Remarks on the Nuclear Shell-Correction Method

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Introduction

In the macroscopic-microscopic method the nuclear binding energy consists of three parts:

$$\boldsymbol{E(Z,A;\mathrm{def}) = E_{\mathrm{mac}}(Z,A;\mathrm{def}) + E_{\mathrm{shell}}(Z,A;\mathrm{def}) + E_{\mathrm{pair}}(Z,A;\mathrm{def})} \ ,$$

The pairing energy $\boldsymbol{E_{\mathrm{pair}}}$ is usually evaluated in the (projected or unprojected) BCS approximation, while the shell energy $\boldsymbol{E_{\mathrm{shell}}}$ is the sum of the proton and neutron contributions

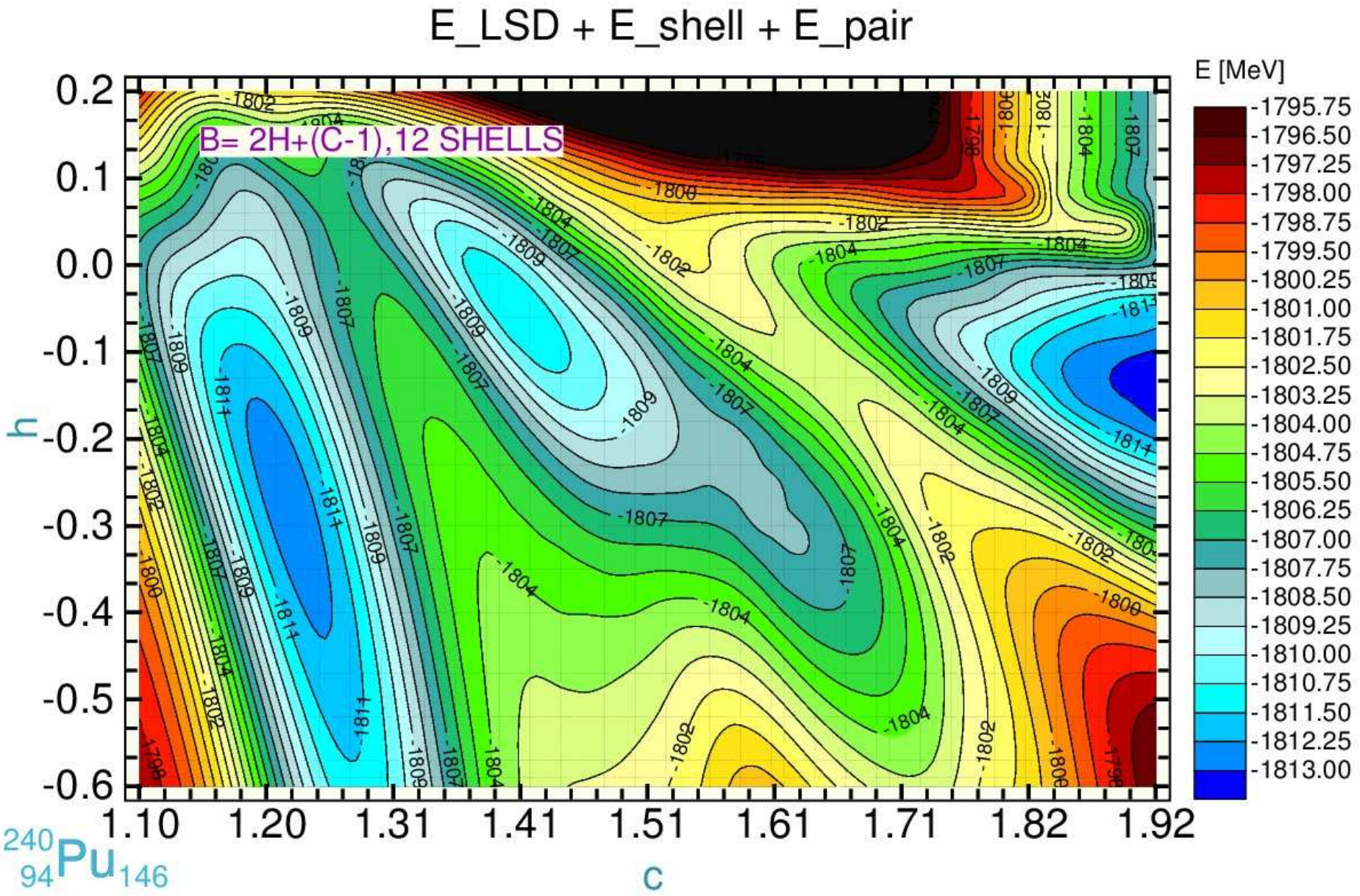
$$\boldsymbol{E_{\mathrm{shell}}(Z,A;\mathrm{def}) = E^{p}_{\mathrm{shell}}(Z;\mathrm{def}) + E^{n}_{\mathrm{shell}}(A-Z;\mathrm{def})} \ .$$

The shell energy of the one kind of particles is equal to the difference

$$\boldsymbol{E_{\mathrm{shell}} = \sum_{i=1}^{\mathcal{N}} e_i - \tilde{E}(\mathcal{N})} \ ,$$

where $\boldsymbol{\mathcal{N}}$ is the number of particles in the system and $\boldsymbol{\tilde{E}}$ is the smooth part of the total single-particle energy. In the following two different methods of evaluating of this smoothed part will be presented.

Example of the potential energy surface



Gauss-Hermite folding

Let $j_n(x, x')$ be a symmetric weight function which has the following properties:

$$\int_{-\infty}^{+\infty} j_n(x, x')\, dx = 1 \quad \text{and} \quad P_k(x) = \int_{-\infty}^{+\infty} P_k(x')\, j_n(x, x')\, dx' \ ,$$

where $P_k(x)$ is an arbitrary polynomial of the order k.

Let us assume that an unknown function $y(x)$ is tabulated in points (x_i, y_i), where $i = 1, 2, ..., N$.
With each point (x_i, y_i) one can associate a function:

$$\tilde{y}_i(x) = \int_{-\infty}^{+\infty} y_i\, \delta(x' - x_i)\, j_n(x, x')\, dx' = y_i\, j_n(x, x_i) \ .$$

Obviously, the integral of the function $\tilde{y}_i(x)$ is:

$$\int_{-\infty}^{+\infty} \tilde{y}_i(x)\, dx = y_i \ .$$

Gauss-Hermite folding, cont.

Let us construct the following function:

$$\tilde{y}(x) = \sum_{i=1}^{N} w_i \, \tilde{y}_i(x) \ .$$

The function $\tilde{y}(x)$ is an approximation of $y(x)$ if the weights w_i are determined from the assumption:

$$\sum_{i=1}^{N} y(x_i) \, \Delta x_i = \int_{-\infty}^{+\infty} \tilde{y}(x) \, dx = \sum_{i=1}^{N} w_i \, y_i \ ,$$

where $\Delta x_i = \frac{1}{2} \, (x_{i+1} - x_{i-1})$. This implies that $w_i = \Delta x_i$.
Finally the folded function $\tilde{y}(x)$ is given by

$$\boxed{\tilde{y}(x) = \sum_{i=1}^{N} y_i \, \Delta x_i \, j_n(x, x_i) \ .}$$

Examples of folding functions

a) Dirac delta: $j(x,x') = \delta(x-x')$, where $\int_{-\infty}^{+\infty} \delta(x-x')dx' = 1$,

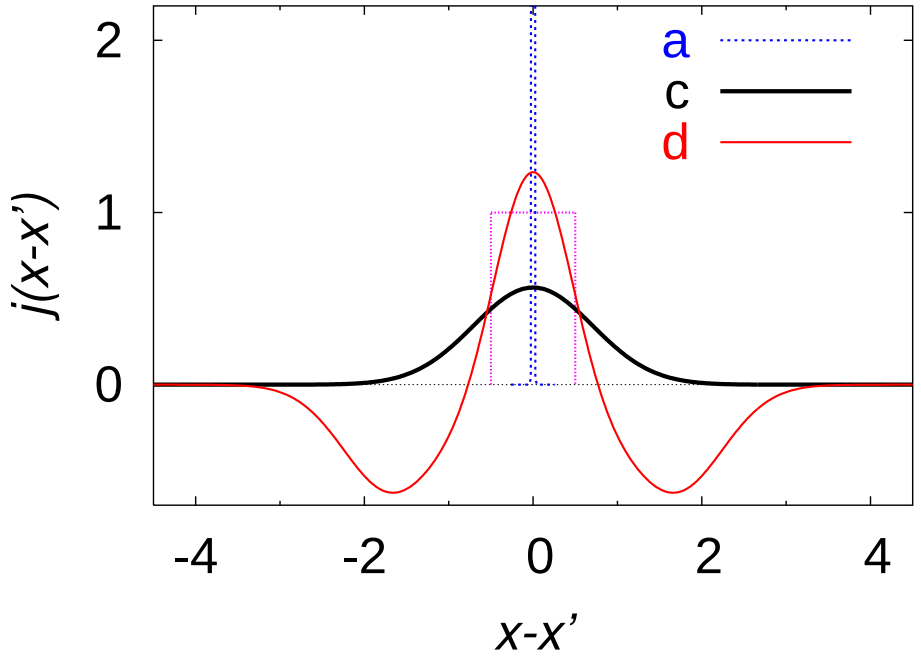
b) Rectangular distribution (with $\theta(x)$ being Heaviside step function):

$$j(x,x') = \frac{1}{2a}\{\theta[x'-(x-a)] - \theta[x'-(x+a)]\},$$

c) Gauss function: $j(x,x') = \frac{1}{\gamma\sqrt{\pi}}\,\mathrm{e}^{-(\frac{x-x'}{\gamma})^2}$,

d) Modified 6th order Gauss-Hermite function:

$$j_n(x,x') = \frac{1}{\gamma\sqrt{\pi}}\,\mathrm{e}^{-(\frac{x-x'}{\gamma})^2}\left[\frac{35}{16} - \frac{35}{8}(\frac{x-x'}{\gamma})^2 + \frac{7}{4}(\frac{x-x'}{\gamma})^4 - \frac{1}{6}(\frac{x-x'}{\gamma})^6\right].$$



Properties of the harmonic oscillator spectrum

The spherical harmonic oscillator $\widehat{H} = \frac{-\hbar^2}{2m}\Delta + \frac{1}{2}m\omega_0^2 r^2$ eigenenergies $e_n = (n + \frac{3}{2})\,\hbar\omega_0$ are degenerated $\mathbf{deg}_n = \frac{1}{2}(n+1)(n+2) \times 2$.

According to the BM-book this degeneracy can be approximated by

$$\mathbf{deg}_n \approx \left(n + \frac{3}{2}\right)^2 = \left(\frac{e_n}{\hbar\omega_0}\right)^2 \quad .$$

The total number of particles ($\mathcal{N}$) occupying all shells up to $n = \mathrm{N}$ is

$$\mathcal{N} = \sum_{n=0}^{\mathrm{N}} \mathbf{deg}_n = \frac{1}{3}(\mathrm{N}+1)(\mathrm{N}+2)(\mathrm{N}+3) \ ,$$

what can be approximated by:

$$\mathcal{N}(\mathrm{N}) \approx \frac{1}{3}(\mathrm{N} + \frac{3}{2})^3 = \frac{1}{3}\left(\frac{e_{\mathrm{N}}}{\hbar\omega_0}\right)^3 \quad .$$

This equation can serve as the average relation between the number of particles and their energies:

$$\mathcal{N}(e) = \tfrac{1}{3}\left(\tfrac{e}{\hbar\omega_0}\right)^3 \ , \quad \text{or} \quad e = (3\mathcal{N})^{1/3}\hbar\omega_0 \ .$$

Last equation leads to the known expression for the average density of s.p levels:

$$g = \frac{\partial \mathcal{N}}{\partial e} = \frac{e^2}{(\hbar\omega_0)^3} = \frac{(3\,\mathcal{N})^{2/3}}{\hbar\omega_0} \ .$$

The sum (E) of the energies of all occupied single-particle levels is

$$E = \sum_{n=0}^{N} e_n \deg_n = \hbar\omega_0 \sum_{n=0}^{N} (n + \frac{3}{2})\,(n+1)\,(n+2)$$

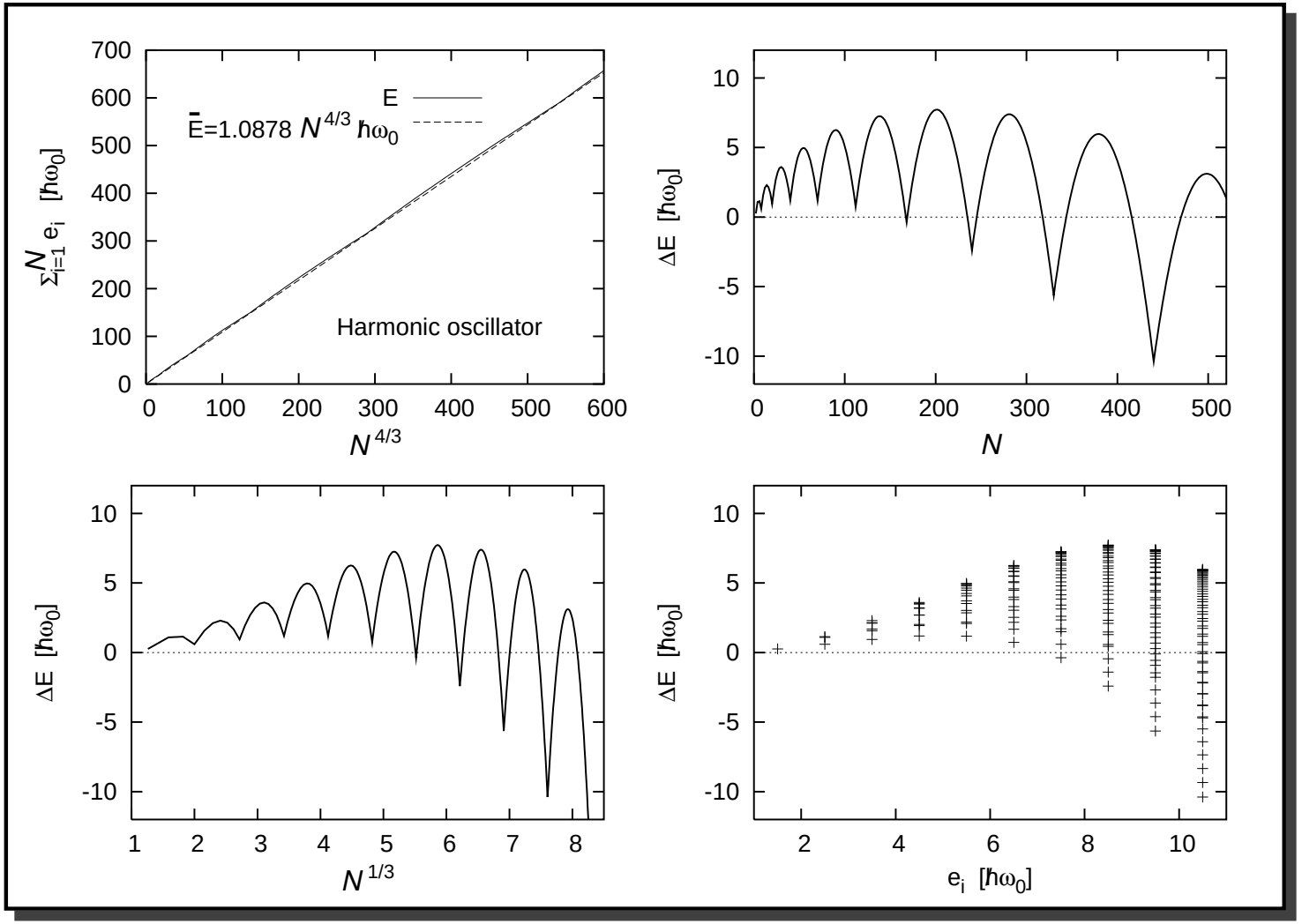
and can be approximated by the integral

$$\overline{E} \approx \int_0^{\mathcal{N}} e(\mathcal{N}')\, d\mathcal{N}' \ .$$

Inserting here the relation $e = (3\mathcal{N})^{1/3}\hbar\omega_0$ one obtains the sum rule:

$$\overline{E} = \overline{\left(\sum_{i=1}^{\mathcal{N}} e_i\right)} \approx \frac{3^{4/3}}{4}\mathcal{N}^{4/3}\hbar\omega_0 \ .$$

Sum of energies of nucleons which occupy the harmonic oscillator levels is proportional to the 4/3 power of the total number of particles in the system.

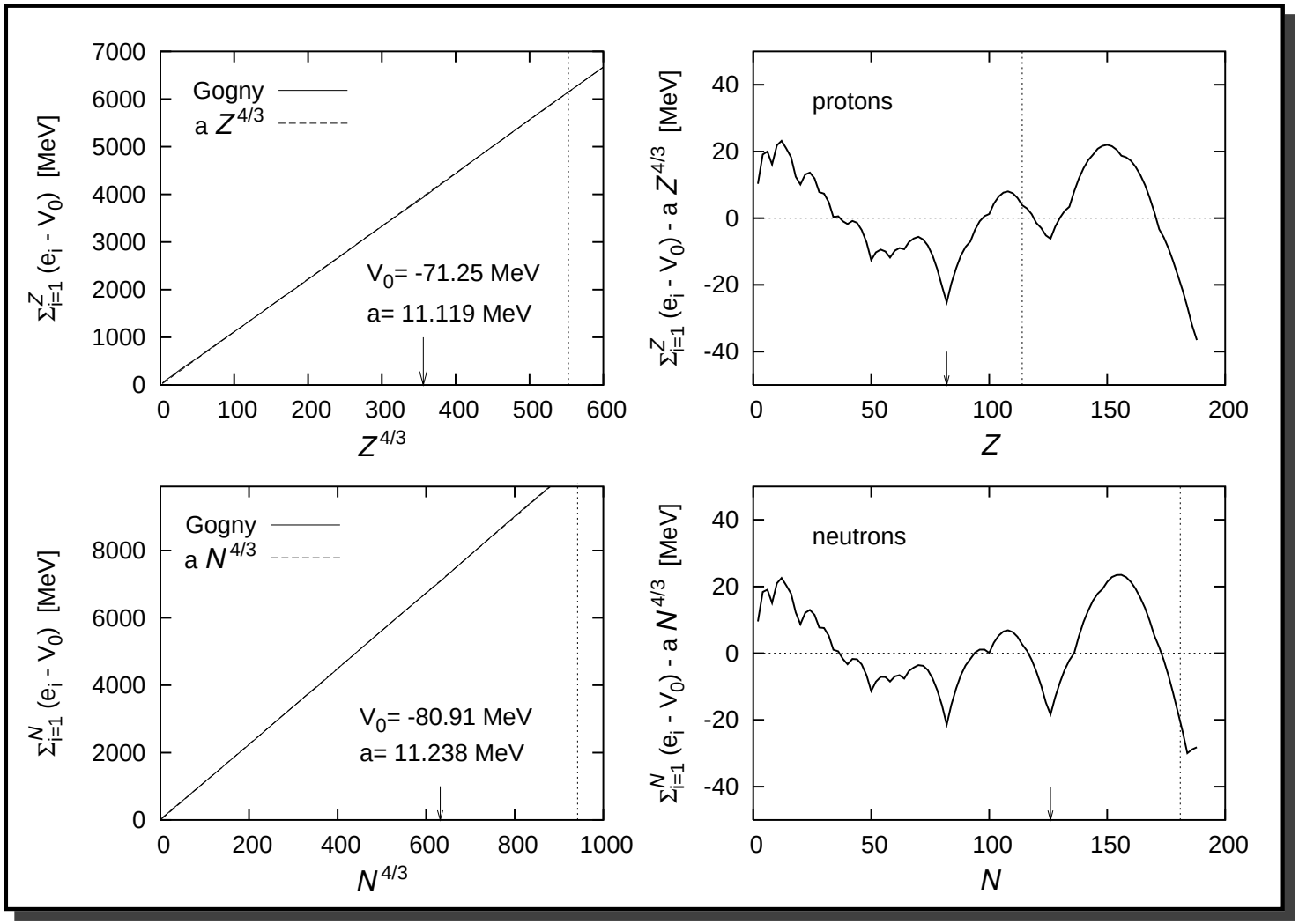


The average distance between the HO major shells can be approximated by:

$$\mathcal{N}_{n+1}^{1/3} - \mathcal{N}_{n}^{1/3} = \frac{1}{3^{1/3}} \frac{e_{n+1} - e_n}{\hbar\omega_0} = 3^{-1/3} \ .$$

Assuming that the minimum of the s.p. potential corresponds to V_0 one can get a more general relation: $\overline{E} = \left(\sum_{i=1}^{\mathcal{N}} e_i \right) \approx a\,\mathcal{N}^{4/3} + V_0\,\mathcal{N}$.

The above relation is even valid for the ^{208}Pb single particle spectrum obtained within the HFB theory with the **Gogny force:**



Average of the sum of the s.p. energies

Let us define a discrete sample of data:

$$S_n = \sum_{i=1}^{n} e_i - \overline{E}(n) = \sum_{i=1}^{n} e_i - a\, n^{4/3} - V_0\, n \ .$$

The parameters a and V_0 can be fixed by minimizing the square deviation of the energy sum and $\overline{E}$:

$$\sum_{n=1}^{\mathcal{N}_{max}} S_n^2 = \min \ ,$$

Using the Gauss-Hermite folding one obtains the average value of S_n:

$$\tilde{S}_{\mathcal{N}} = \frac{1}{\gamma\sqrt{\pi}} \sum_{n=2,4}^{\mathcal{N}_{max}} \frac{2}{3\, n^{2/3}}\, S_n\, \mathrm{e}^{-\left(\frac{\mathcal{N}^{1/3}-n^{1/3}}{\gamma}\right)^2} f_6\left(\frac{\mathcal{N}^{1/3}-n^{1/3}}{\gamma}\right) \ ,$$

where $f_6(x) = \frac{35}{16} - \frac{35}{8}x^2 + \frac{7}{4}x^4 - x^6$ is the correction polynomial.

The smoothed energy over particle number of an even or odd $\mathcal{N}$ system is

$$\tilde{E}(\mathcal{N}) = \tilde{S}_{\mathcal{N}} + a\mathcal{N}^{4/3} + V_0\mathcal{N} \ .$$

Strutinsky smoothed energy

In this method one evaluates first the smooth s.p. particle level density $\tilde{g}(e)$ by folding the discrete spectrum of the eigenenergies e_i

$$g(e) = \sum_i \delta(e - e_i) \quad \longrightarrow \quad \tilde{g}(e) = \frac{1}{\gamma s} \sum_i j\left(\frac{e - e_i}{\gamma s}\right) ,$$

where $j(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} (\frac{35}{16} - \frac{35}{8} x^2 + \frac{7}{4} x^4 - x^6)$.

According to Strutinsky the smoothed s.p. energy is given by the integral

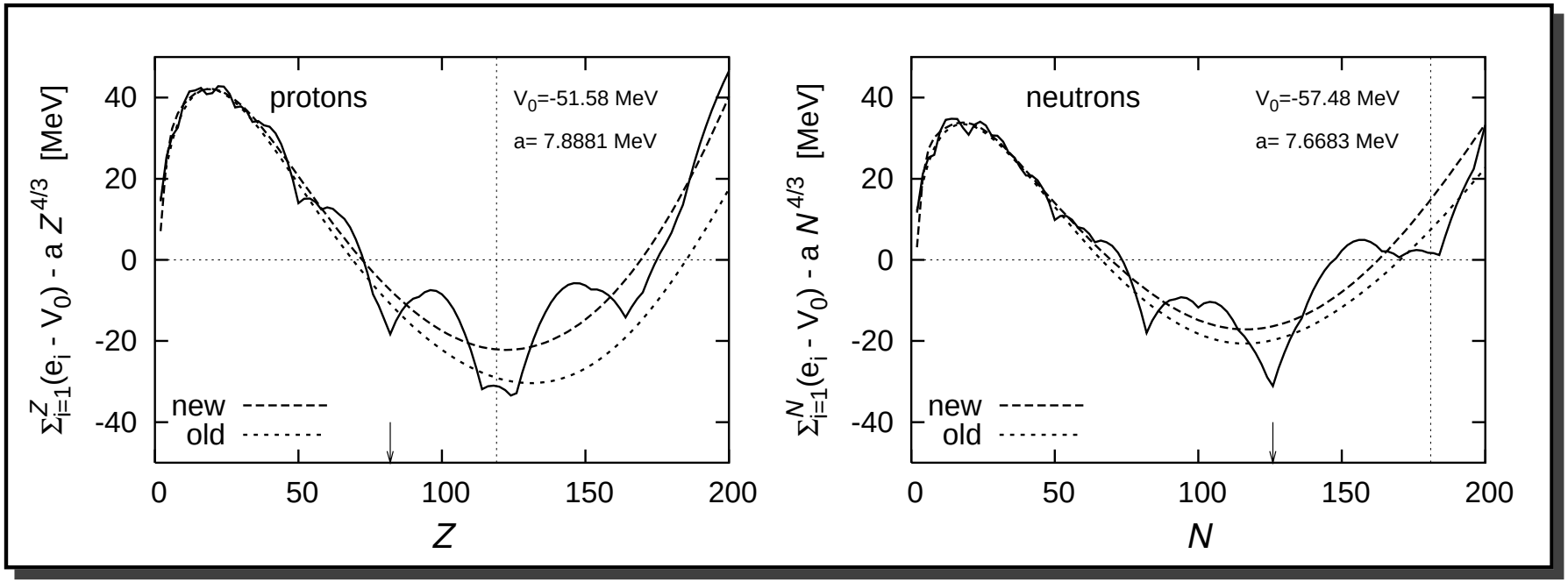
$$\tilde{E}_{\mathrm{Str}} = \int_{-\infty}^{\lambda} 2\, e\, \tilde{g}(e)\, de , \qquad \mathcal{N} = \int_{-\infty}^{\lambda} 2\, \tilde{g}(e)\, de .$$

where λ is the Fermi energy in the system without the shell structure.

Note: The Strutinsky energy $\tilde{E}_{\mathrm{Str}}$ is not equal to the average sum of the s.p. energies $\tilde{E}$ and it corresponds to the system which only conserves on average (not exactly) the number of nucleons.

Comparison of the both smoothed energies

Sum of the s.p. energies $\boldsymbol{E}$ obtained with the Saxon-Woods potential [a] for ^{208}Pb and its smooth part $\tilde{\boldsymbol{E}}$ evaluated by folding in the $\mathcal{N}$-space (new) as well as that $\tilde{\boldsymbol{E}}_{\mathbf{Str}}$ obtained within the Strutinsky method (old). From all the curves the average HO trend is subtracted. The arrows indicate positions of the Fermi energies and the vertical lines mark the end of the bound spectra.



[a] Chepurnov parameters

Difference between the both types of smoothing

The sum of the single-particle energies is approximated roughly by

$$\overline{\left(\sum_{i=1}^{\mathcal{N}} e_i\right)} \approx a\,\mathcal{N}^{4/3} + V_0\,\mathcal{N}\ ,$$

Let us assume that $\mathcal{N}_i$ and $\mathcal{N}_{i+1}$ are two neighboring magic numbers. The Strutinsky prescription for the half filled shell $\mathcal{N} = (\mathcal{N}_{i+1} - \mathcal{N}_i)/2$ is

$$\tilde{E}_{\rm Str} = a\mathcal{N}^{4/3} + V_0\mathcal{N}\ .$$

The average in the $\mathcal{N}$-space is given by the integral

$$\tilde{E} = \frac{1}{\Delta}\int_{\mathcal{N}-\Delta/2}^{\mathcal{N}+\Delta/2} (an^{4/3} + V_0 n)\,dn\ ,$$

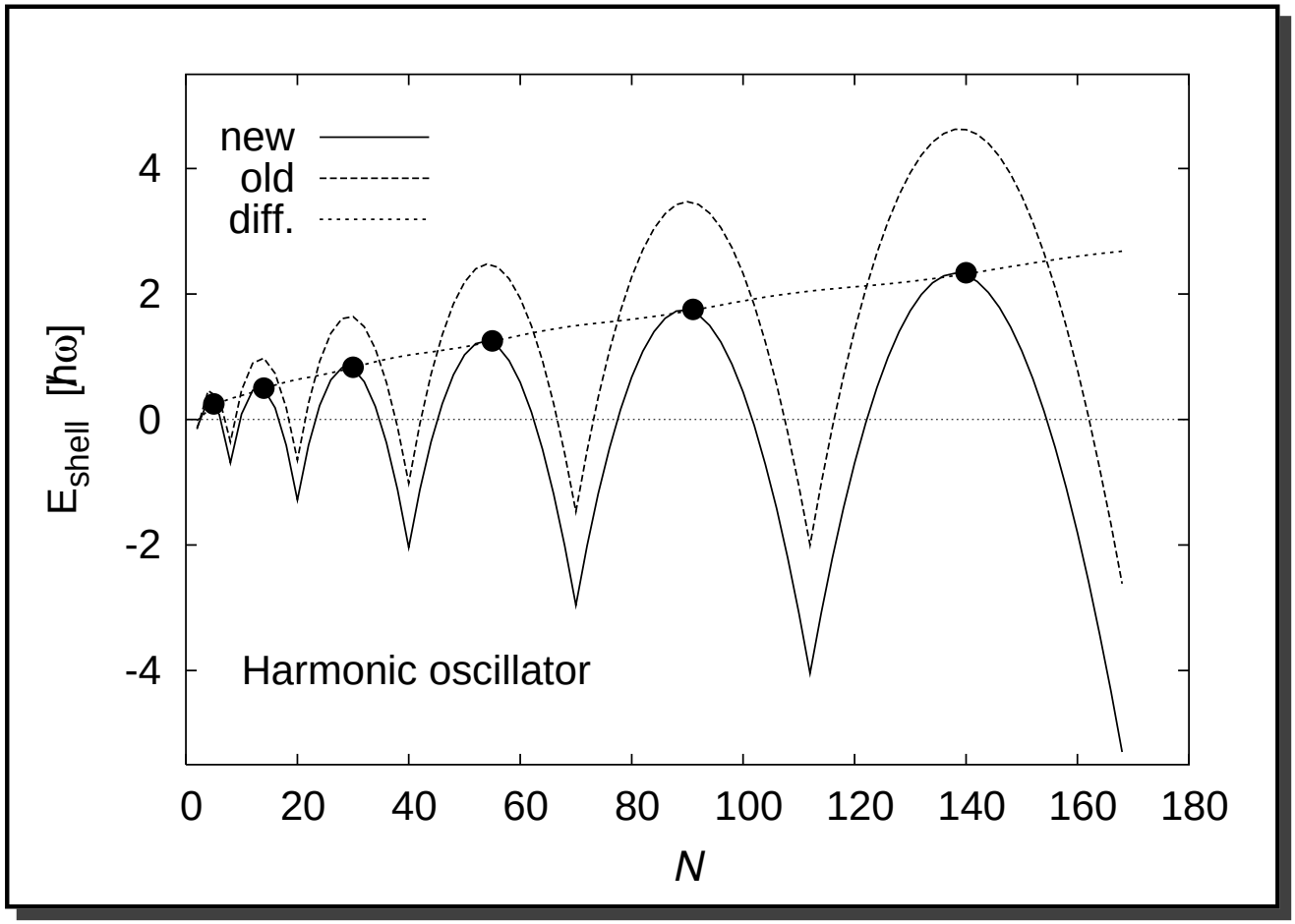
where $\Delta = \mathcal{N}_{i+1} - \mathcal{N}_i$ is the degeneracy of the level.
So, the difference between the both smoothed energies is

$$\boxed{\tilde{E} - \tilde{E}_{\rm Str} \approx \tfrac{1}{54}\,a\,\tfrac{\Delta^2}{\mathcal{N}^{2/3}}\ ,}$$

where $a \approx 3^{4/3}/4\,\hbar\omega_0$.

Spherical harmonic oscillator case

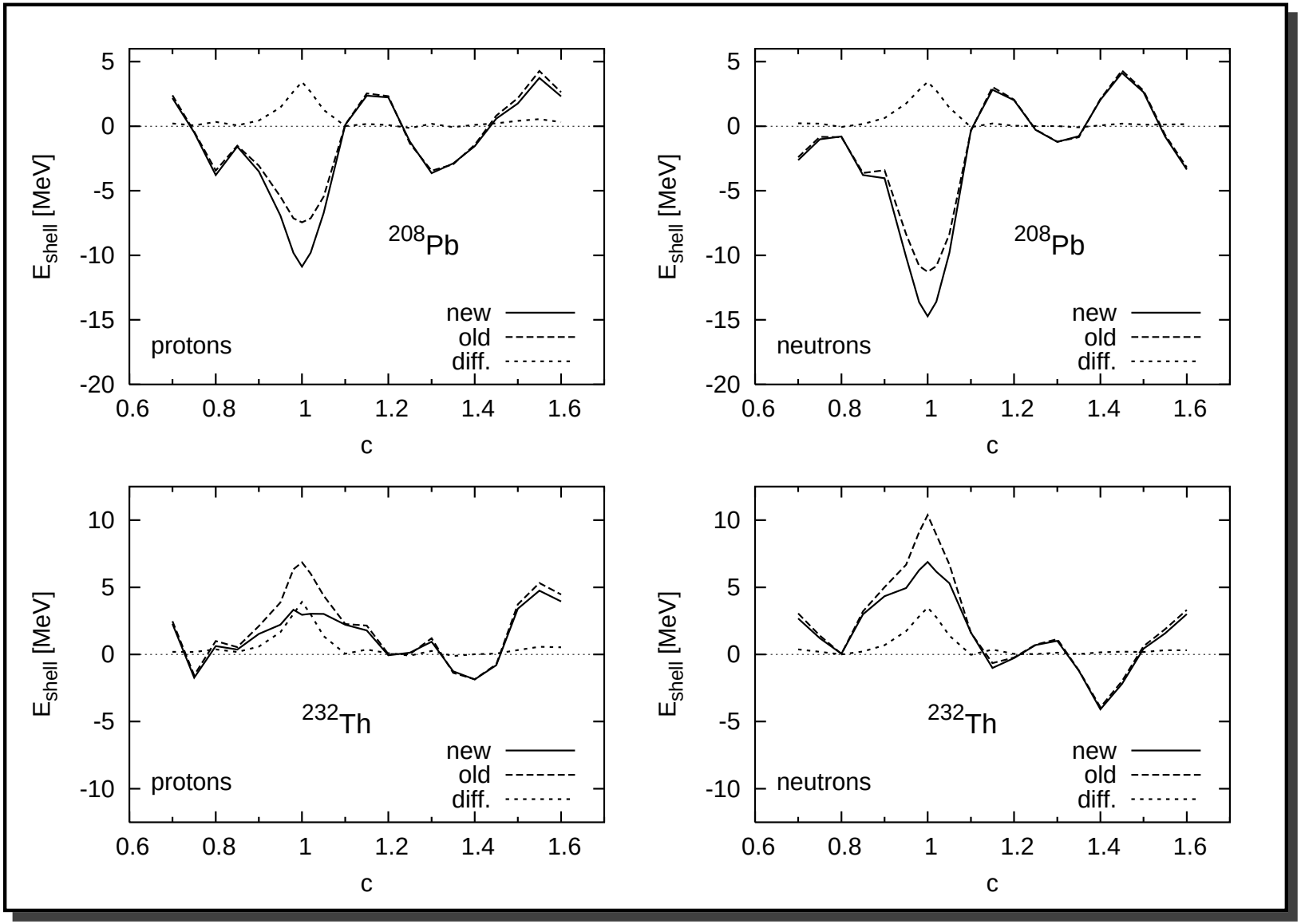
The shell energy $\boldsymbol{E_{\mathbf{shell}} = \sum_{i=1}^{N} e_i - \tilde{E}}$ for the spherical harmonic oscillator single-particle levels evaluated in the both approaches



The difference between the old and new shell energies is marked by the dots while its estimates by a simple formula is represented by the black points.

Deformed Saxon-Woods potential case

a

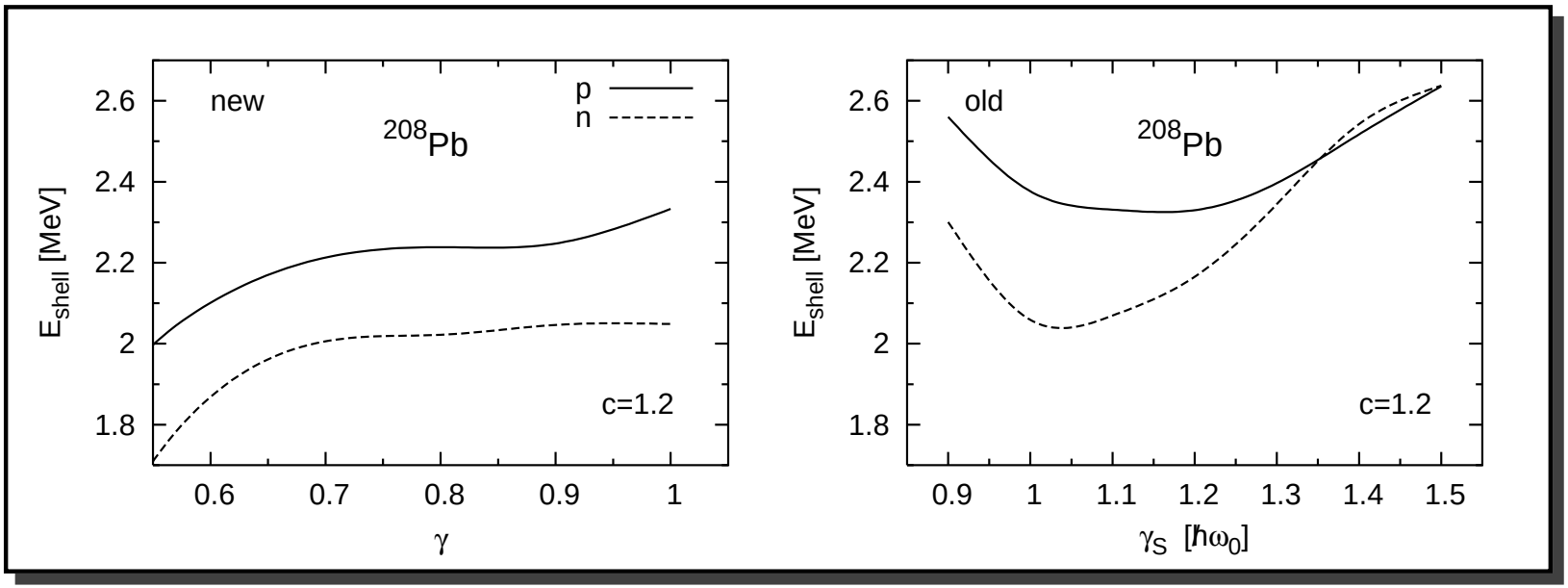


[a]The deformation c is the relative elongation defined as in the Funny-Hills paper.

Plateau condition

The proton and neutron shell energies $E_{\mathbf{shell}}$ obtained with the Saxon-Woods potential for ^{208}Pb at deformation $c = 1.2$ with the smooth part $\tilde{E}$ evaluated by folding in the $\mathcal{N}$-space (l.h.s.) and that $\tilde{E}_{\mathbf{Str}}$ obtained within the Strutinsky method (r.h.s.) as function of the smearing parameters γ (dimensionless) and γ_S (in $\hbar\omega_0$).

a



[a]The deformation c is the relative elongation defined as in the Funny-Hills paper.

Deformed harmonic oscillator case

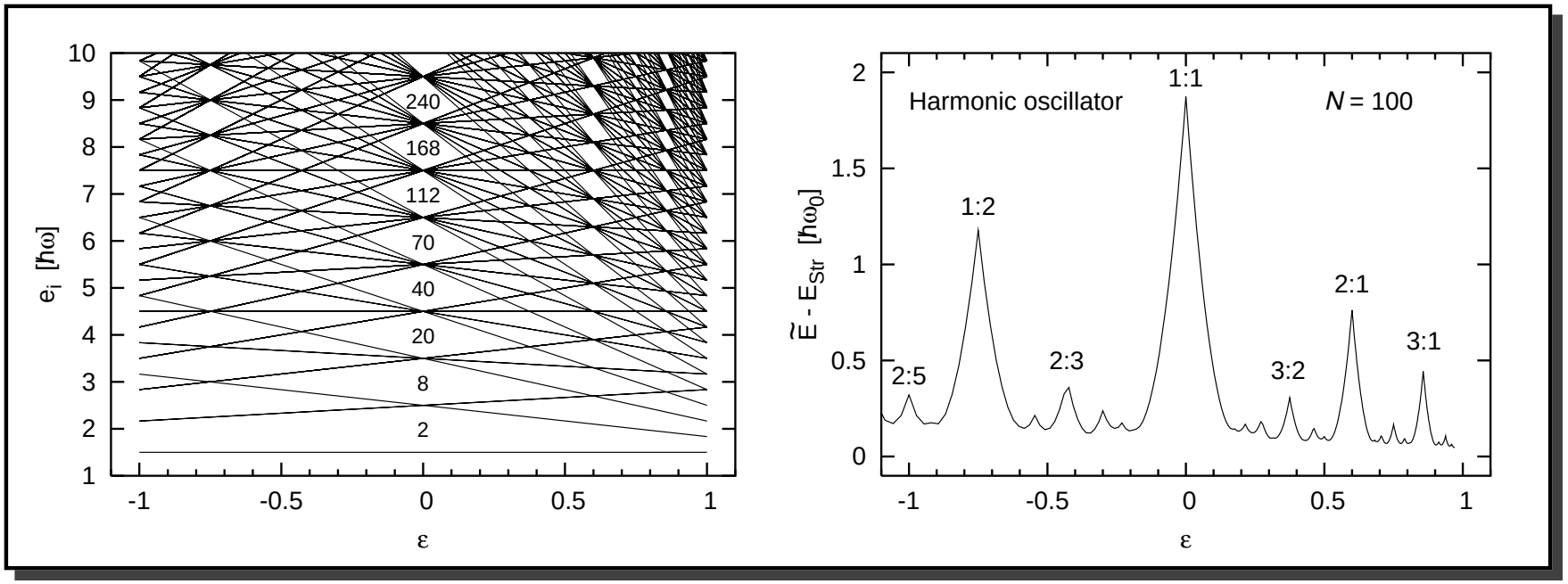
The eigenenergies of the axially deformed harmonic oscillator

$$\widehat{H} = \frac{-\hbar^2}{2m}\Delta + \frac{1}{2}m\left[\omega_\perp^2(x^2+y^2) + \omega_z^2 z^2\right]$$

are

$$E_{n_\perp N_z} = \hbar\omega_\perp(n_\perp + 1) + \hbar\omega_z(n_z + \frac{1}{2}) \ .$$

[a]



The pikes are visible when the ratio of the HO frequencies $\omega_\perp/\omega_z$ is equal to the ratio of small integers.

[a] Here ε is the Nilsson quadrupole deformation and $\omega_\perp/\omega_z = (1+\varepsilon/3)/(1-2\varepsilon/3)$.

Summary and conclusions

- An alternative method of evaluating of the smooth part of the total single-particle energy is presented. One performs here the folding of the sums of nucleon energies in the particle number space, not in the energies of individual nucleons as it was done in the traditional Strutinsky method.
- The averaging in the $\mathcal{N}$-space is more consistent with the definition of the macroscopic energy which represents the average dependence on Z and A of the nuclear binding energy.
- The new shell energy is systematically smaller (by a couple MeV) than the old one for spherical nuclei (and some shape isomers) but for deformed nuclei systems the both energies are close each other.
- The difference between the smooth energies evaluated using the both averaging methods can serve as a tool to find semi-magic structure in the deformed nuclei.

'Technical' conclusions

- The sum of nucleon energies follows the harmonic oscillator sum rule.
- The new estimate of the smoothed energy is by a few MeV smaller than the Strutinsky one for nuclei with the large degeneracy of the s.p. levels, while for the non-degenerated systems they are close each other.
- The sum over $\mathcal{N}$ of the new estimates of the shell energies is close to zero for sufficiently large number of particles, while such a sum for the traditional Strutinsky shell correction grows systematically with $\mathcal{N}$ when the s.p. levels are degenerate.
- The amplitudes of the both shell energies are almost the same when the number of particle varies.
- The plateau condition for the $\mathcal{N}$ averaging is better fullfield than in the Strutinsky averaging over energy.
- The new estimates of the shell energy are more stable for the energy cut-off in the s.p. spectrum because one smoothes only the difference from the HO sum rule.

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Gauss-Hermite Approximation Formula

Let us consider an ensemble of N points $\{x_i\}$ distributed uniformly in the interval $[a, b]$. To each point x_i corresponds a point y_i, and we assume there exists a function $y(x)$ such that: $y_i = y(x_i)$.

The folded function $\widetilde{y}(x)$ is given by

$$\widetilde{y}(x) = \sum_{i=1}^{N} y_i \, \Delta x_i \, j_n(x, x_i) \ .$$

The Riemann integral of the function $y(x)$ between bounds a and b should be equal to the integral of $\widetilde{y}(x)$:

$$\int_a^b y(x)\, dx \approx \sum_{i=1}^{N} y(x_i)\, \Delta x_i = \int_{-\infty}^{\infty} \widetilde{y}(x)\, dx \ ,$$

where Δx_i is set to: $\Delta x_i = \frac{1}{2}\,(x_{i+1} - x_{i-1})$ with $x_0 = a$ and $x_{N+1} = b$ and

$$\int_{-\infty}^{\infty} j(x, x_i)\, dx = 1 \ .$$

Gauss-Hermite folding, cont.

The function $y(x)$ approximated by the Gauss-Hermite folding reads:

$$\widetilde{y}(x) = \frac{1}{\gamma\sqrt{\pi}} \sum_{i=1}^{N} y_i \, \Delta x_i \exp\left\{ -\left(\frac{x - x_i}{\gamma} \right)^2 \right\} f_n\left(\frac{x - x_i}{\gamma} \right) \ ,$$

where

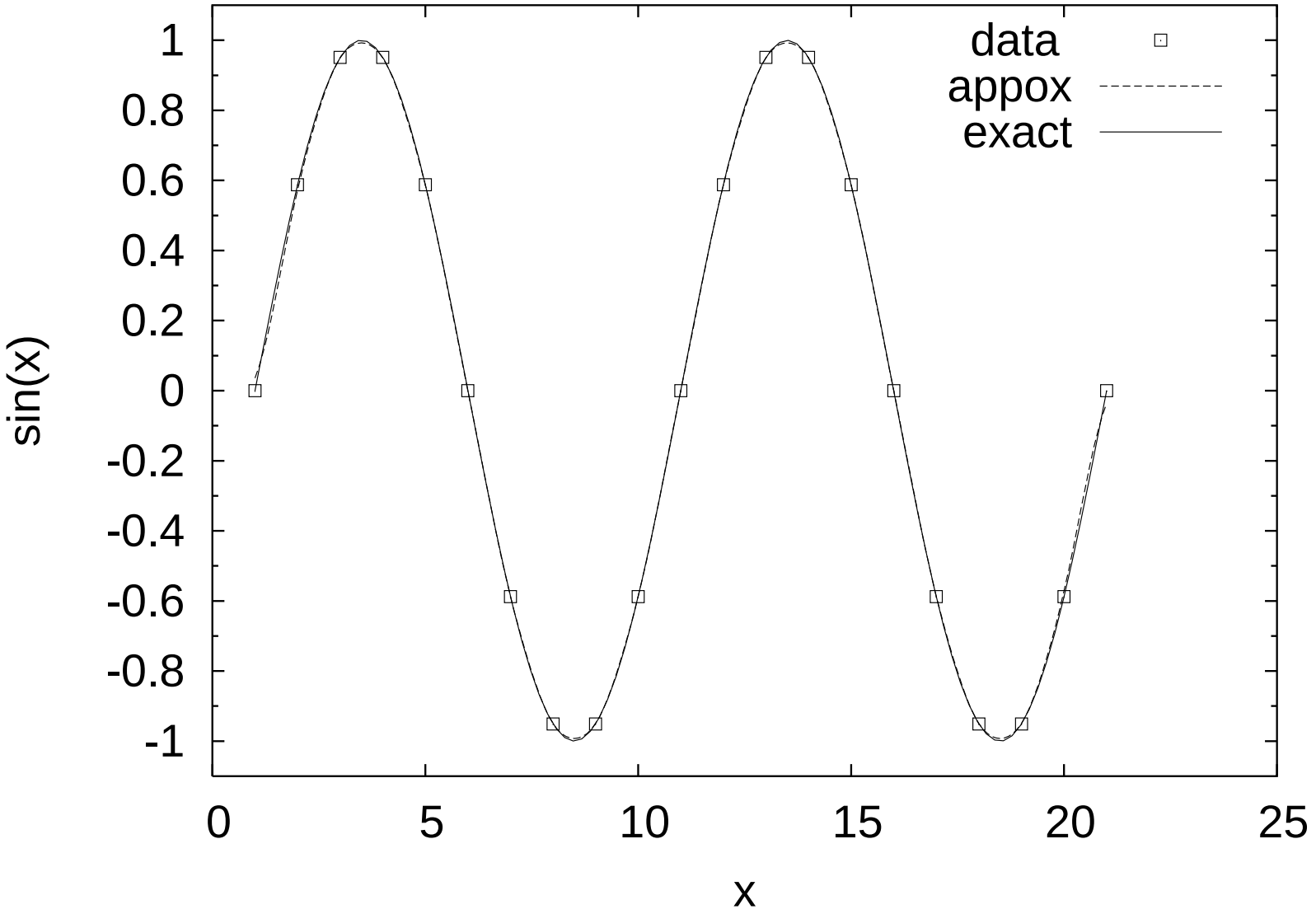
$$\begin{aligned} f_0(u) &= 1 \ , \\ f_2(u) &= \tfrac{3}{2} - u^2 \ , \\ f_4(u) &= \tfrac{15}{8} - \tfrac{5}{2}u^2 + \tfrac{1}{2}u^4 \ , \\ f_6(u) &= \tfrac{35}{16} - \tfrac{35}{8}u^2 + \tfrac{7}{4}u^4 - \tfrac{1}{6}u^6 \ , \end{aligned}$$

The polynomials $f_n(u)$ are found from the Strutinsky requirement

$$P_k(x) = \int_{-\infty}^{+\infty} P_k(x') \, j_n(x, x') \, dx' \ ,$$

where $k \leq n$ are the even natural numbers and P_k is an arbitrary polynomial of the order k.

Example of one-dimensional approximation



The sinus function approximated by the $\mathbf{2^{nd}}$ order Gauss-Hermite folding.

Multidimensional case

Let assume that the data points are stored in a m-dimensional array $Y[1:N_1, 1:N_2, ..., 1:N_m]$ which corresponds to the ordinates $X_i[1:N_i]$, where $i = 1, 2, ..., m$.

The ensemble of the Hermite polynomials $H_i(x)$ forms a complete basis of orthogonal functions in which an arbitrary m-dimensional function $F(\vec{r}) \equiv F(x_1, x_2, ..., x_m)$ can be expanded

$$F(x_1, x_2, ..., x_m) = \sum_{i_1=0}^{\infty} \sum_{i_2=0}^{\infty} .... \sum_{i_m=0}^{\infty} C_{i_1 i_2 ... i_m} H_{i_1}(x_1) H_{i_2}(x_2) ... H_{i_m}(x_m) \ .$$

It means that one can perform independent foldings in each x_i coordinate. So, the approximation of the function $Y(X)$ can be written as:

$$\widetilde{Y}(x_1, x_2, \ ... \ , x_m) = \sum_{i_1=0}^{N_1} \Delta x_{i_1} \sum_{i_2=0}^{N_2} \Delta x_{i_2} ... \sum_{i_m=0}^{N_m} \Delta x_{i_m} \cdot \ Y[i_1, i_2, \ ... \ , i_m] \, j_n(x_1, X_1[i_1]) ... j_n(x_m, X_m[i_m]) \ .$$

and Δx_{i_k} are the distances between the mesh-points.

Example of the approximation in 4 dimensions

The approximation of the four-dimensional $\cos(r)$ function by the 2^{nd} order Gauss-Hermite folding on basis of $p = 5$ and $p = 7$ closest to the given points in function of the smearing parameter γ:

$1/\gamma$	δ_{avr}	$\delta_{\min}$	$\delta_{\max}$	δ_{avr}	$\delta_{\min}$	$\delta_{\max}$
	$p = 5$			$p = 7$		
0.98	0.0081	-0.0296	0.0530	0.0030	-0.0073	0.0241
1.00	0.0072	-0.0261	0.0485	**0.0029**	**-0.0074**	**0.0242**
1.02	0.0065	-0.0233	0.0452	0.0030	-0.0076	0.0249
1.04	0.0060	-0.0210	0.0428	0.0032	-0.0080	0.0260
1.06	0.0057	-0.0192	0.0414	0.0035	-0.0086	0.0276
1.08	**0.0057**	**-0.0179**	**0.0409**	0.0040	-0.0093	0.0295
1.10	0.0059	-0.0171	0.0411	0.0046	-0.0102	0.0320

Here δ_{avr} is the root mean square deviation and $r = \sqrt{x_1^2 + x_2^2 + x_3^2 + x_4^2}$.

Example of the approximation in 4 dimensions

The functions are tabulated in 21 equidistant points along each coordinate. The smearing parameter $\gamma = \mathbf{0.93}$ or $\gamma = \mathbf{1}$ is chosen in case of the $\boldsymbol{p = 5}$ or $\boldsymbol{p = 7}$ point basis used when folding, respectively.

Function Y	Range	$Y_{\min}$	$Y_{\max}$	p	δ_{avr}	$\delta_{\min}$	$\delta_{\max}$
$\sin(r)/r$	$-2\pi : 2\pi$	-0.2172	1	5	0.0011	-0.0029	0.0128
				7	0.0005	-0.0012	0.0059
$x_1^2 + x_2^2 + x_3^2 + x_4^2$	-2 : 2	0	8	5	0.0053	-0.0218	0.0102
				7	0.0013	-0.0017	0.0014
$(x_1 \cdot x_2 \cdot x_3 \cdot x_4)^2$	-2 : 2	0	256	5	0.0076	-0.2491	0.1161
				5	0.0017	-0.0191	0.0102
$x_1 \cdot x_2 \cdot x_3 \cdot x_4$	-2 : 2	-16	16	5	0.0014	-0.0180	0.0180
				7	0.0001	-0.0017	0.0017

The root mean square deviation $\boldsymbol{\delta_{\text{avr}}}$ as well as the maximal in plus difference ($\boldsymbol{\delta_{\max}}$) and the minimal in minus one ($\boldsymbol{\delta_{\min}}$) are evaluated for the $\boldsymbol{N = 149057}$ mesh and inter-mesh points (in the middle) excluding the points which lie on two outer layers (i.e two first or last rows or columns).

ghost.f

```
C-----------------------------------------------------------------------
C   The 2nd order Gauss-Hermite folding (a la V.M. Strutinsky) of a function
C   defined on a sample of equidistant points in the n-dimensional space
C-----------------------------------------------------------------------
      subroutine ghost(nna,npts,xdn,dx,y,yref,gamma,x,fun,dfun)
      parameter (ndim=4,id=2,nid=2*id+1)
      dimension y(npts),xdn(ndim),dx(ndim),x(ndim),dfun(ndim),nna(ndim)
C
C     The data points which should be approximated by the function fun(x) have
C     to be stored in the main program as the n-dimensional array:
C     dimension y(nna(1),nna(2),....,(nna(ndim)) ,
C     where nna(i) is the number of points related to the x_i coordinate.
C     The total number of points in y is npts=nna(1)*nna(2)*.....*nna(ndim).
C     The equidistant grid beginning at xdn(i) with step dx(i) is assumed
C     for each coordinate. The value and gradient of the approximated function
C     in the the point x(ndim) are stored in fun and dfun respectively.
C     REMARK:  In order to increase the accuracy of the approximation one
C     preforms the folding of the differences y(i)-yref, where yref is the
C     function value around which the approximation should be the best.
C     A reasonable choice of yref is the average of the input points i.e.
C     yref=(sum y(i))/npts. The folding is performed using 2*id+1 points
C     closest to point x in each direction and gamma is the smearing width.
C     (C) Copr. 2004 Krzysztof Pomorski, email: pomorski@kft.umcs.lublin.pl
C
      dimension f(ndim,nid),df(ndim,nid),fdf(ndim),ni(ndim),nnn(ndim)
      gami=1./gamma
      fun=0.
      nnn(1)=1
      do 2 i=1,ndim
      dfun(i)=0.
      if(i.gt.1) nnn(i)=nnn(i-1)*nna(i-1)
      xx=(x(i)-xdn(i))/dx(i)+1.
      ni(i)=int(xx+0.5)
      fnorm=0.
      do 1 j=1,nid
      t=gami*(xx-(ni(i)+j-id-1))
      gauss=exp(-t**2)
      f(i,j)=gami*gauss*(1.5-t**2)
      fnorm=fnorm+f(i,j)
    1 df(i,j)=gami**2*gauss*(2.*t**3-5.*t)/dx(i)
      do 2 j=1,nid
      f(i,j)=f(i,j)/fnorm
    2 df(i,j)=df(i,j)/fnorm
      nbox=nid**ndim
      do 6 k=1,nbox
      l=1
      ff=1.
      do 3 m=1,ndim
    3 fdf(m)=1.
      icur=k-1
      nn=nid**(ndim-1)
      do 5 i=ndim,1,-1
      j=icur/nn+1
      ff=ff*f(i,j)
      do 4 m=1,ndim
      if(m.eq.i) fdf(m)=fdf(m)*df(i,j)
    4 if(m.ne.i) fdf(m)=fdf(m)*f(i,j)
      l=l+nnn(i)*(min(nna(i),max(1,ni(i)+j-id-1))-1)
      icur=icur-(j-1)*nn
    5 nn=nn/nid
      fun=fun+(y(l)-yref)*ff
      do 6 m=1,ndim
    6 dfun(m)=dfun(m)+(y(l)-yref)*fdf(m)
      fun=fun+yref
      return
      end
```