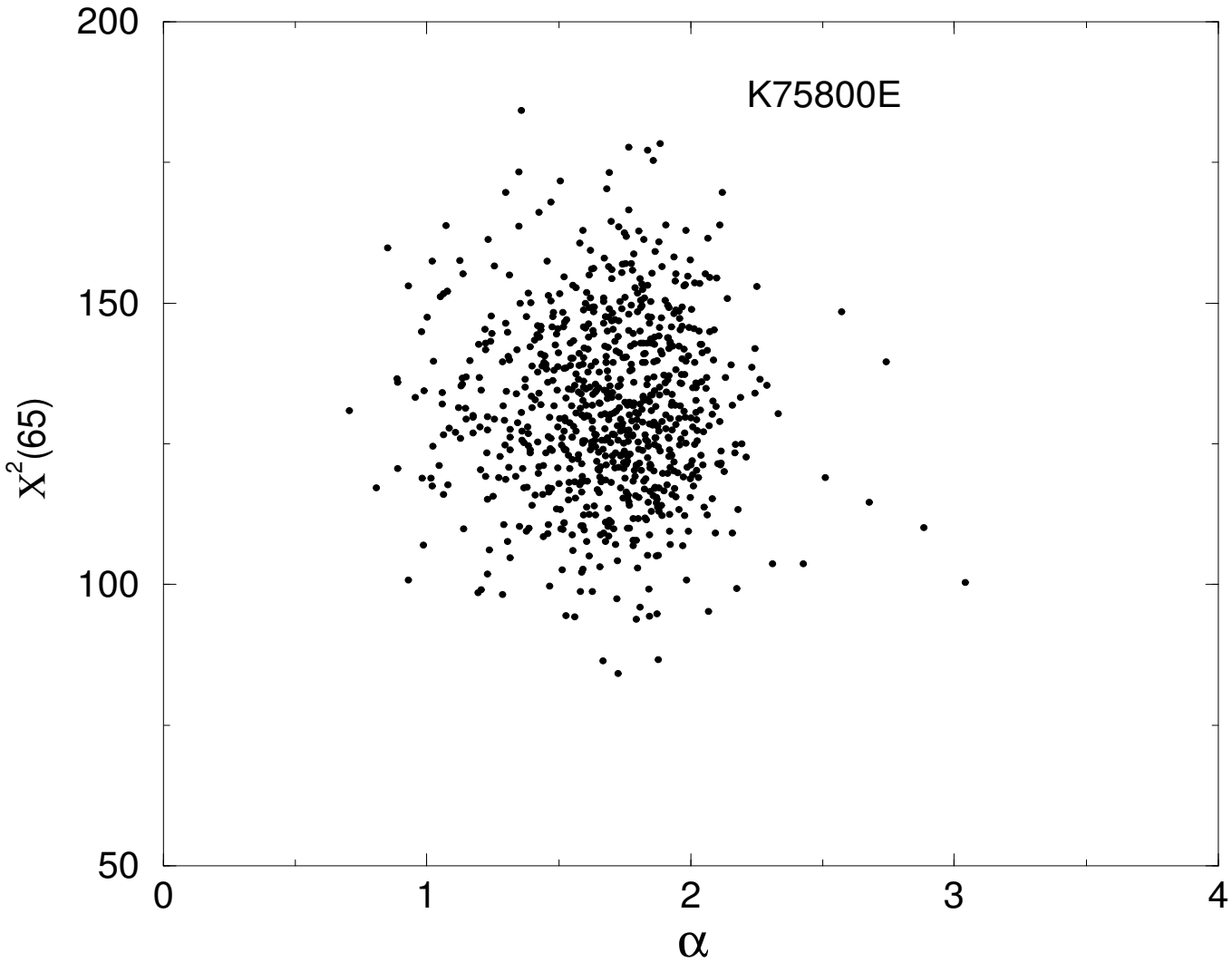
$\bar{\alpha} = \frac{1}{N}\Sigma_i(\alpha_i)$
$\sigma_\alpha^2 = \frac{N}{N-1}\Sigma_i(\alpha_i - \bar{\alpha})^2,$

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

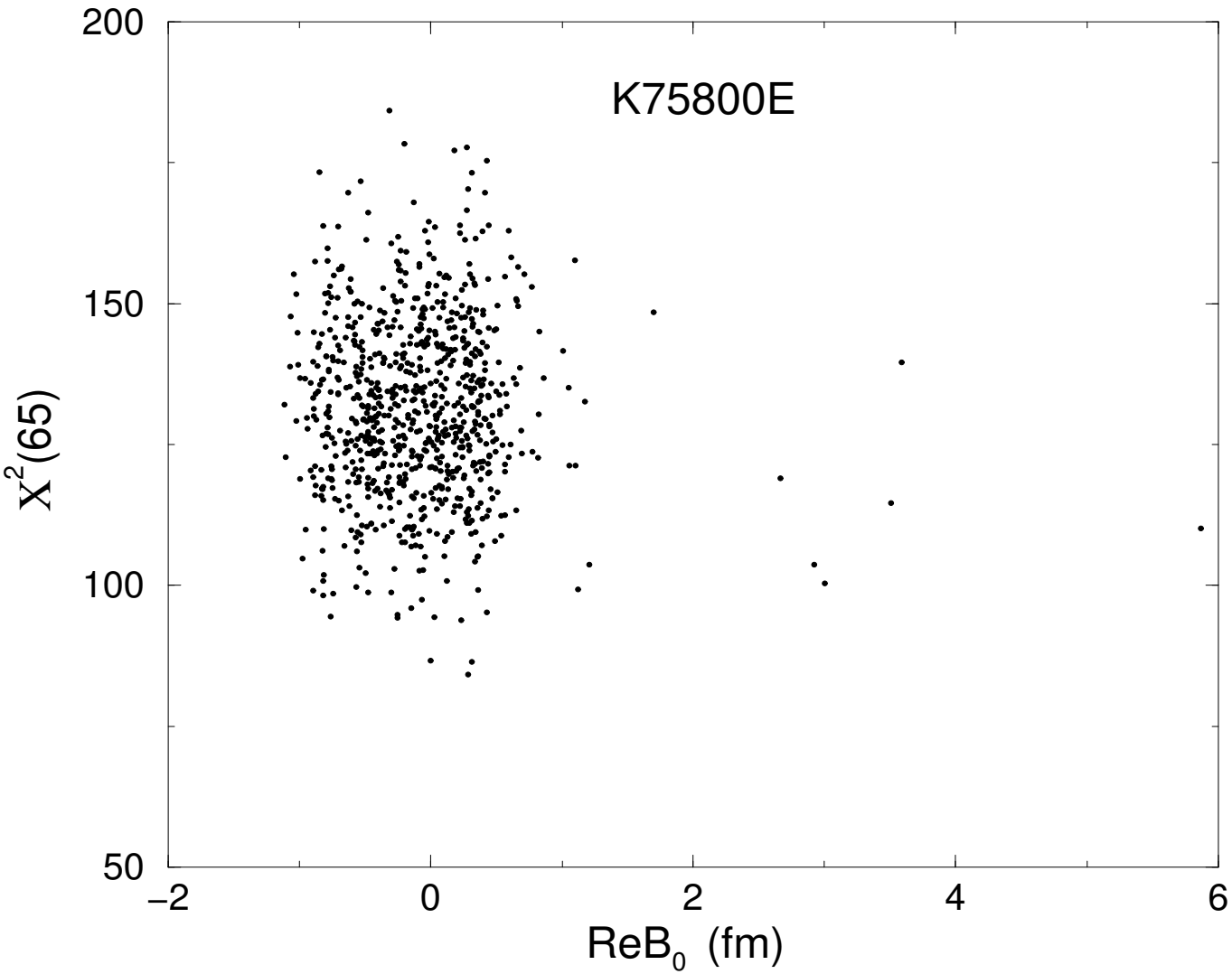
and correlations

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

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



Relusts for KM-based fits



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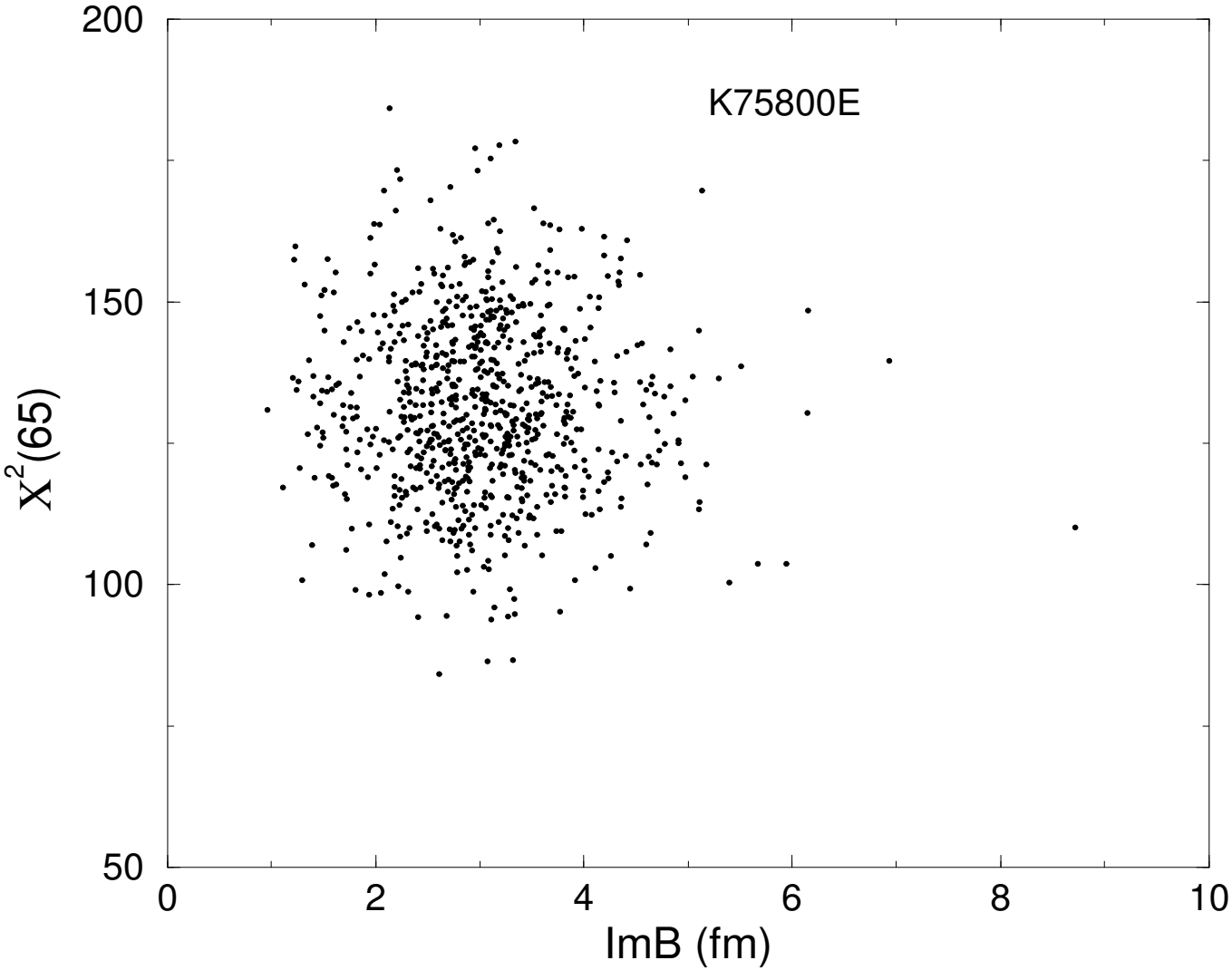

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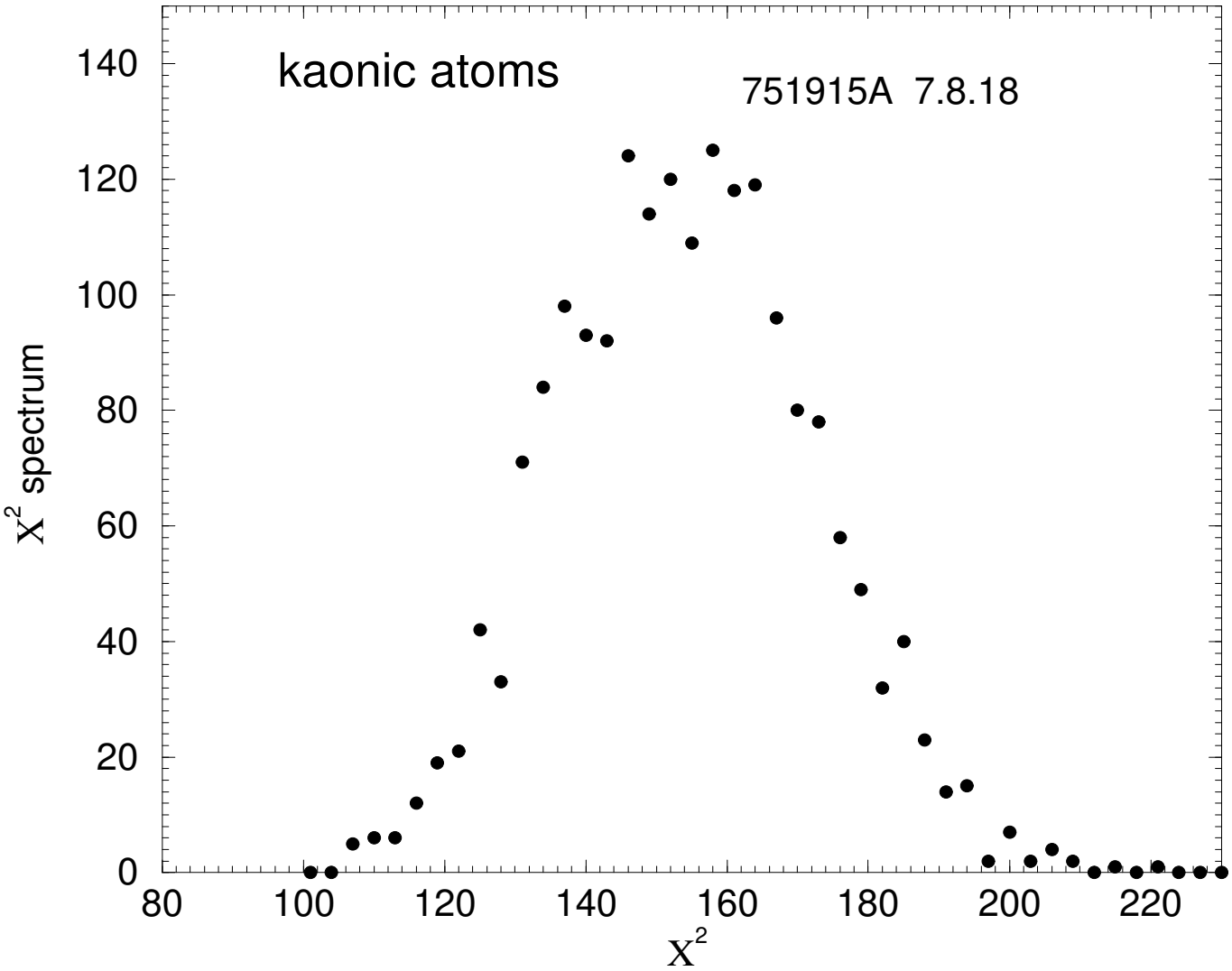
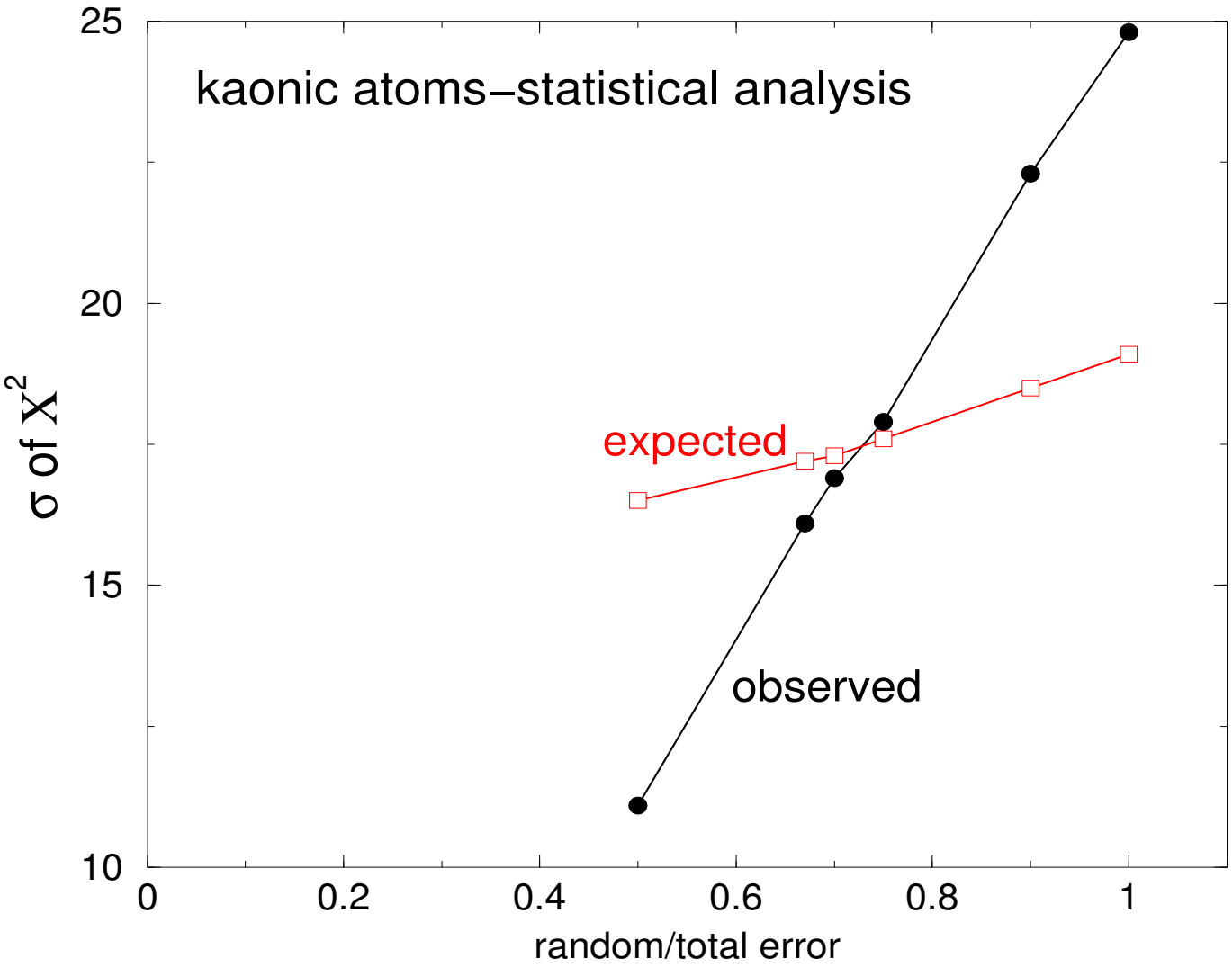


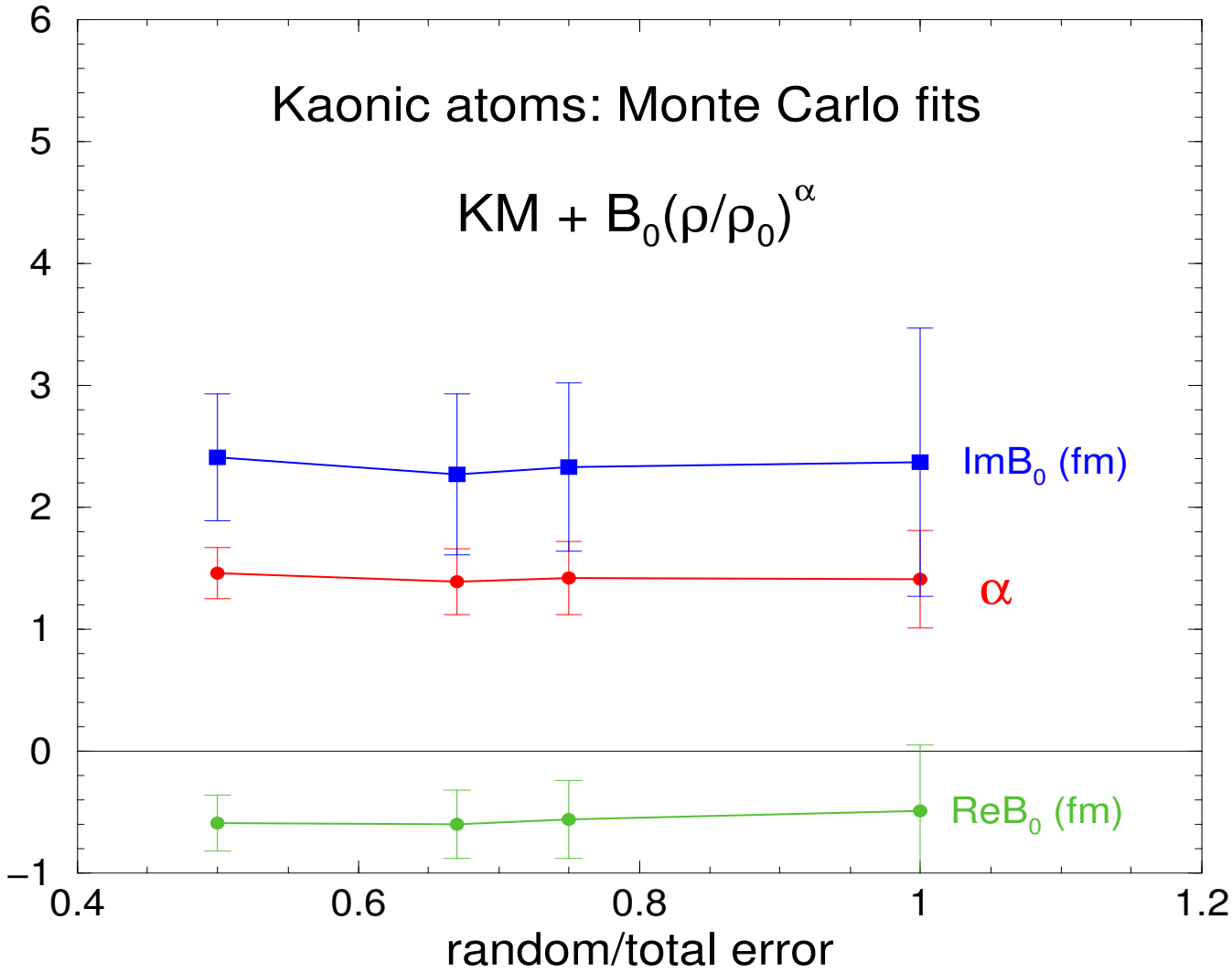
Passing the 'upper and lower 16% test' for a Gaussian.

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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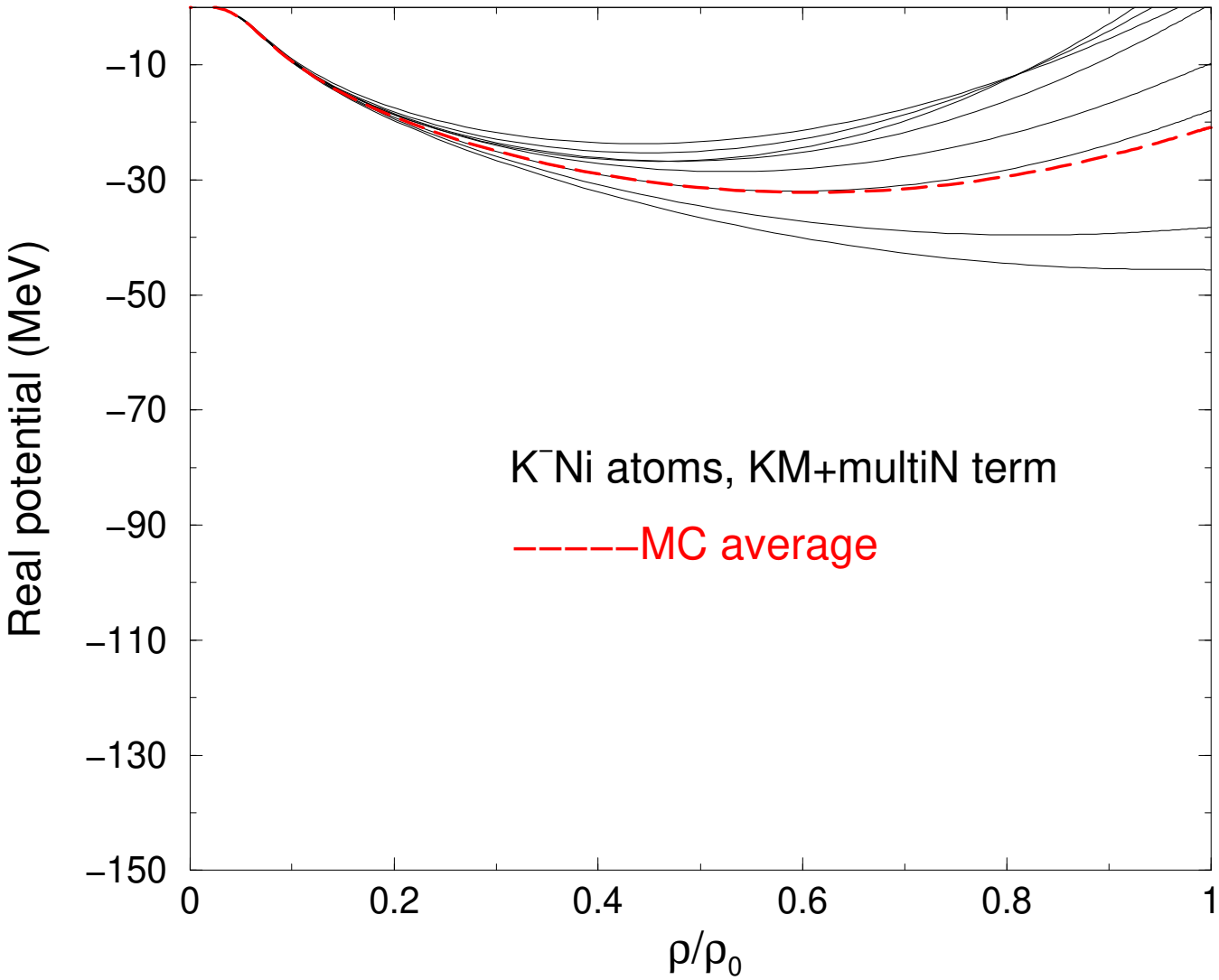
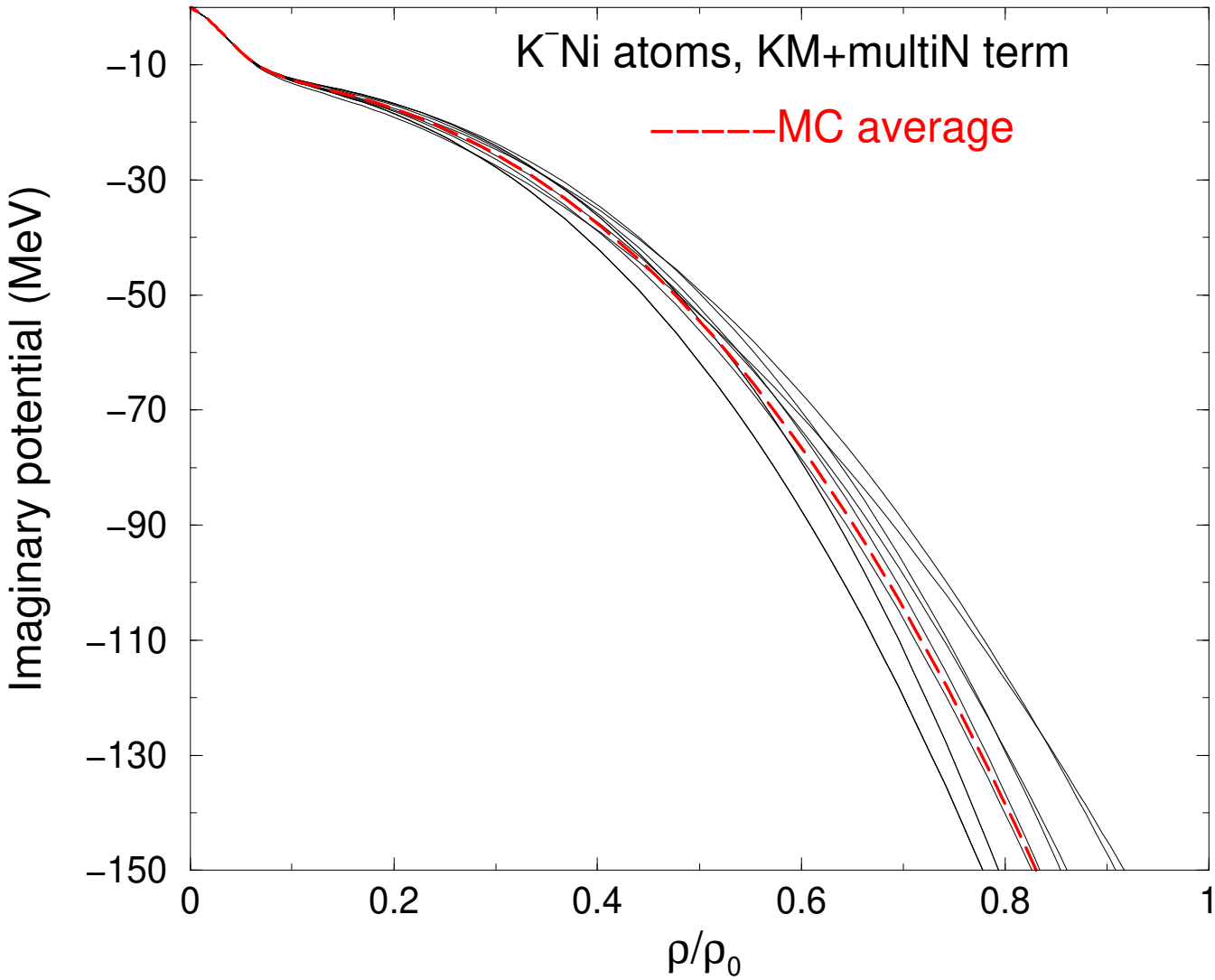
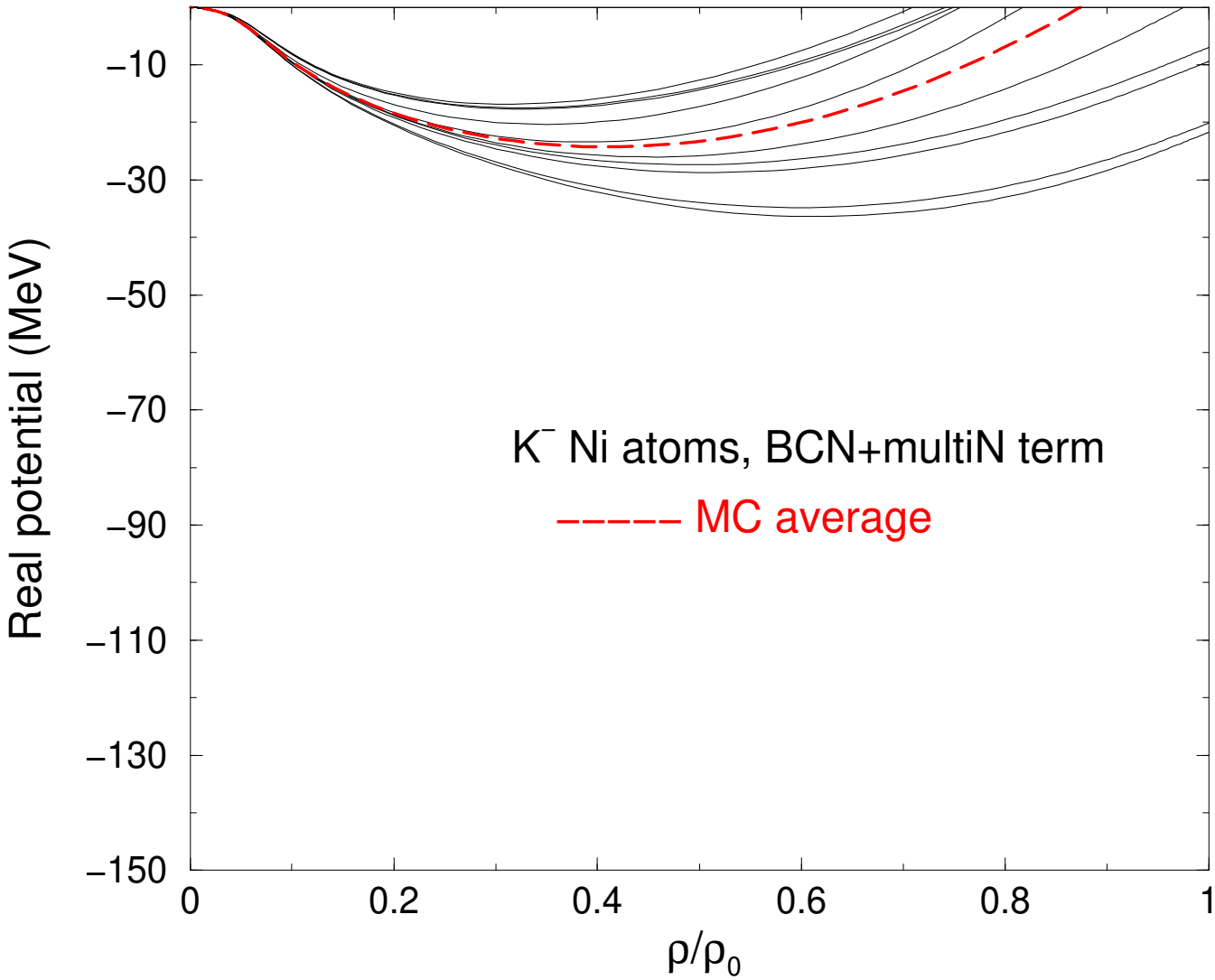
$\alpha = 1.46 \pm 1.85$.
From the Monte-Carlo technique we get
$\chi^2(65)$=119.4, (this is NOT χ^2_{ave})
Re$B_0 = -0.55 \pm 0.33$ fm,
Im$B_0 = 2.39 \pm 0.72$ fm,
$\alpha = 1.44 \pm 0.31$.

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+multiN term
−−−−−MC average


K⁻Ni atoms, KM+multiN term
------MC average
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
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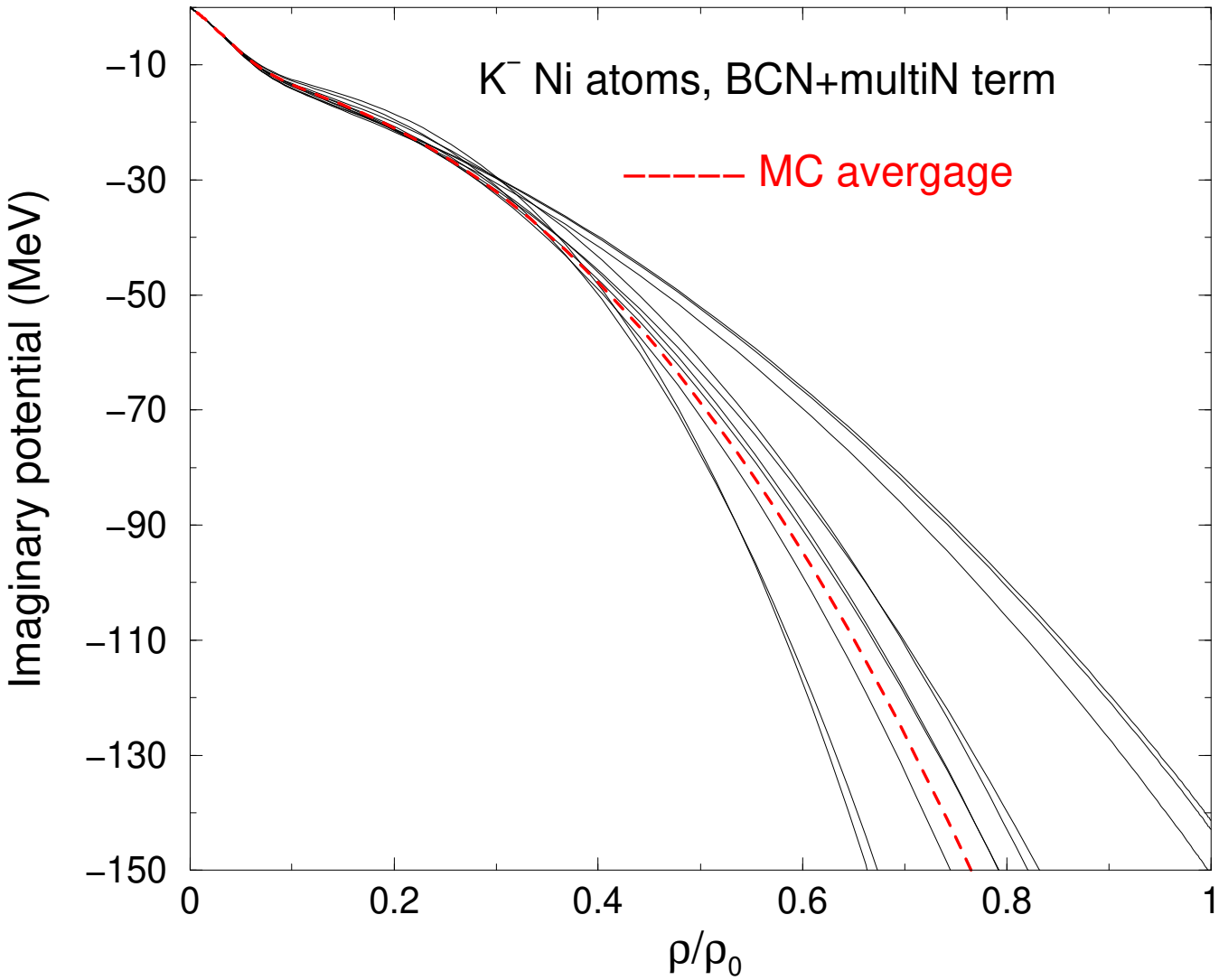
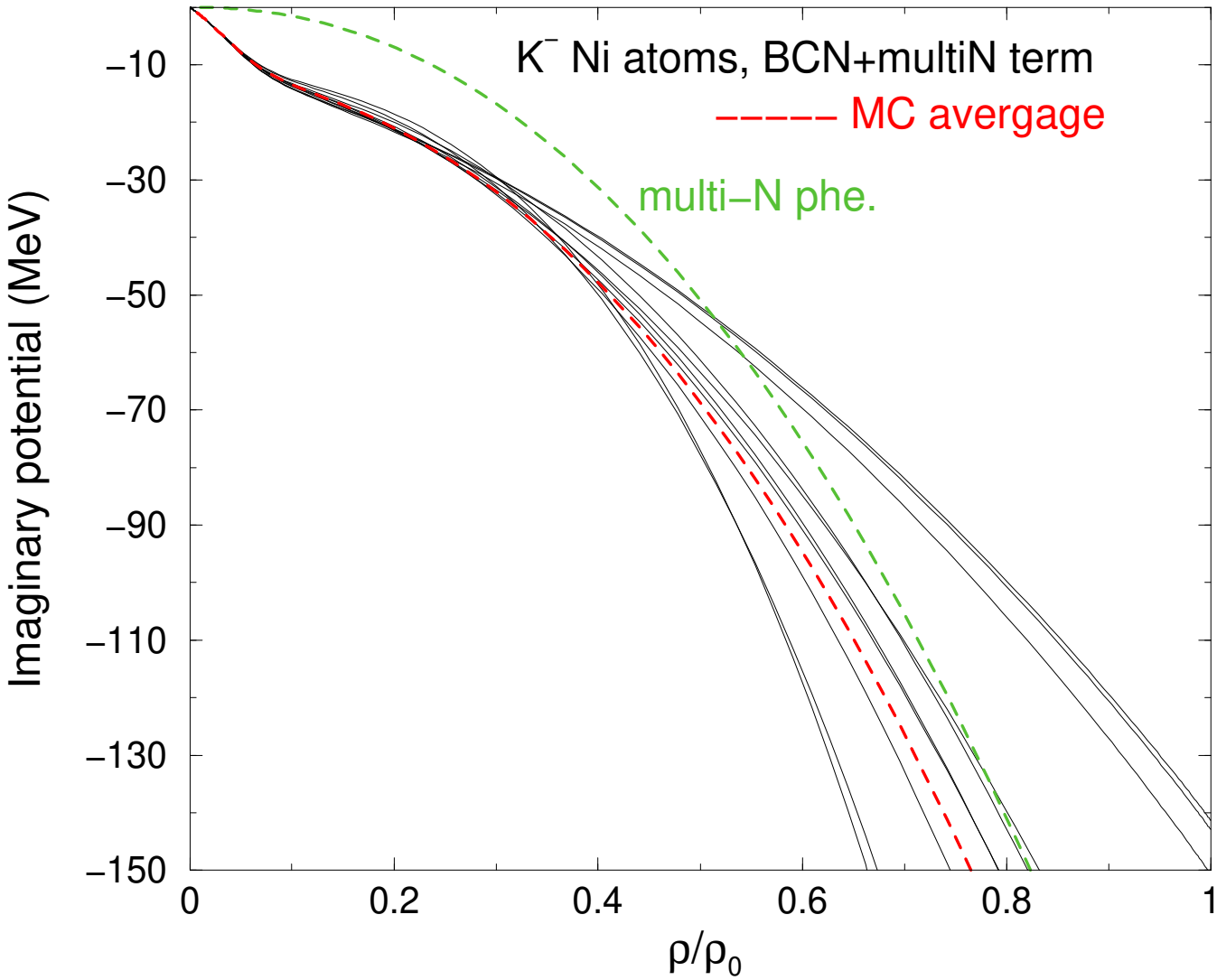
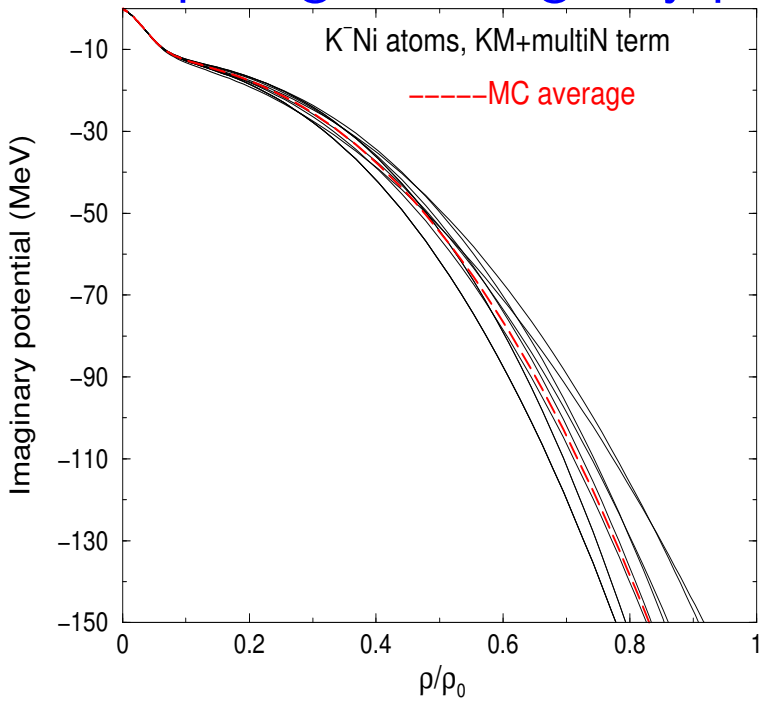
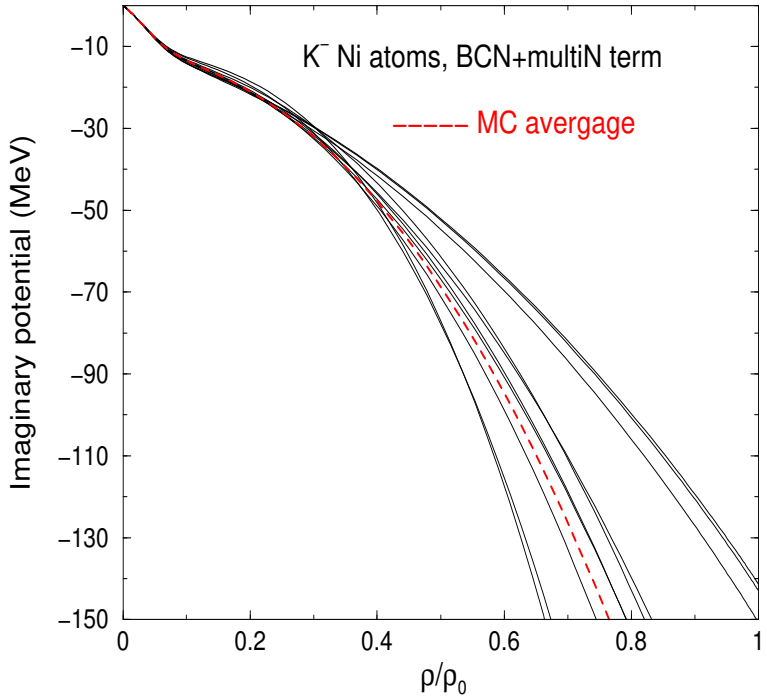
0
0.2
0.4
0.6
0.8
1
ρ/ρ0
K⁻ Ni atoms, BCN+multiN term
MC average

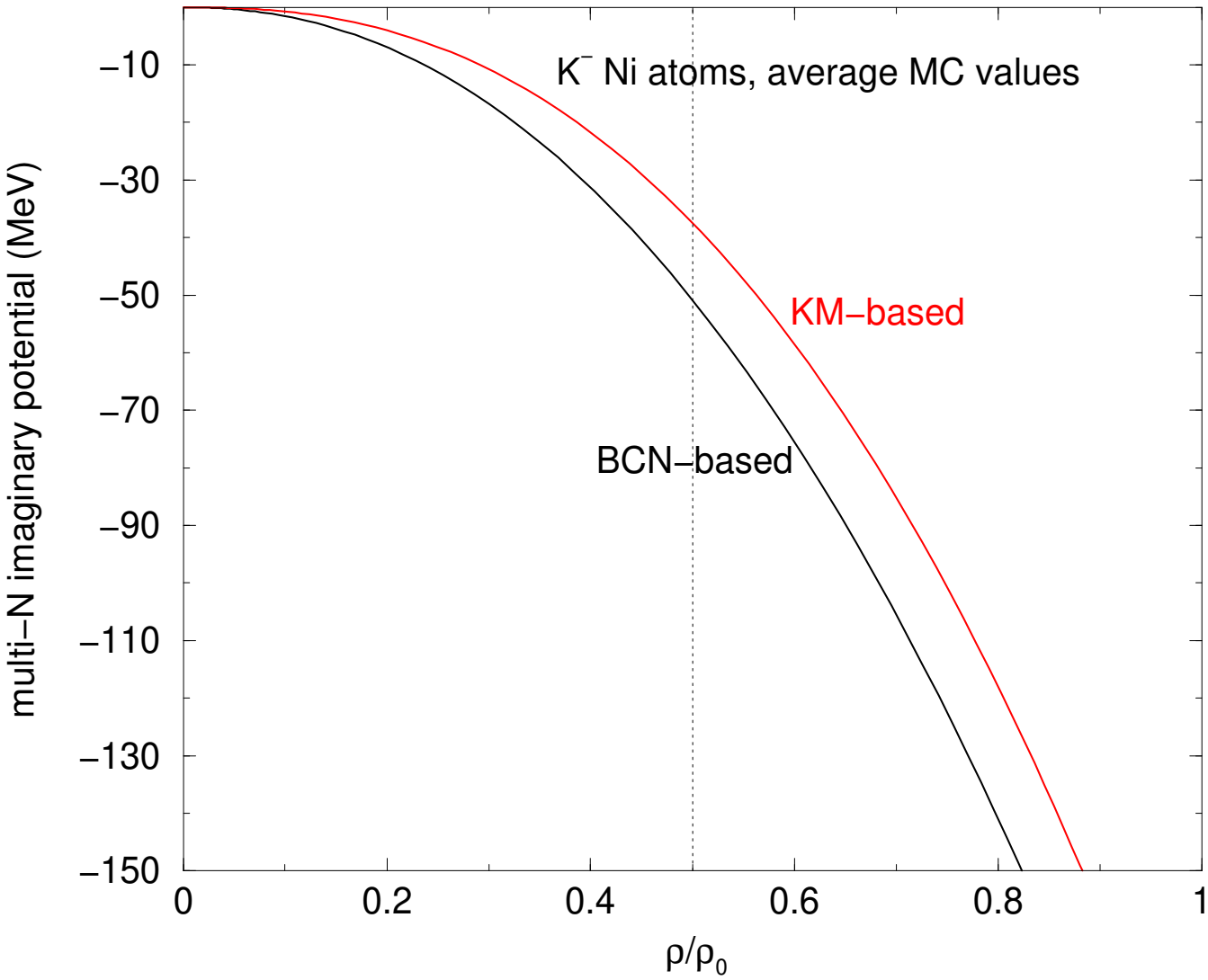

K⁻ Ni atoms, BCN+multiN term
MC avergage
Imaginary potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0


K⁻ Ni atoms, BCN+multiN term
MC avergage
multi–N phe.
Imaginary potential (MeV)
–10
–30
–50
–70
–90
–110
–130
–150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0

Comparing full imaginary potentials, KM based to BCN based






K⁻ Ni atoms, average MC values
KM–based
BCN–based
multi–N imaginary potential (MeV)
−10
−30
−50
−70
−90
−110
−130
−150
0
0.2
0.4
0.6
0.8
1
ρ/ρ0

Testing BCN's (KN+KNN) potential on some N=Z targets

for O, Mg, Si, S we find χ^2 per point=33

global (KM 1N + phen. term) χ^2 per point=3
global (BCN 1N + phen. term) χ^2 per point=4.6

Fraction of multinucleon absorptions at rest from Bubble-Chamber experiments

$$K^- + N \rightarrow Y + \pi$$
$$K^- + N + N \rightarrow Y + N$$

0.26±0.03 on a mixture of C, F and Br (Berkeley, 1968)
0.28±0.03 on Ne (BNL, 1971)
0.19±0.03 on C (CERN, 1977)
Results from nuclear emulsions quote larger uncertainties.

We therefore adopt as a best estimate of experimental K^- multinucleon absorption-at-rest fraction an average value of 0.25±0.05 for C and heavier nuclei.

Apply fraction of *single*-nucleon absorptions 0.75±0.05 as an additional constraint.

The level width Γ is obtained from the eigenvalue $E_{K^-} - i\Gamma/2$ when solving the Klein-Gordon equation with an optical potential, ($E_{K^-} = m_{K^-} - B_{K^-}$). It is also related to the imaginary part of the potential by the overlap integral of $\mathrm{Im}\, V_{K^-}$ and $|\psi|^2$,

$$\Gamma = -2 \frac{\int \mathrm{Im}\, V_{K^-} \, |\psi|^2 \, d\vec{r}}{\int [1 - (B_{K^-} + V_{\mathrm{C}})/\mu_K] \, |\psi|^2 \, d\vec{r}}$$

where B_{K^-}, V_{C} and μ_K are the K^- binding energy, Coulomb potential and reduced mass, respectively, and ψ is the K^- wave function of the particular state concerned.

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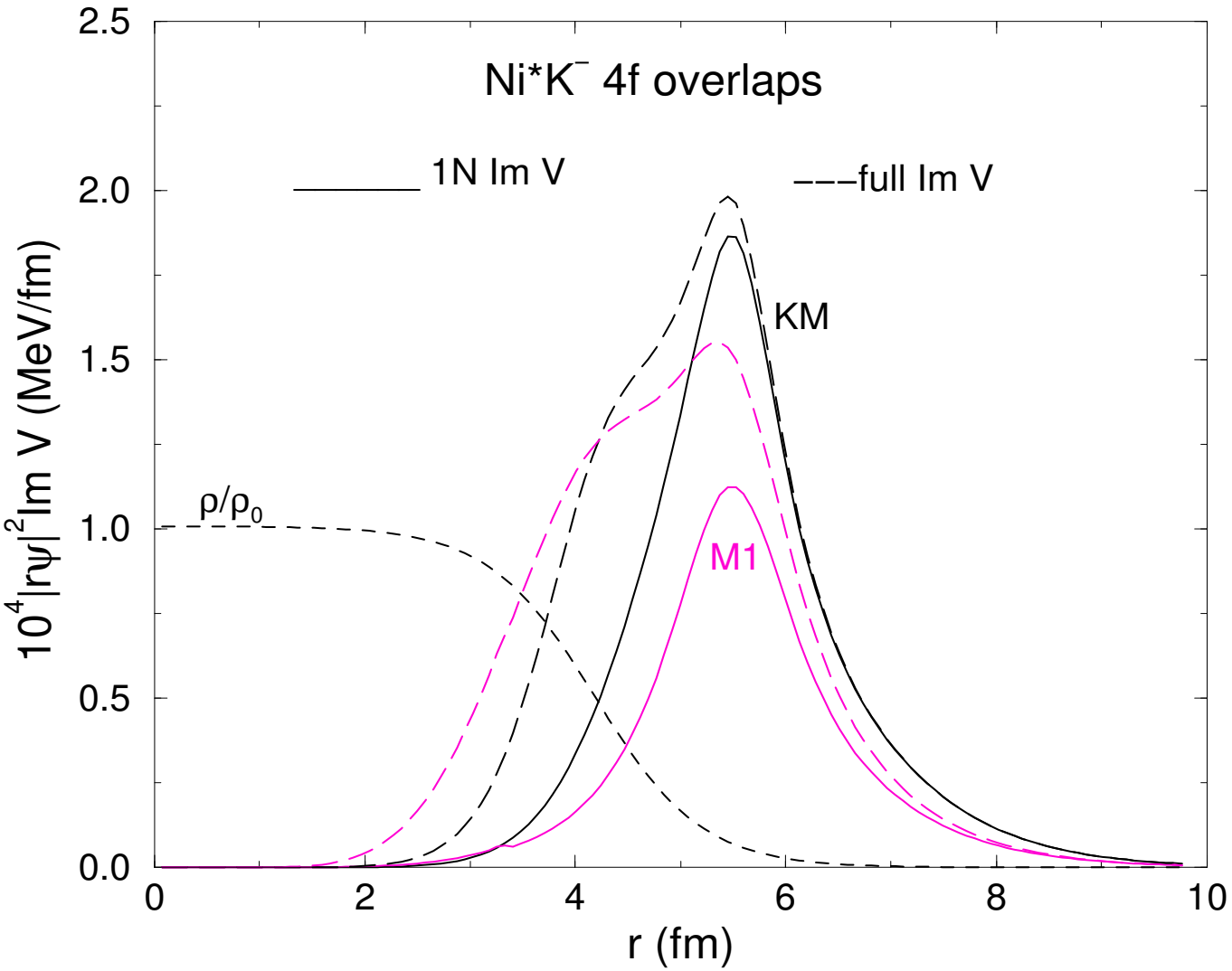
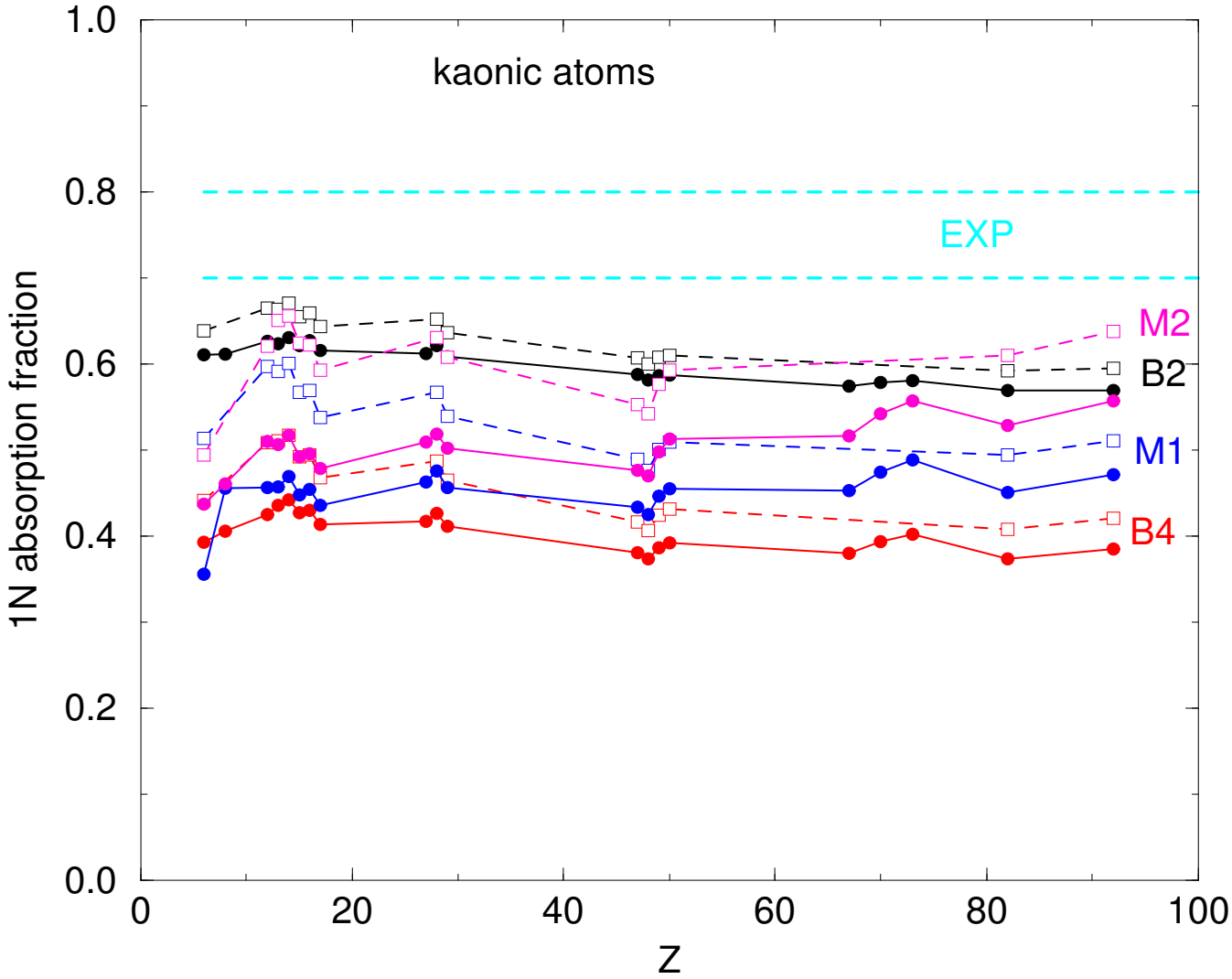
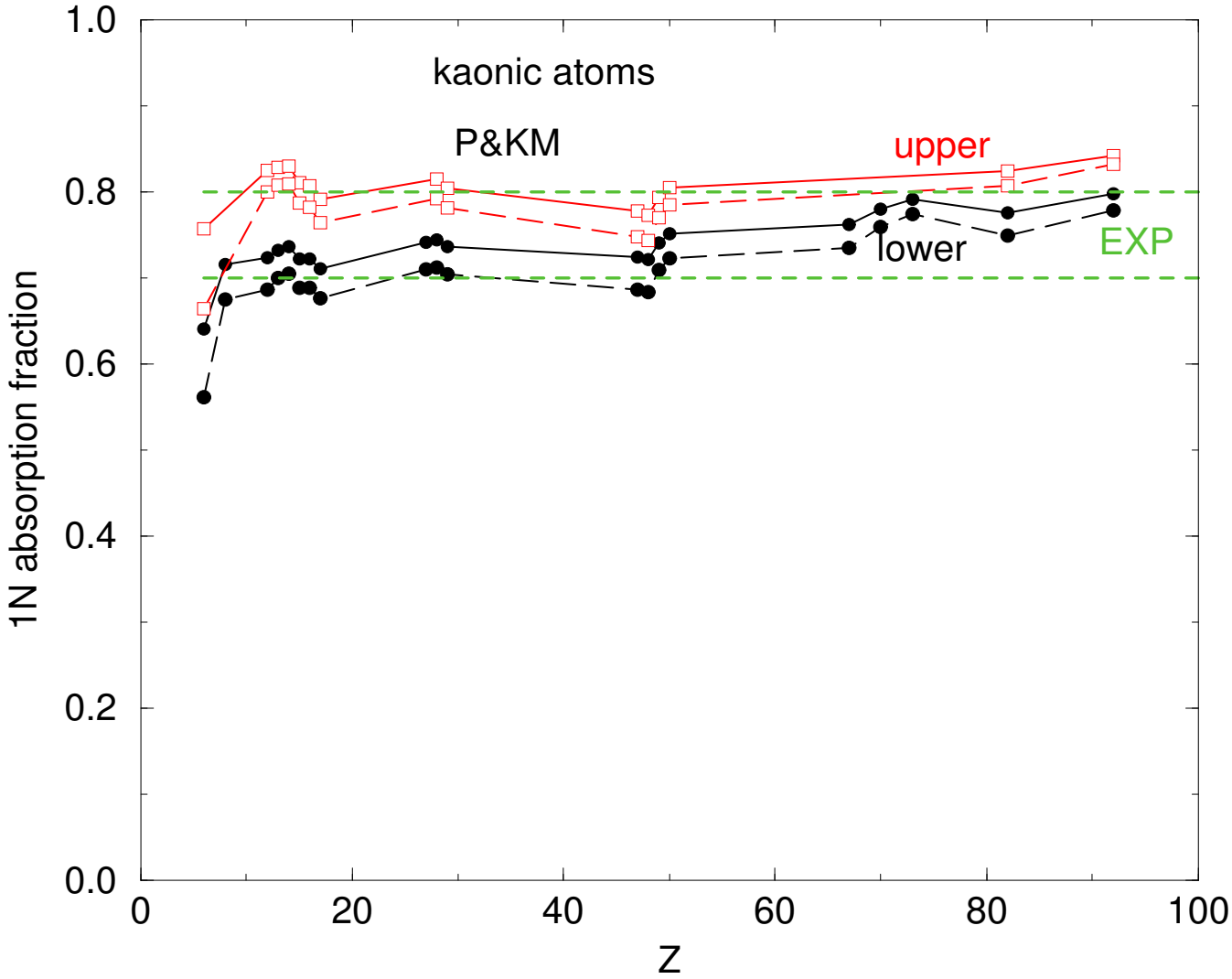
where B_{K^-}, V_{C} and μ_K are the K^- binding energy, Coulomb potential and reduced mass, respectively, and ψ is the K^- wave function of the particular state concerned.

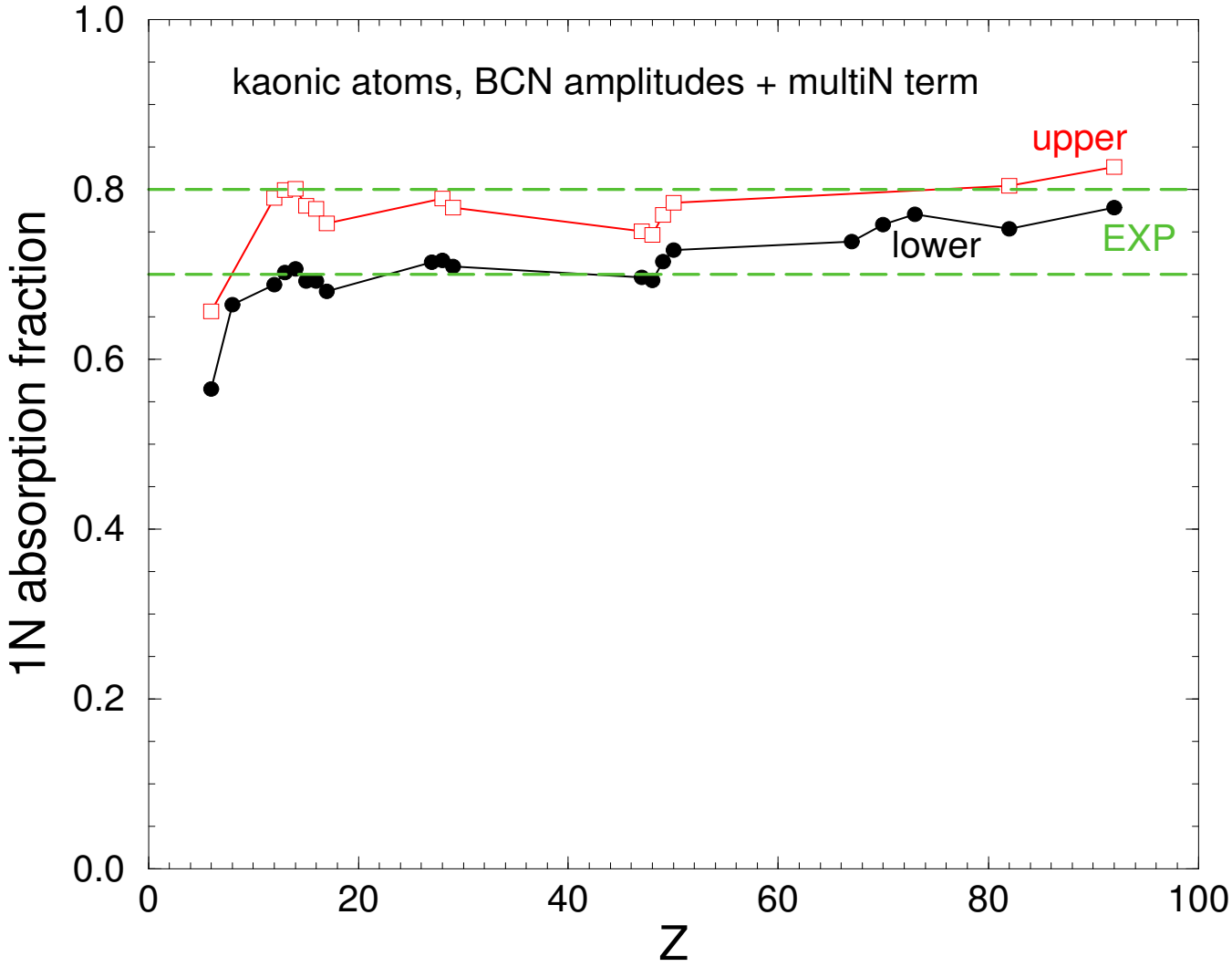
When the *best fit* optical potential is $V^{(1)}_{K^-} + V^{(2)}_{K^-}$, the sum of a single-nucleon part and a multinucleon part, it is straight forward to calculate the fraction of single-nucleon absorptions, separately for any nucleus and for any specific kaonic atom state.

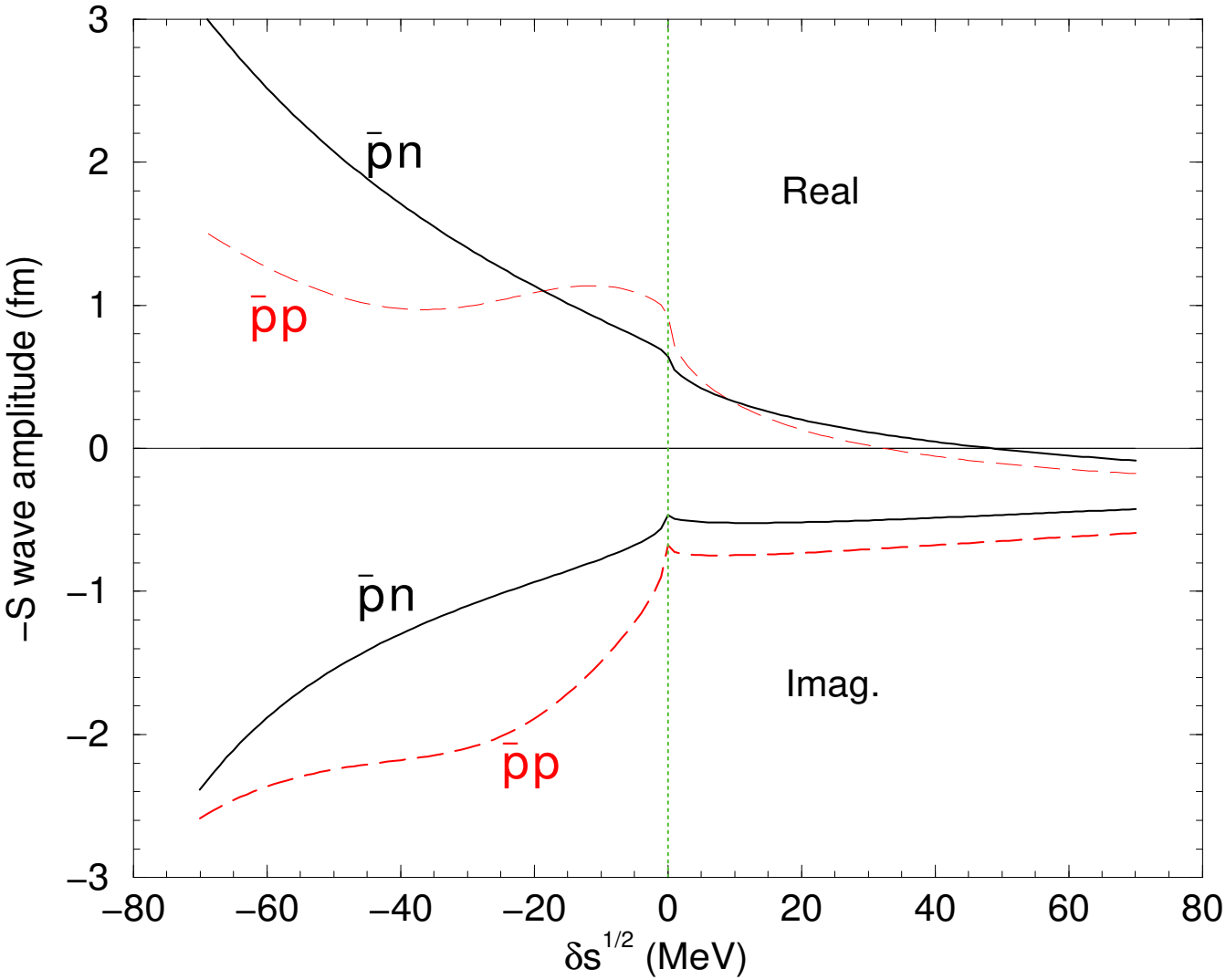


single N absorption fraction $\neq$ Im(VKN)/[Im(VKN)+Im(VKNN)]

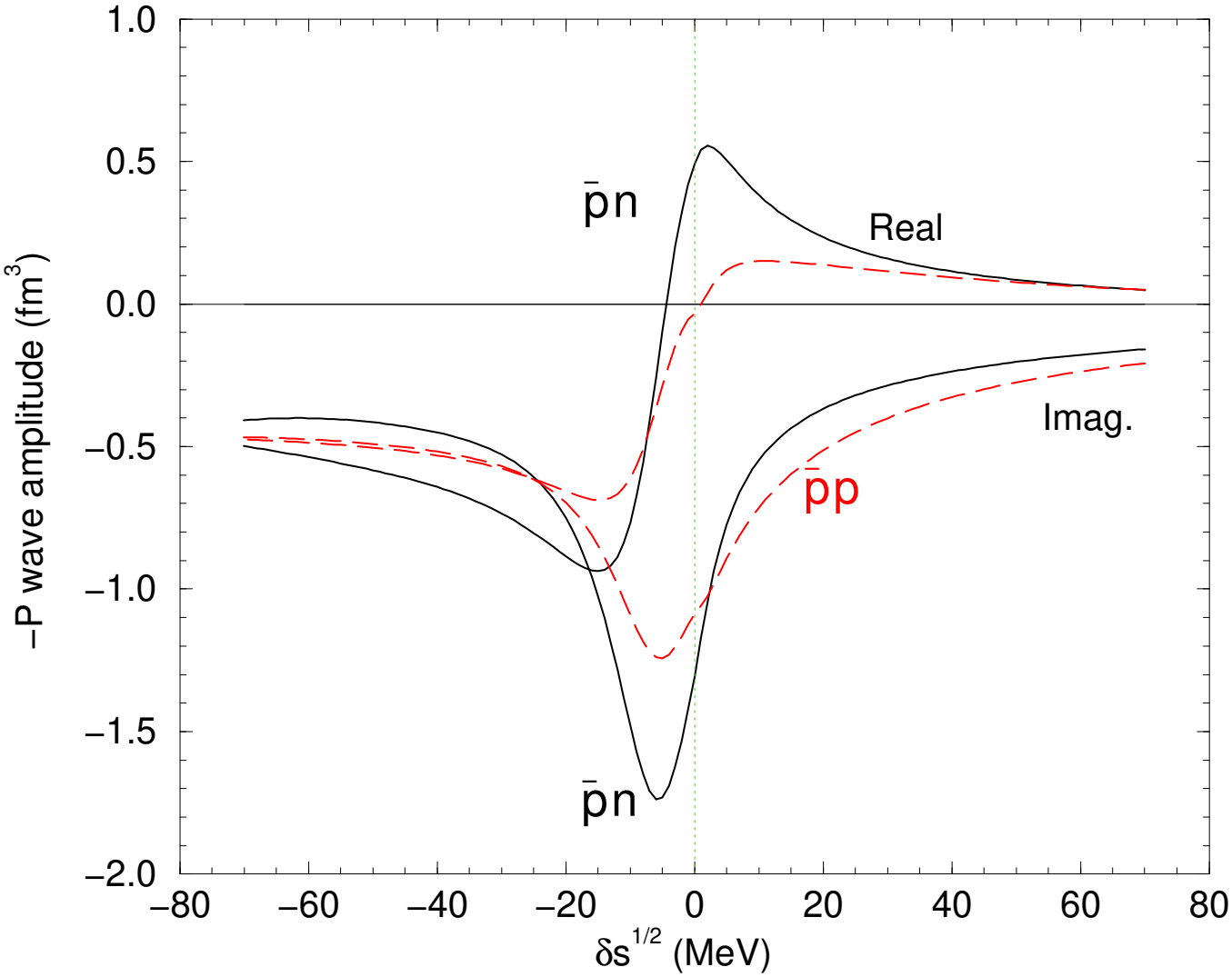

kaonic atoms
EXP
M2
B2
M1
B4
1N absorption fraction
Z
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100


kaonic atoms
P&KM
upper
lower
EXP
1N absorption fraction
Z
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100


kaonic atoms, BCN amplitudes + multiN term
upper
lower
EXP
1N absorption fraction
Z
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100



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.

Summary

- Modern $\bar{K}$-nucleon scattering amplitudes are unable to lead to acceptable optical potentials for kaonic atoms.
- Conventional χ^2 fits of additional phenomenological term lead to good fits but unacceptable uncertainties of parameters.
- Monte Carlo methods achieve significantly improved accuracies for the phenomenological parameters.
- Based on single-nucleon absorption fractions one can select the Kyoto-Munich (KM), Prague (P) and the Barcelona (BCN) amplitudes.
- For the first time one may get empirically the part of the optical potential that represent multinucleon interactions.