4th-year course

Lecture 1: Nuclear masses

York, UK, 2025, Tuesday 11 February 2025 11:00-12:00, Check in code 293110

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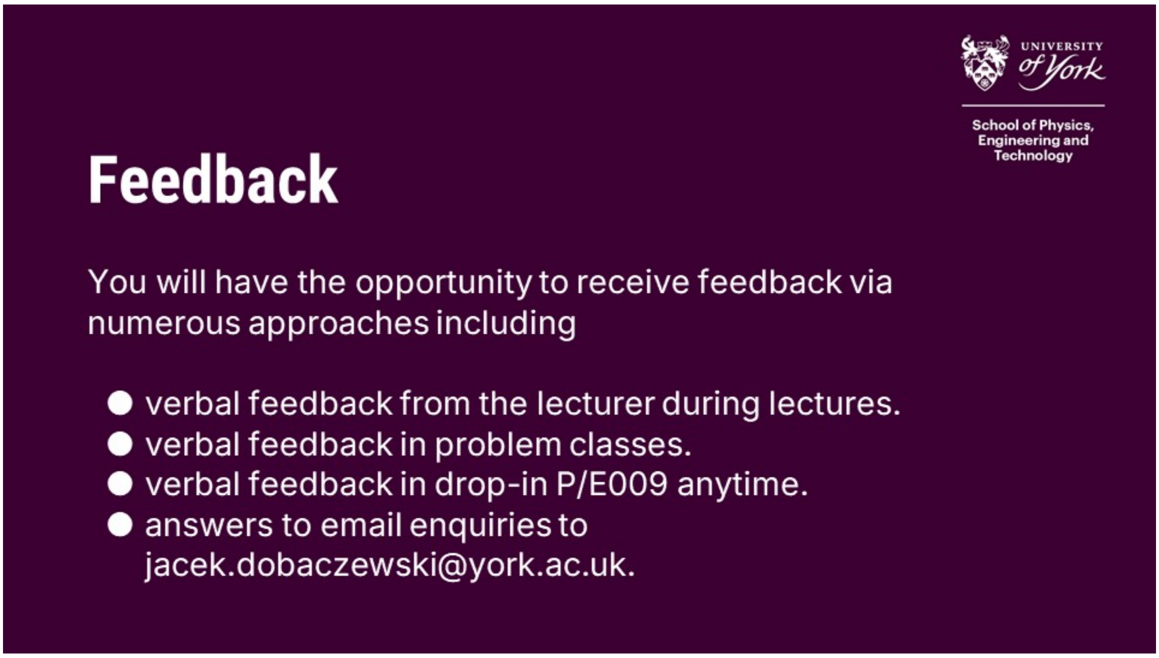

UNIVERSITY of York
School of Physics, Engineering and Technology

Feedback

You will have the opportunity to receive feedback via numerous approaches including

- verbal feedback from the lecturer during lectures.
- verbal feedback in problem classes.
- verbal feedback in drop-in P/E009 anytime.
- answers to email enquiries to jacek.dobaczewski@york.ac.uk.

This course will be delivered in the jupyter-notebook format

To run it, please download it from the [anaconda (https://www.anaconda.com/)](https://www.anaconda.com/) website.

This notebook and all files referred to and linked to, along with its pdf transcript, are available on VLE.

In [1]:
```
# Import of modules

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

# Not really needed, but nicer plots
import seaborn as sns
sns.set()
```

Experimental nuclear masses

$$M(A,Z) = Z(m_P + m_e) + (A - Z)m_N - E_{atomic}(A,Z) - E_B(A,Z)$$

$M(A,Z)$ is the mass of the neutral atom

Z is the atomic number

A is the mass number; the number of neutrons is thus $N = A - Z$

m_P is the mass of a proton, m_e is the mass of an electron, m_N is the mass of a neutron

$E_{atomic}(A,Z)$ is the binding energy of all electrons in the neutral atom

$E_B(A,Z)$ is the nuclear binding energy

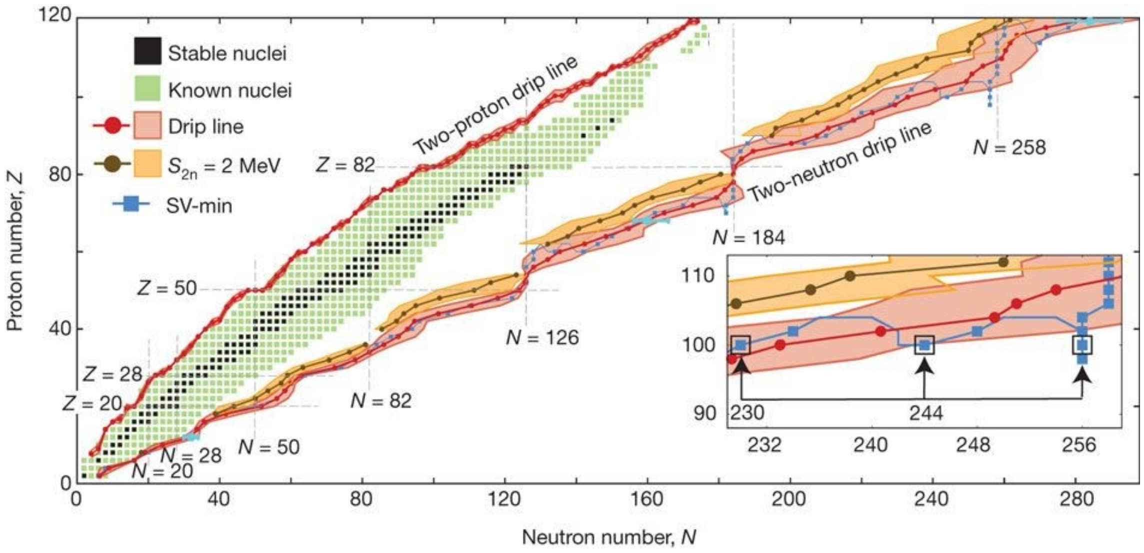
$$E = mc^2, \quad \text{and} \quad c = 1$$

We express all energies and masses in mega-electronovolts (MeV), or eV, keV, or meV.

1 MeV is the energy that an elementary charge e gains in en electrostatic potential of one million volts

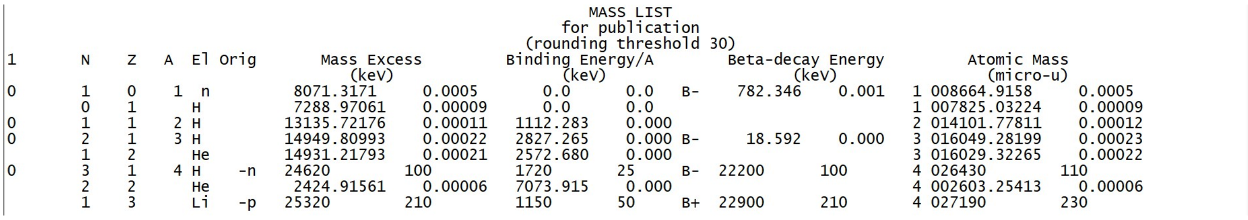
The Segré chart (Table of Nuclides (https://atom.kaeri.re.kr/nuchart/))

J.Erler et al., Nature 486, 509 (2012) (https://www.nature.com/articles/nature11188)



Download the experimental mass table

The 2020 Atomic Mass Evaluation (https://www-nds.iaea.org/amdc/ame2020/massround.mas20.txt)


```
                                                               MASS LIST
                                                            for publication
                                                        (rounding threshold 30)
1       N    Z   A  El orig       Mass Excess         Binding Energy/A        Beta-decay Energy        Atomic Mass
                                     (keV)                  (keV)                    (keV)               (micro-u)
0       1    0    1   n        8071.3171     0.0005       0.0      0.0   B-    782.346    0.001   1 008664.9158     0.0005
        0    1      H          7288.97061    0.00009      0.0      0.0                            1 007825.03224    0.00009
0       1    1    2 H         13135.72176    0.00011   1112.283   0.000                           2 014101.77811    0.00012
0       2    1    3 H         14949.80993    0.00022   2827.265   0.000 B-     18.592   0.000     3 016049.28199    0.00023
        1    2      He        14931.21793    0.00021   2572.680   0.000                           3 016029.32265    0.00022
0       3    1    4 H    -n   24620       100          1720       25     B-   22200     100       4 026430        110
        2    2      He         2424.91561    0.00006   7073.915   0.000                           4 002603.25413    0.00006
        1    3      Li   -p   25320       210          1150       50     B+   22900     210       4 027190        230
```

In the python-readable format

```
1    0    1    1         0.000000
2    1    1    2         2.224566
3    2    1    3         8.481795
4    1    2    3         7.718040
5    3    1    4         6.880000
6    2    2    4        28.295660
7    1    3    4         4.600000
```

In [2]:

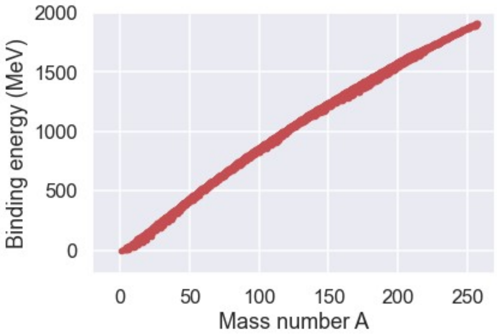
```
AME2016k = []
AME2016N = []
AME2016Z = []
AME2016A = []
AME2016B = []
mydata = np.loadtxt("mass16round-sum.txt")

for i in range(0,len(mydata)):
     AME2016k.append(mydata[i][0])    #Python starts counting on 0
     AME2016N.append(mydata[i][1])
     AME2016Z.append(mydata[i][2])
     AME2016A.append(mydata[i][3])
     AME2016B.append(mydata[i][4])

print (len(mydata))
```

```
2453
```

Current inventory of measured nuclear binding energies contains 2453 entries

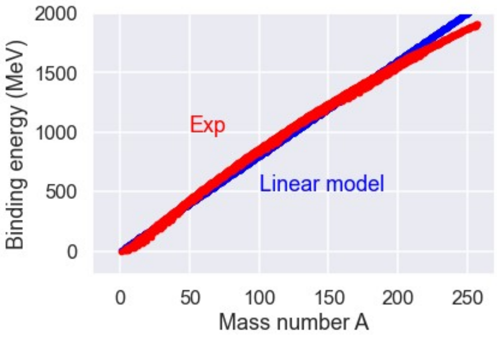
In [3]:

```
plt.plot(AME2016A,AME2016B,'r.')
plt.axis([-20, 270, -200, 2000])
#plt.axis([-2, 22, -10, 210])
plt.xlabel('Mass number A')
plt.ylabel('Binding energy (MeV)')
plt.show()
```

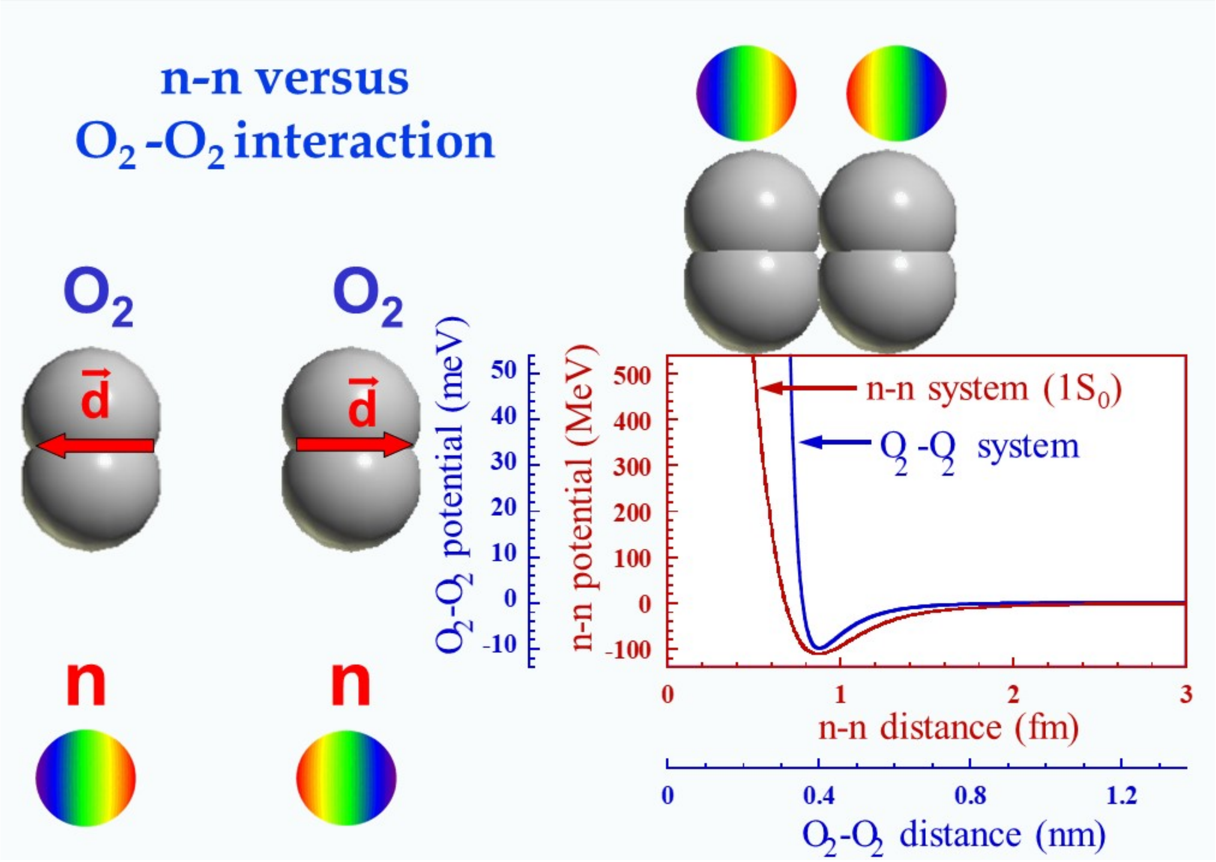


In [4]:

```
aV = 8

BindingLD= []
for i in range(0,len(mydata)):
    A = AME2016A[i]
    e = aV * A
    BindingLD.append(e)

plt.plot(AME2016A,BindingLD,'.',color='blue')
plt.plot(AME2016A,AME2016B,'.',color='red')
plt.axis([-20, 270, -200, 2000])
#plt.axis([-2, 22, -10, 210])
#plt.axis([38, 52, 240, 510])
plt.xlabel('Mass number A')
plt.ylabel('Binding energy (MeV)')
plt.text(50,1000,'Exp',color='red')
plt.text(100,500,'Linear model',color='blue')
plt.show()
```



The origin of nuclear binding [arxiv.nucl-th/0301069 (https://arxiv.org/abs/nucl-th/0301069)](https://arxiv.org/abs/nucl-th/0301069), J.H. Rose et al. [PRL 53 (1984) 344 (https://doi-org.libproxy.york.ac.uk/10.1103/PhysRevLett.53.344)](https://doi-org.libproxy.york.ac.uk/10.1103/PhysRevLett.53.344)



Liquid-drop model and liquid-drop mass formula

$$E_B(A,Z) = a_V A - a_S A^{\frac{2}{3}} - a_C \frac{Z^2}{A^{\frac{1}{3}}} - a_I \frac{(A-2Z)^2}{A} + \delta(A)$$

a_V is the volume energy coefficient

a_S is the surface energy coefficient

a_C is the Coulomb energy coefficient

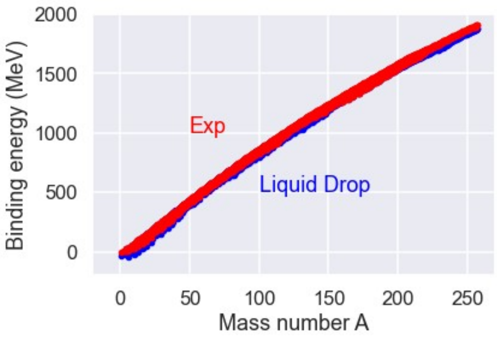
a_I is the symmetry energy coefficient

$\delta(A)$ is the pairing-energy term

$$\delta(A) = \begin{cases} a_P A^{-3/4} & \text{for even-even nuclei} \\ 0 & \text{for odd nuclei} \\ -a_P A^{-3/4} & \text{for odd-odd nuclei} \end{cases}$$

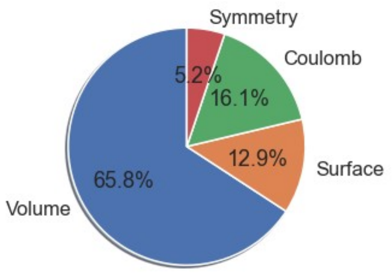
In [5]:

```
# Generating the liquid-drop parameters

# values given in the 1980 book of Ring & Schuck,
# "The Nuclear Many-Body Problem", {Springer-Verlag, Berlin, 1980}

aV = 15.98
aS = 18.56
aC = 0.717
aI = 28.1
aP = 34

# modifiers

#aV = 17
#aS = 0
#aC = 0
#aI = 0
#aP = 0

# Generating the liquid-drop binding energies

onethird=1/3
twothird=2/3
threefourth = 3/4

BindingLD= []
for i in range(0,len(mydata)):
    A = AME2016A[i]
    N = AME2016N[i]
    Z = AME2016Z[i]
    e = aV * A - aS * A**twothird -aC * Z**2/A**onethird -aI * (A-2*Z)**2/A
    if (N % 2) == 0 and (Z % 2) == 0:
        e = e + aP * A**(-threefourth)
    if (N % 2) == 1 and (Z % 2) == 1:
        e = e - aP * A**(-threefourth)
    BindingLD.append(e)

plt.plot(AME2016A,BindingLD,'.',color='blue')
plt.plot(AME2016A,AME2016B,'.',color='red')
plt.axis([-20, 270, -200, 2000])
#plt.axis([-2, 22, -10, 210])
#plt.axis([38, 52, 240, 510])
plt.xlabel('Mass number A')
plt.ylabel('Binding energy (MeV)')
plt.text(50,1000,'Exp',color='red')
plt.text(100,500,'Liquid Drop',color='blue')
plt.show()
```



In [6]:

```
BindingLDatA= []

onethird=1/3
twothird=2/3
threefourth = 3/4

N = 126
Z = 82
A = N+Z
eV = aV * A
eS = aS * A**twothird
eC = aC * Z**2/A**onethird
eI = aI * (A-2*Z)**2/A
eP = 0
if (N % 2) == 0 and (Z % 2) == 0:
    eP = + aP * A**(-threefourth)
if (N % 2) == 1 and (Z % 2) == 1:
    eP = - aP * A**(-threefourth)

BindingLDatA.append(eV)
BindingLDatA.append(eS)
BindingLDatA.append(eC)
BindingLDatA.append(eI)
# BindingLDatA.append(eP)

# Pie chart, where the slices will be ordered and plotted counter-clockwise:
# labels = ['Volume', 'Surface', 'Coulomb', 'Symmetry', 'Pairing']
labels = ['Volume', 'Surface', 'Coulomb', 'Symmetry']
# sizes = [eV, eS, eC, eI, eP]
sizes = [eV, eS, eC, eI]
# explode = (0.1, 0, 0, 0)  # only "explode" the 1st slice)
explode = (0, 0, 0, 0)  # do not "explode")

fig1, ax1 = plt.subplots()
ax1.pie(sizes, explode=explode, labels=labels, autopct='%1.1f%%',shadow=True, startangle=90)
ax1.axis('equal')  # Equal aspect ratio ensures that pie is drawn as a circle.
```

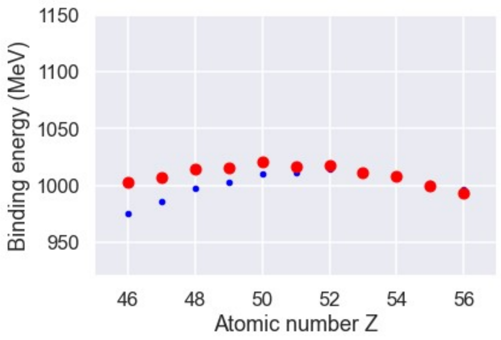


The symmetry energy.

Let us have look at the chain of isobars (nuclei having the same mass number A), which have the same volume and surface energies.

In [7]:

```
# Generating data for the isobaric A=120 chain

AME2016B120=[]
AME2016Z120=[]
LDB120=[]
for i in range(0,len(mydata)):
    A = AME2016A[i]
    if (A==120):
        AME2016B120.append(AME2016B[i])
        AME2016Z120.append(AME2016Z[i])
        LDB120.append(BindingLD[i])

plt.plot(AME2016Z120,LDB120,'.',color='blue')
plt.plot(AME2016Z120,AME2016B120,'o',color='red')
plt.axis([45, 57, 920, 1150])
plt.xlabel('Atomic number Z')
plt.ylabel('Binding energy (MeV)')
plt.show()
```



The pairing energy.

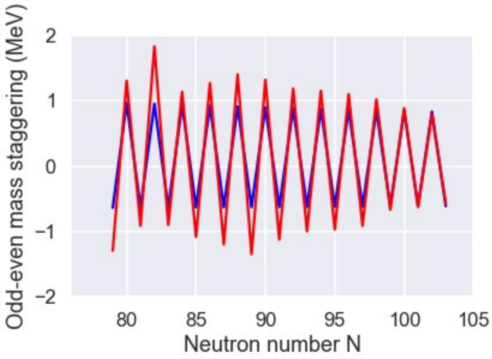
Odd-even mass staggering.

$$OES_N(N,Z) = E_B(N,Z) - \frac{1}{2}(E_B(N+1,Z) + E_B(N-1,Z))$$

$$OES_Z(N,Z) = E_B(N,Z) - \frac{1}{2}(E_B(N,Z+1) + E_B(N,Z-1))$$

In [8]:

```
# Generating data for the odd-even staggering in the isotopic chain Z=68 (erbium)

AME2016N68=[]
AME2016n68=[]
AME2016B68=[]
LDB68=[]
AME2016b68=[]
LDb68=[]
AME2016S68=[]
LDS68=[]
for i in range(0,len(mydata)):
    Z = AME2016Z[i]
    if (Z==68):
        AME2016B68.append(AME2016B[i])
        AME2016n68.append(AME2016N[i])
        LDB68.append(BindingLD[i])
for i in range(1,len(LDB68)-1):
    am=AME2016B68[i-1]
    a0=AME2016B68[i]
    ap=AME2016B68[i+1]
    AME2016S68.append(a0-(am+ap)/2)

    am=LDB68[i-1]
    a0=LDB68[i]
    ap=LDB68[i+1]
    LDS68.append(a0-(am+ap)/2)

    AME2016N68.append(AME2016n68[i])

plt.plot(AME2016N68,LDS68,'-',color='blue')
plt.plot(AME2016N68,AME2016S68,'-',color='red')
plt.axis([76, 105, -2, 2])
plt.xlabel('Neutron number N')
plt.ylabel('Odd-even mass staggering (MeV)')
plt.show()
```



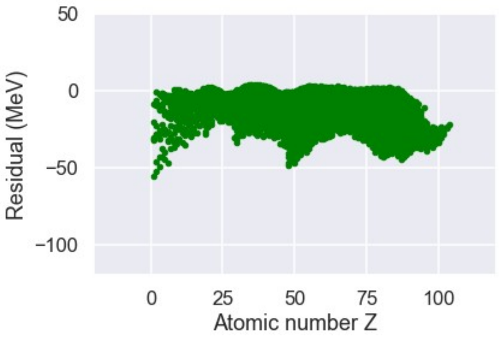
Residuals of the liquid-drop mass formula

Differences between theory (model) and experiment

In [9]:

```
# Generating the liquid-drop parameters

# values given in the 1980 book of Ring & Schuck

aV = 15.98
aS = 18.56
aC = 0.717
aI = 28.1
aP = 34

# modifiers

#aV = 16
#aS = 0
#aC = 0
#aI = 0
#aP = 0

# Generating the liquid-drop binding energies

onethird=1/3
twothird=2/3
threefourth = 3/4

import math

RMSdeviation=0
ResidualLD= []
for i in range(0,len(mydata)):
    A = AME2016A[i]
    N = AME2016N[i]
    Z = AME2016Z[i]
    e = aV * A - aS * A**twothird -aC * Z**2/A**onethird -aI * (A-2*Z)**2/A
    if (N % 2) == 0 and (Z % 2) == 0:
        e = e + aP * A**(-threefourth)
    if (N % 2) == 1 and (Z % 2) == 1:
        e = e - aP * A**(-threefourth)
    ResidualLD.append(e-AME2016B[i])
    RMSdeviation=RMSdeviation+ResidualLD[i]**2

RMSdeviation=math.sqrt(RMSdeviation/len(mydata))

print ('RMS deviation=',RMSdeviation)

plt.plot(AME2016Z,ResidualLD,'.',color='green')
plt.axis([-20, 270, -100, 50])
plt.axis([-20, 160, -100, 50])
plt.axis([-20, 120, -120, 50])
plt.xlabel('Neutron number N')
plt.xlabel('Mass number A')
plt.xlabel('Atomic number Z')
plt.ylabel('Residual (MeV)')
plt.show()
```

```
RMS deviation= 17.615879844163686
```



2020 parameterization of the liquid-drop mass formula

published in:

Bethe–Weizsäcker semiempirical mass formula coefficients 2019 update based on AME2016

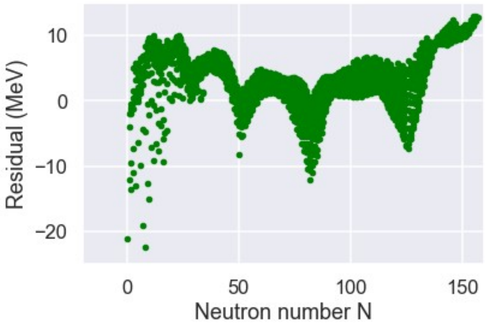
Djelloul Benzaid, Salaheddine Bentridi, Abdelkader Kerraci, Naima Amrani

Nuclear Science and Techniques, 31:9, 3 January 2020 (https://doi.org/10.1007/s41365-019-0718-8)

$$\delta(A) = \begin{cases} a_P A^{-1/2} & \text{for even-even nuclei} \\ 0 & \text{for odd nuclei} \\ -a_P A^{-1/2} & \text{for odd-odd nuclei} \end{cases}$$

In [10]:
```
# Generating the liquid-drop parameters

# values given in the recent paper, Benzaid et al. (2020)

aV = 14.64
aS = 14.08
aC =  0.64
aI = 21.07
aP = 11.54

# modifiers

#aV = 14.5
#aS = 0
#aC = 0
#aI = 0
#aP = 0

# Generating the liquid-drop binding energies

onethird=1/3
twothird=2/3
onehalf =1/2

RMSdeviation=0
ResidualLD= []
for i in range(0,len(mydata)):
    A = AME2016A[i]
    N = AME2016N[i]
    Z = AME2016Z[i]
    e = aV * A - aS * A**twothird -aC * Z**2/A**onethird -aI * (A-2*Z)**2/A
    if (N % 2) == 0 and (Z % 2) == 0:
        e = e + aP * A**(-onehalf)
    if (N % 2) == 1 and (Z % 2) == 1:
        e = e - aP * A**(-onehalf)
    ResidualLD.append(e-AME2016B[i])
    RMSdeviation=RMSdeviation+ResidualLD[i]**2

RMSdeviation=math.sqrt(RMSdeviation/len(mydata))

print ('RMS deviation=',RMSdeviation)

plt.plot(AME2016N,ResidualLD,'.',color='green')
plt.axis([-20, 270, -25, 15])
plt.axis([-20, 160, -25, 15])
#plt.axis([-20, 120, -25, 15])
plt.xlabel('Mass number A')
plt.xlabel('Neutron number N')
#plt.xlabel('Atomic number Z')
plt.ylabel('Residual (MeV)')
plt.show()
```

```
RMS deviation= 4.938714487029749
```



Nuclear DFT - a primer

The binding energy E is defined as an integral of the energy density $\mathcal{H}(r)$, which depends on the kinetic density $\tau(r)$ and particle density $\rho(r)$:

$$E \equiv \int dr\, \mathcal{H}(r), \quad \text{for} \quad \mathcal{H}(r) = \frac{\hbar^2}{2m}\tau(r) - \frac{1}{2}C\rho^2(r), \quad \rho(r) = \sum_{i=1}^{A} \phi_i(r)\phi_i^*(r), \quad \tau(r) = \sum_{i=1}^{A}(\nabla\phi_i(r))(\nabla\phi_i^*(r))$$

Density Functional Theory (DFT) is based on a variational method, whereupon the single-particle (Kohn-Sham) orbitals $\phi_i(r)$ are obtained as:

$$\delta_{\phi_i^*(r)} E[\tau(r),\rho(r)] = 0 \quad \Longrightarrow \left[-\frac{\hbar^2}{2m}\Delta - C\rho(r)\right]\phi_i(r) = \epsilon_i\phi_i(r)$$

DFT looks like a mean-field approximation, it smells like a mean-field approximation, and it seems to be a mean-field approximation, but DFT is NOT a mean-field approximation. **There exists an EXACT functional $E[\rho(r)]$ for which DFT**

gives the EXACT energy and the EXACT density.

Mass table based on the UNEDF0 Skyrme density functional:

M. Kortelainen et al., Phys. Rev. C 82, 024313 (2010) (https://journals.aps.org/prc/abstract/10.1103/PhysRevC.82.024313)

Download the mass table

Skyrme UNEDF0 even-even nuclei (http://massexplorer.frib.msu.edu/content/DFTMassTables.html)

In [11]:

```
UNEDF0k = []
UNEDF0N = []
UNEDF0Z = []
UNEDF0A = []
UNEDF0B = []
mydata2 = np.loadtxt("All_Even-Even_Nuclei.UNEDF0-cut.txt")

for i in range(0,len(mydata2)):
    UNEDF0k.append(i)    #Python starts counting on 0
    UNEDF0Z.append(mydata2[i][0])
    UNEDF0N.append(mydata2[i][1])
    UNEDF0A.append(mydata2[i][2])
    UNEDF0B.append(mydata2[i][3])
for i in range(0,len(mydata2)):
    UNEDF0B[i]=-UNEDF0B[i]

print (len(mydata2))
```

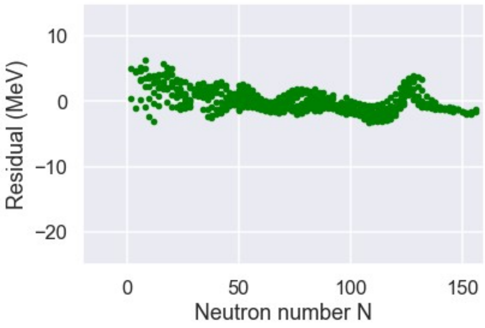
```
2243
```

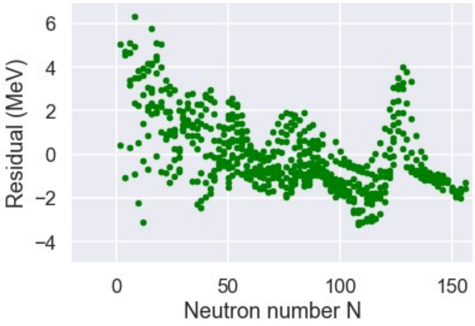
Database of calculated UNEDEF0 even-even nuclei 2243 entries

In [12]:

```
ResidualUN=[]
ResidualA=[]
ResidualN=[]
ResidualZ=[]
BindingUN=[]
BindingAM=[]
for i in range(0,len(mydata)):
    N = AME2016N[i]
    Z = AME2016Z[i]
    for j in range(0,len(mydata2)):
        if (N == UNEDF0N[j] and Z == UNEDF0Z[j]):
#            print (i,j)
            ResidualUN.append(UNEDF0B[j]-AME2016B[i])
            ResidualA.append(N+Z)
            ResidualN.append(N)
            ResidualZ.append(Z)
            BindingUN.append(UNEDF0B[j])
            BindingAM.append(AME2016B[i])

RMSdeviation=0
for i in range(0,len(ResidualUN)):
    RMSdeviation=RMSdeviation+ResidualUN[i]**2

RMSdeviation=math.sqrt(RMSdeviation/len(ResidualUN))

print ('RMS deviation=',RMSdeviation)

plt.plot(ResidualN,ResidualUN,'.',color='green')
plt.axis([-20, 270, -25, 15])
plt.axis([-20, 160, -25, 15])
#plt.axis([-20, 120, -25, 15])
plt.xlabel('Mass number A')
plt.xlabel('Neutron number N')
#plt.xlabel('Atomic number Z')
plt.ylabel('Residual (MeV)')
plt.show()

plt.plot(ResidualN,ResidualUN,'.',color='green')
plt.axis([-20, 270, -25, 15])
plt.axis([-20, 160, -5, 7])
#plt.axis([-20, 120, -25, 15])
plt.xlabel('Mass number A')
plt.xlabel('Neutron number N')
#plt.xlabel('Atomic number Z')
plt.ylabel('Residual (MeV)')
plt.show()
```

```
RMS deviation= 1.6593899570797244
```

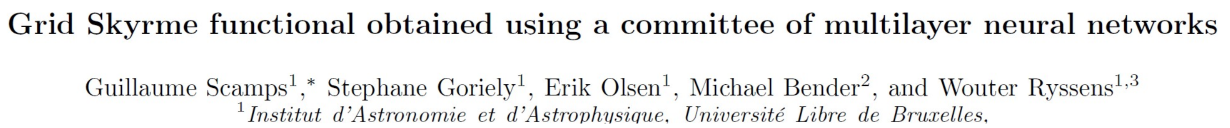




Modern nuclear DFT + corrections:

[arXiv2011.07904 (https://arxiv.org/abs/2011.07904)](https://arxiv.org/abs/2011.07904)

[The European Physical Journal A volume 57, Article number: 333 (2021) (https://link.springer.com/article/10.1140/epja/s10050-021-00642-1)](https://link.springer.com/article/10.1140/epja/s10050-021-00642-1)



Grid Skyrme functional obtained using a committee of multilayer neural networks

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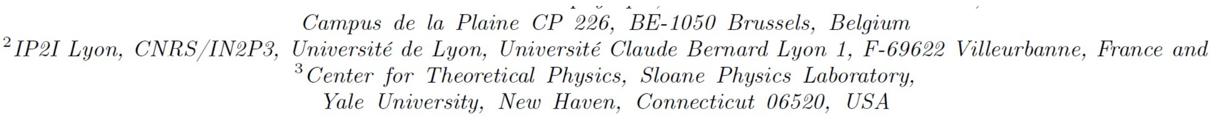

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RMS error on the 2408 known masses of 661 keV

Modern nuclear Liquid Drop + corrections:

[Atomic Data and Nuclear Data Tables 109–110 (2016) 1–204 (http://dx.doi.org/10.1016/j.adt.2015.10.002)](http://dx.doi.org/10.1016/j.adt.2015.10.002)

Nuclear ground-state masses and deformations: FRDM(2012)

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The error of the mass model is 559.5 keV for 2149 nuclei

Take-home messages

Nucleon-nucleon potential has a minimum around 0.9 fm and therefore nuclear matter in equilibrium has a binding energy per particle of about 8 MeV.

Nuclear binding energy (positive) can be described as a sum of five terms:

(1) large positive volume term, (2) large negative surface term, (3) large negative Coulomb term, (4) relatively small negative symmetry term, and (5) small pairing term with alternating sign

Coulomb and symmetry terms are responsible for the stability valey turning for large A towards more neutron-rich nuclei

Pairing term is responsible for the odd-even mass staggering along isotopic and isotonic chains

Liquid-drop mass formula describes experimental masses with the RMS deviation of about 5 MeV

Modern nuclear DFT describes experimental masses with the RMS deviation of about 1.7 MeV

With correctons, the modern nuclear DFT and liquid-drop mass formula describe experimental masses with the RMS deviation of about 0.6 MeV

In [ ]: