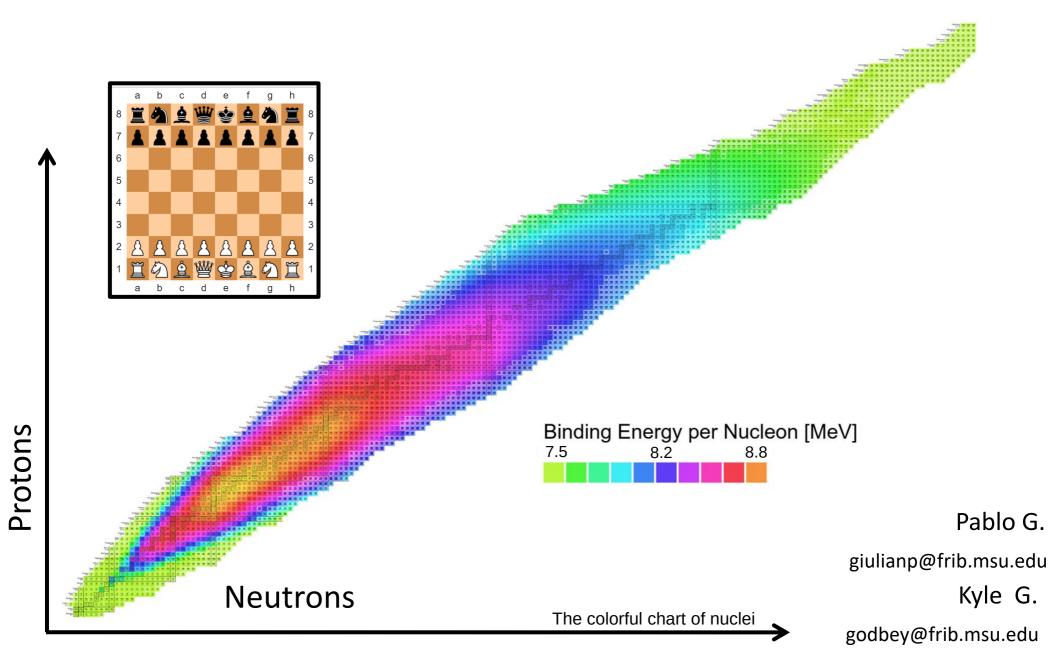
Nuclear Theory









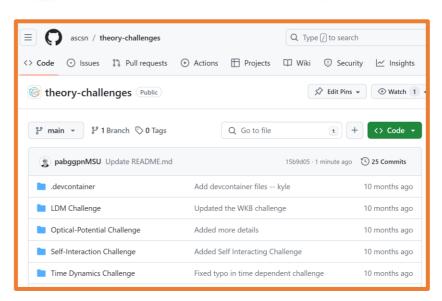
Hand-on session set-up



Advanced Scientific Computing and Statistics Network



https://github.com/ascsn/theory-challenges



For today

Who am I?

Why theory?

Building models

Building a (simple) nuclear model

Quantum mechanics

Building (better) nuclear models

Challenges (Hands-On Session)

For today

Who am I?

Why theory?

Building models

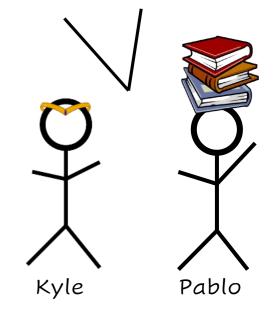
Building a (simple) nuclear model

Quantum mechanics

Building (better) nuclear models

Challenges (Hands-On Session)











Undegrad



PhD



Postdoc



Me Universidad Simon Bolivar





Undegrad



PhD



Postdoc



San Francisco

San Francisco

REBRASKA

Chicap

REBRASKA

LOS Angeles

COCCGARC

MISSOUR

MASSUR

MASSUR

SAN Antonio

LOUISAMA

HOUston

Monterey

Guadalajara

Mexco

Mexico City

Manni

Havana

Sant

Domint

Guadalajara

Guatemala

Carebean Sea

Costa Rica

Sant

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STATE OF

ROSAMA

Manaus

Venezuela





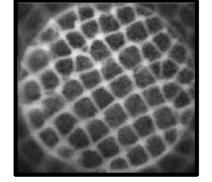
Michigan





Pattern formation in vibrated sand







Undegrad



PhD



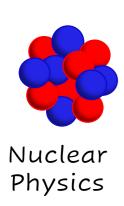
Postdoc

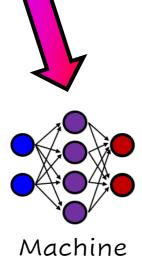




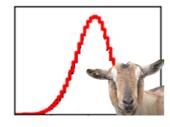








Learning



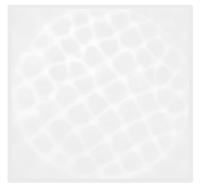
Bayesian Statistics



Michigan

Pattern formation in vibrated sand





Nuclear

Physics

Education

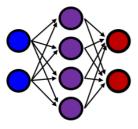
Undegrad

Outreach

Community



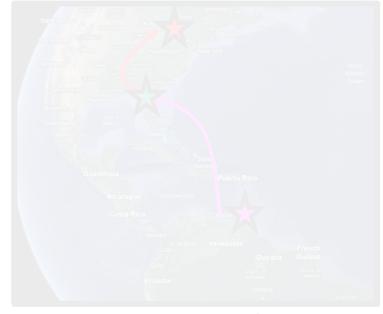




Machine Learning



Bayesian Statistics



Venezuela





Michigan





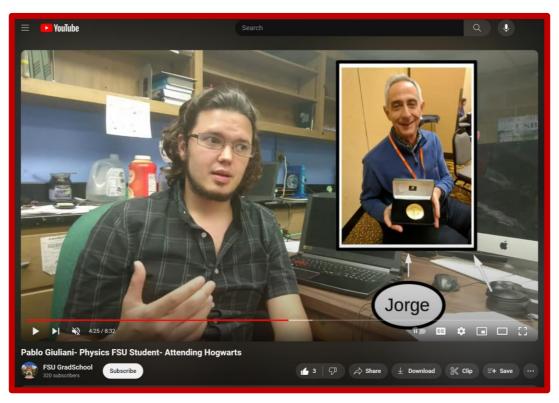
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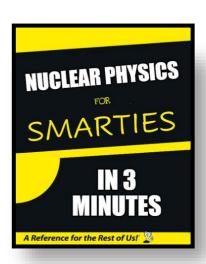


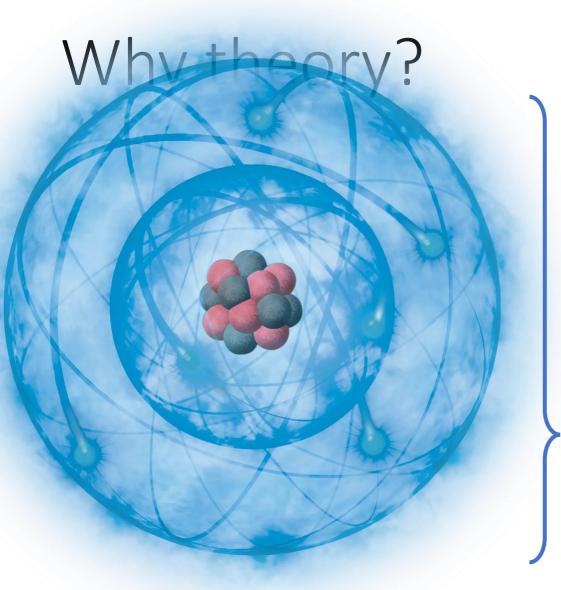
PhD



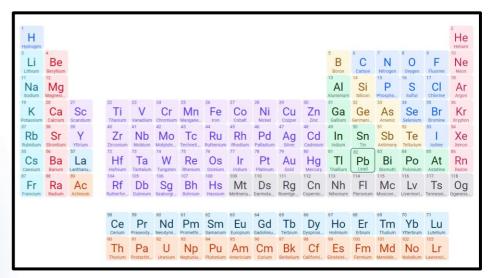




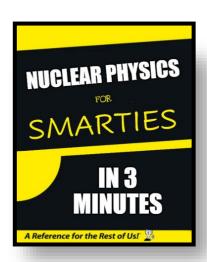




Chemical Periodic Table

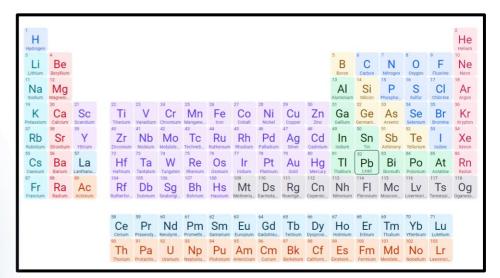


An atom

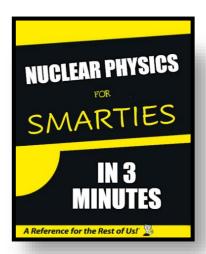


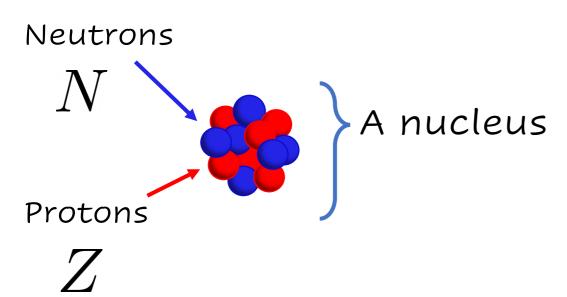
Nucleus Electrons

Chemical Periodic Table

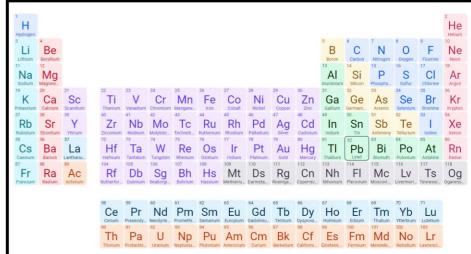


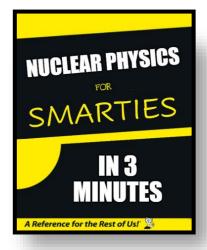
An atom

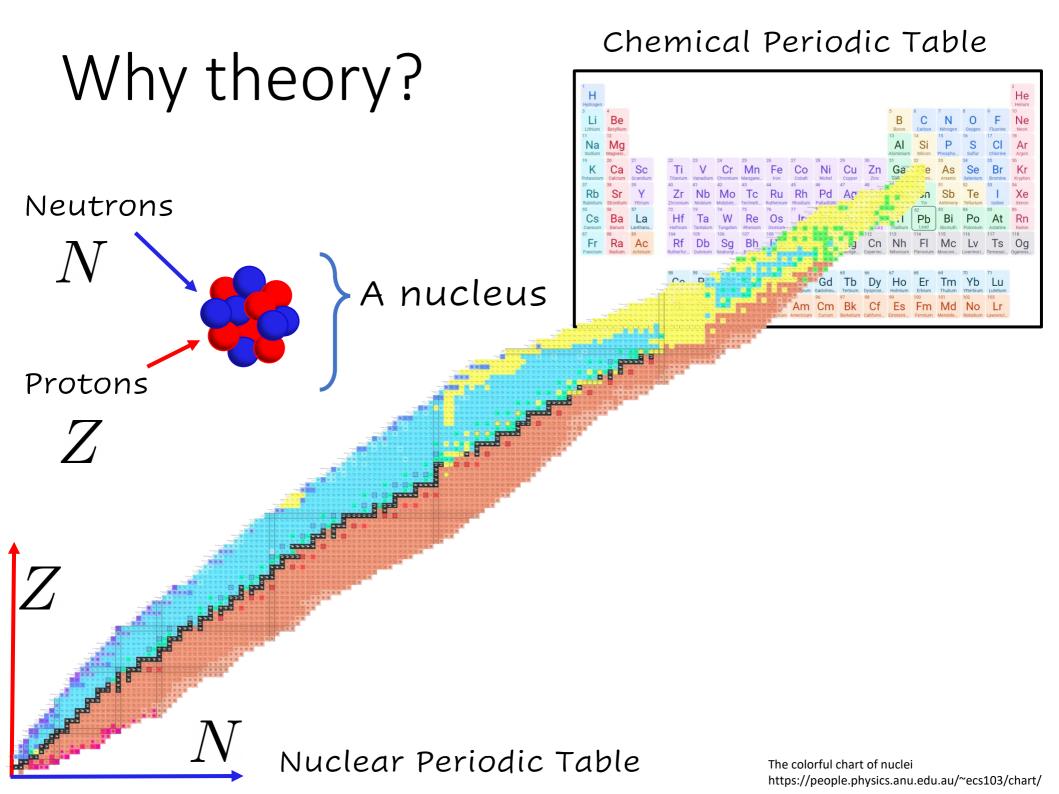


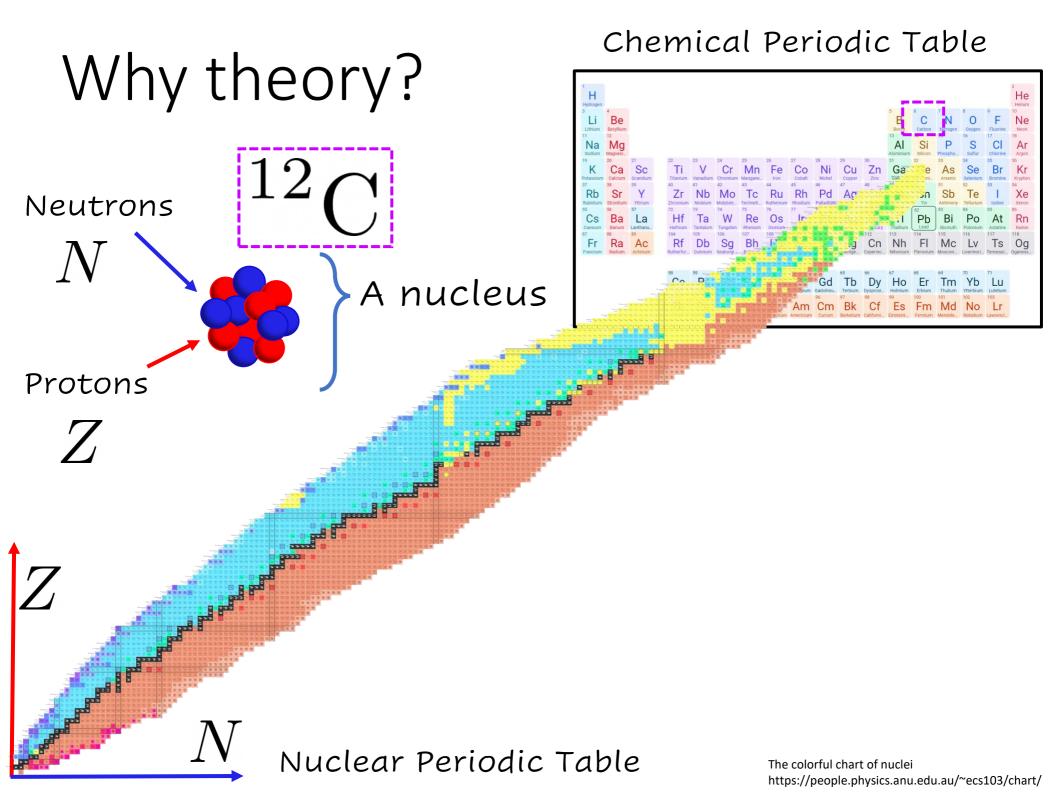


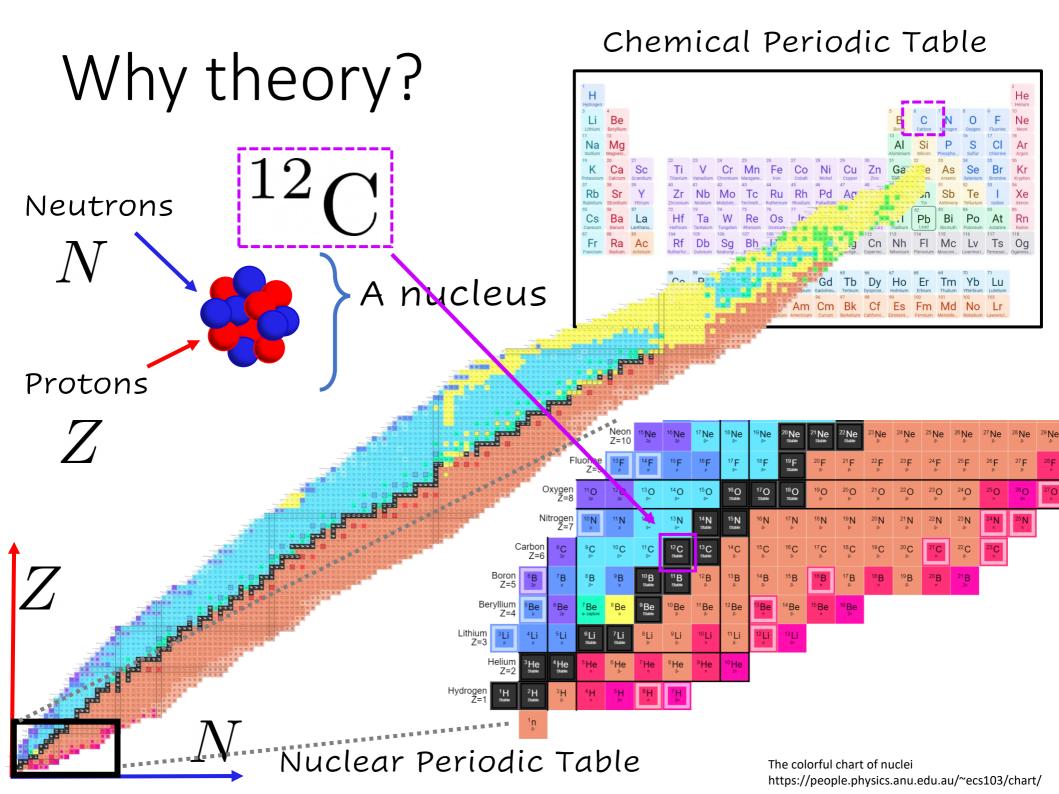
Chemical Periodic Table

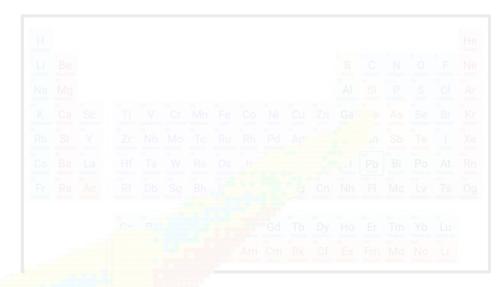












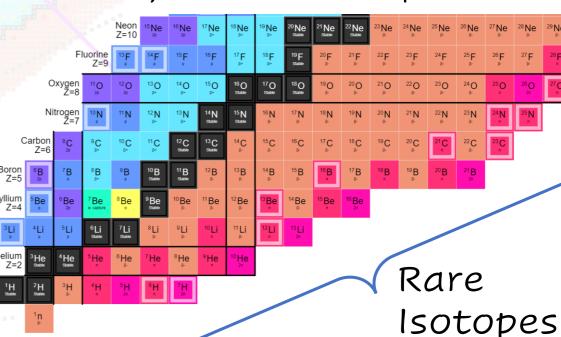
Rare Isotopes

Chemical Periodic Tabl



FRIB

Facility for Rare Isotope Beams



Nuclear Periodic Table

The colorful chart of nuclei https://people.physics.anu.edu.au/~ecs103/chart/

"It is a big device, but without the people around it, its nothing"



Premiering 2024



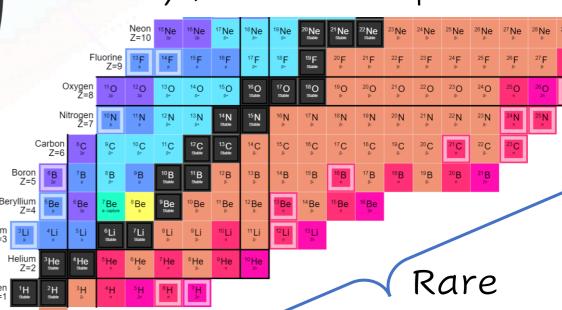
Teaser

Thanks Agnes Mocsy!



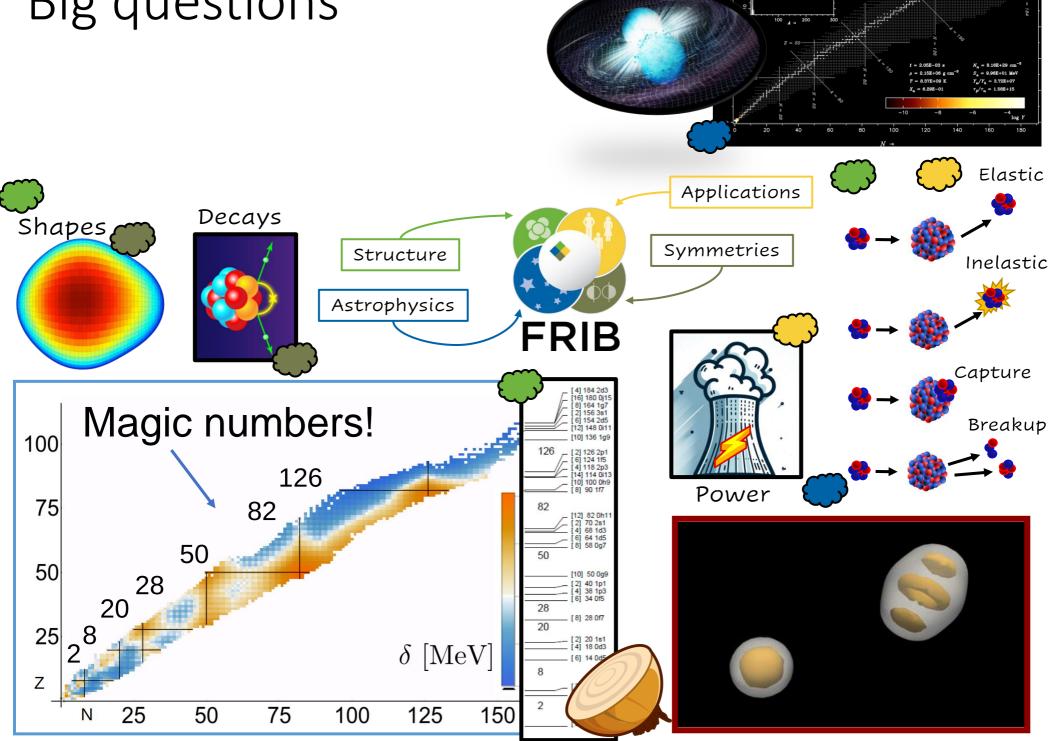
FRIB

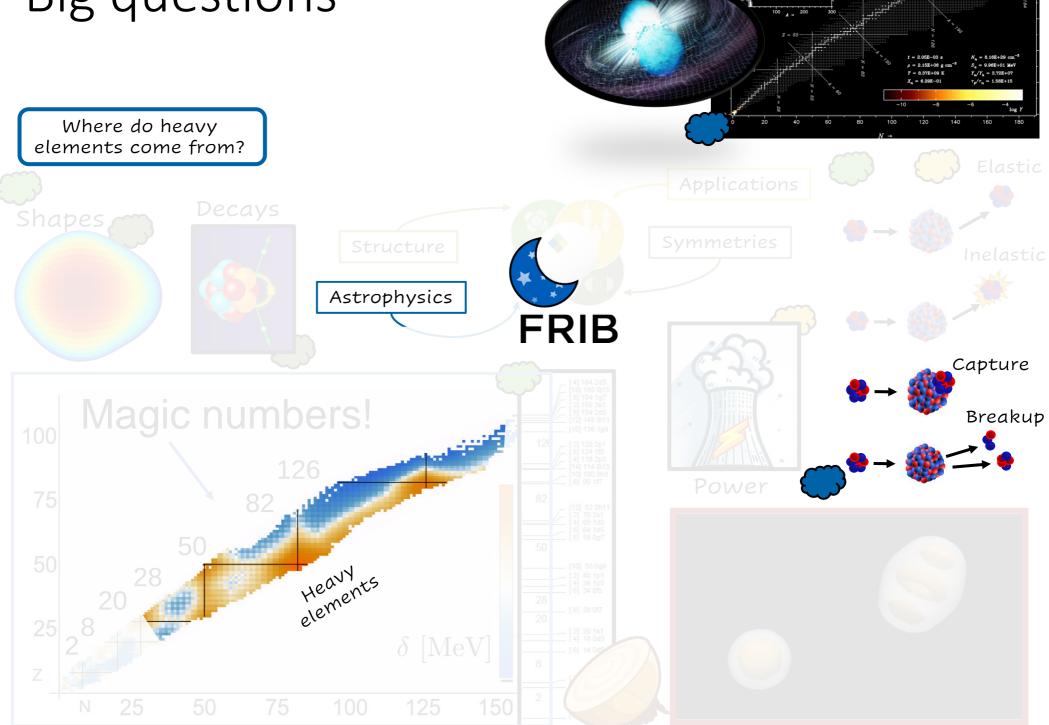
Facility for Rare Isotope Beams

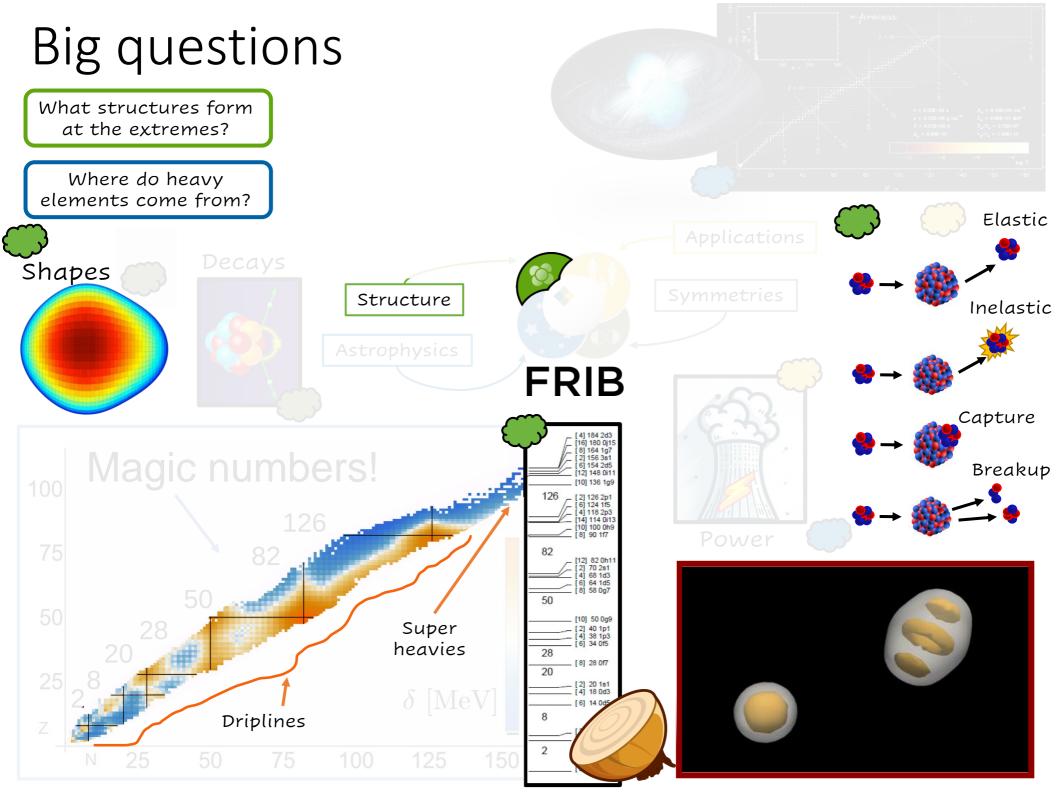


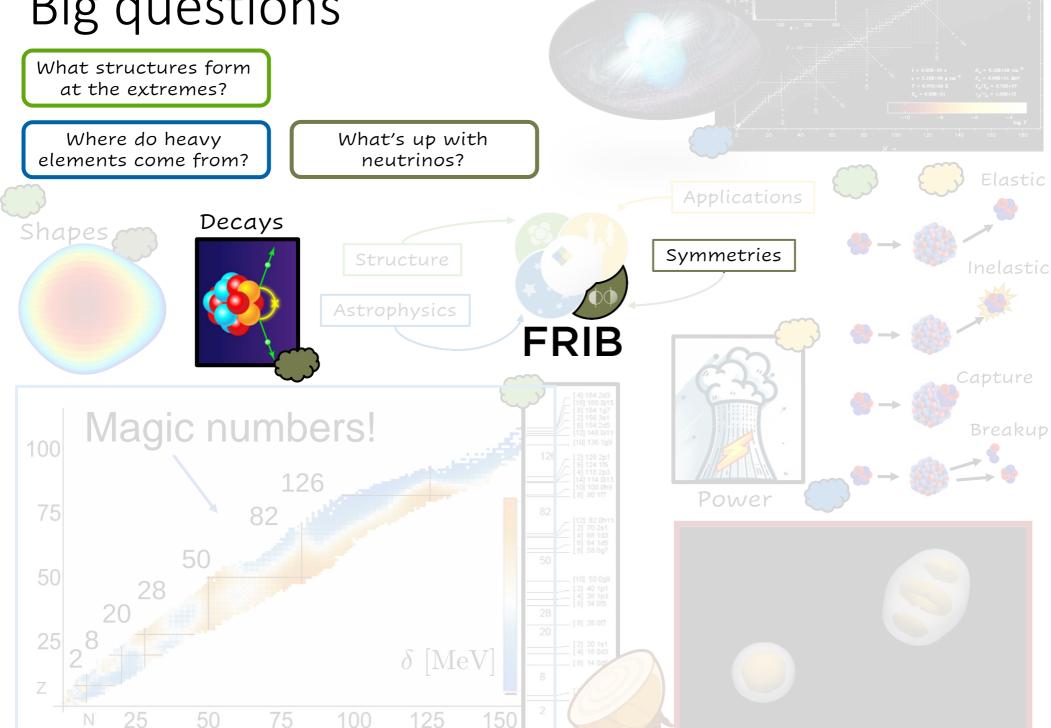
Isotopes

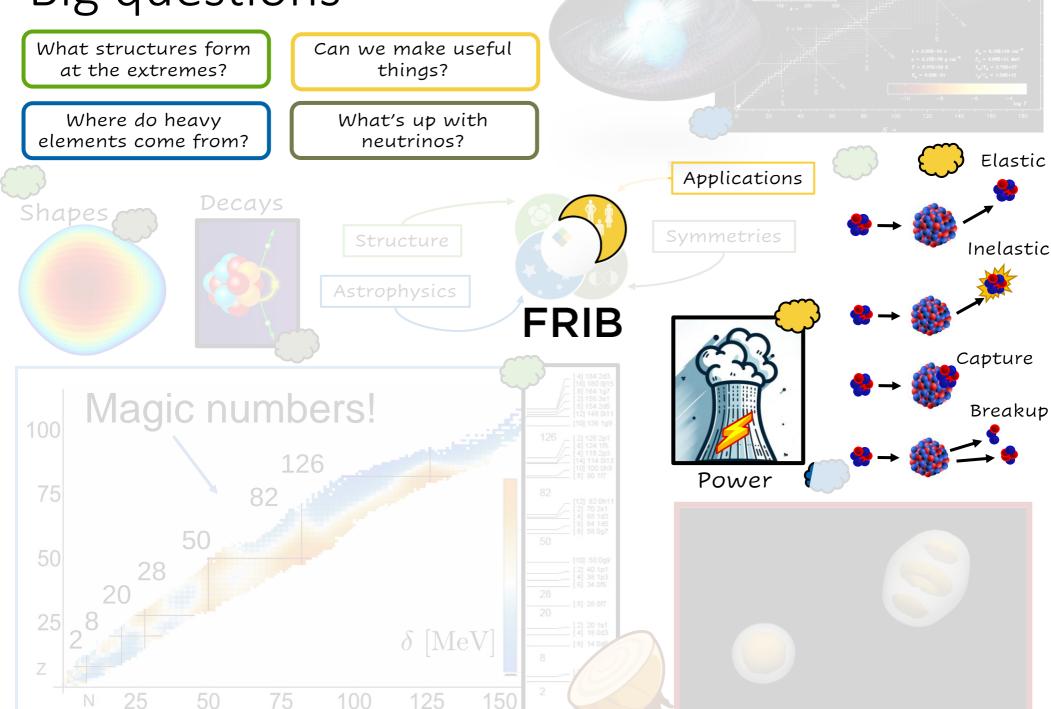
We have fun





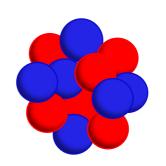






All of this is really, really hard to study Applications Symmetries Structure Astrophysics **FRIB**

All of this is really, really hard to study

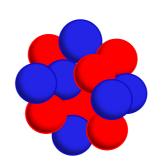


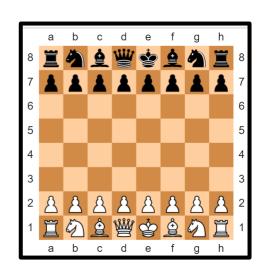


1) Rules are unclear

$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

All of this is really, really hard to study





1) Rules are unclear

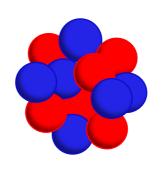


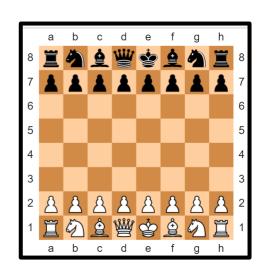
 $\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$

You can watch

... from far away

All of this is really, really hard to study





1) Rules are unclear



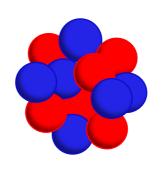
You can watch

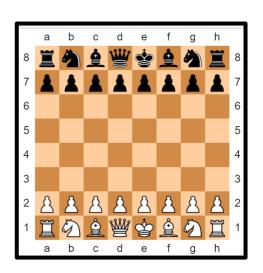
... from far away

...and is dark

$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

All of this is really, really hard to study





1) Rules are unclear



You can watch

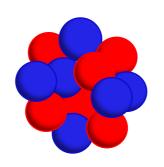
... from far away

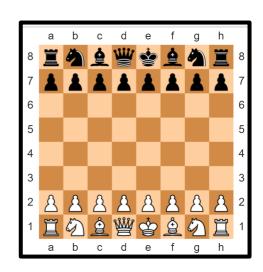
...and is dark

...and half the screen is broken

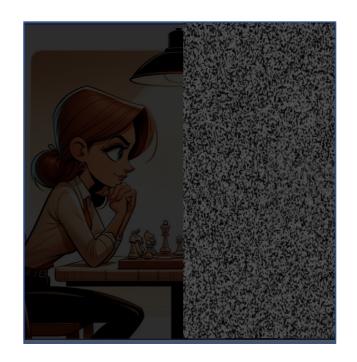
$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

All of this is really, really hard to study





1) Rules are unclear



 $\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$

You can watch

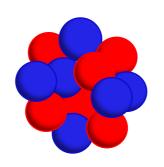
... from far away

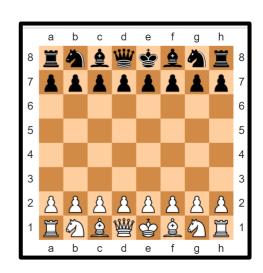
...and is dark

...and half the screen is broken

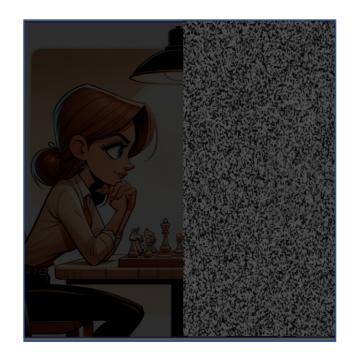
...and you are wearing sunglasses

All of this is really, really hard to study





1) Rules are unclear



 $\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$

You can watch

... from far away

...and is dark

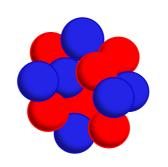
...and half the screen is broken

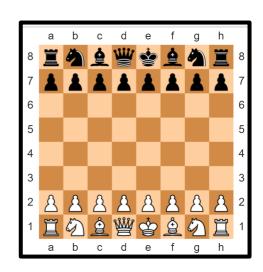
...and you are wearing sunglasses

... and only one instant at a time

All of this is really, really hard to study

Experiment!





1) Rules are unclear



 $\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$

You can watch

... from far away

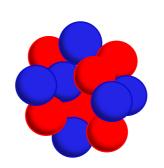
...and is dark

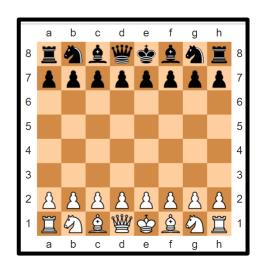
...and half the screen is broken

...and you are wearing sunglasses

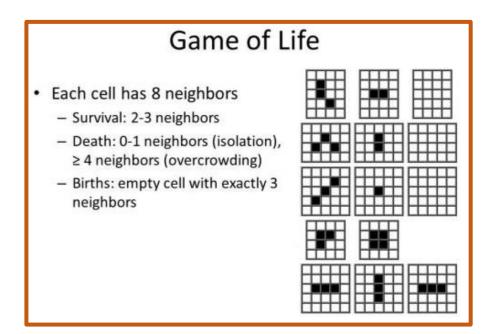
... and only one instant at a time

All of this is really, really hard to study



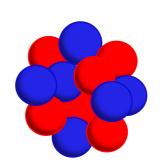


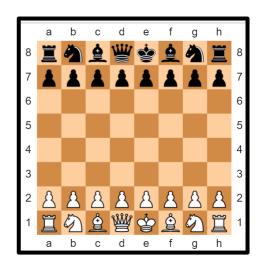
- 1) Rules are unclear
- 2) Emergent complexity



The Challenge

All of this is really, really hard to study





- 1) Rules are unclear
- 2) Emergent complexity

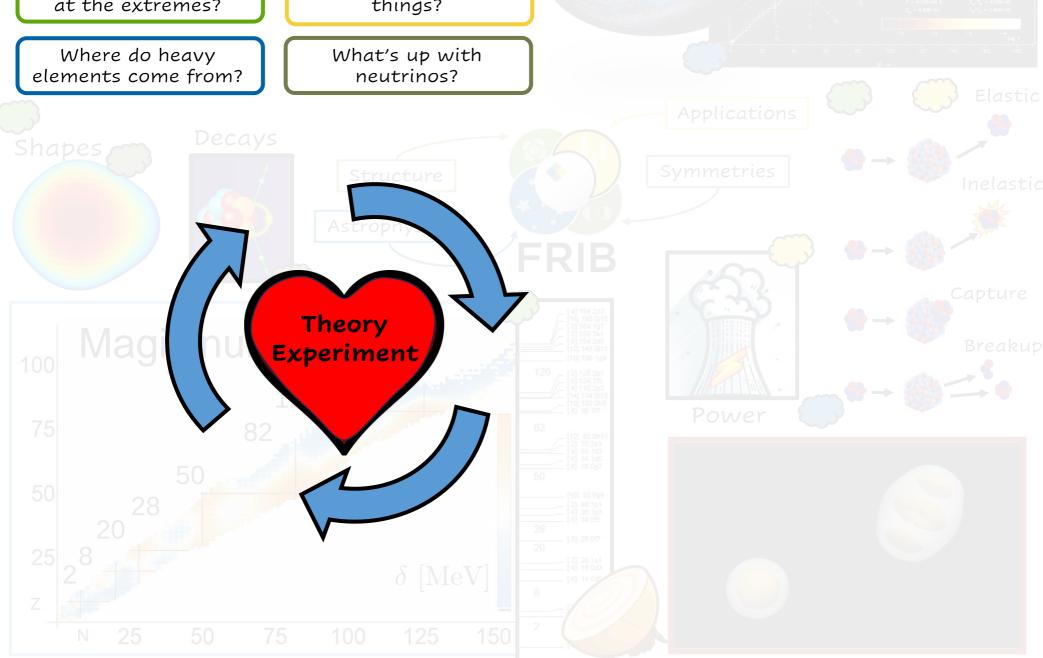


Game of Life • Each cell has 8 neighbors - Survival: 2-3 neighbors - Death: 0-1 neighbors (isolation), ≥ 4 neighbors (overcrowding) - Births: empty cell with exactly 3 neighbors

We need theory

What structures form at the extremes?

Can we make useful things?



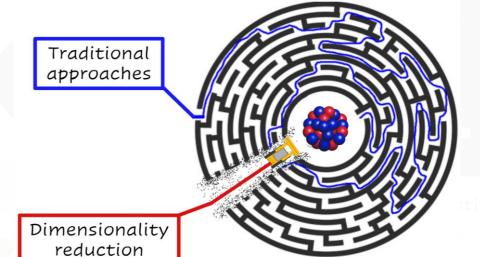
We need theory

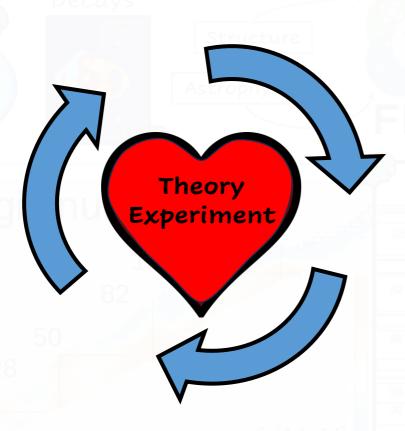
What structures form at the extremes?

Where do heavy elements come from?

Can we make useful things?

What's up with neutrinos?







Video of me talking

My research is to use machine learning and statistics to propel this cycle

For today

Who am 1?

Why theory?

Building models



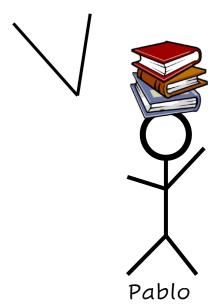
Building a (simple) nuclear model

Quantum mechanics

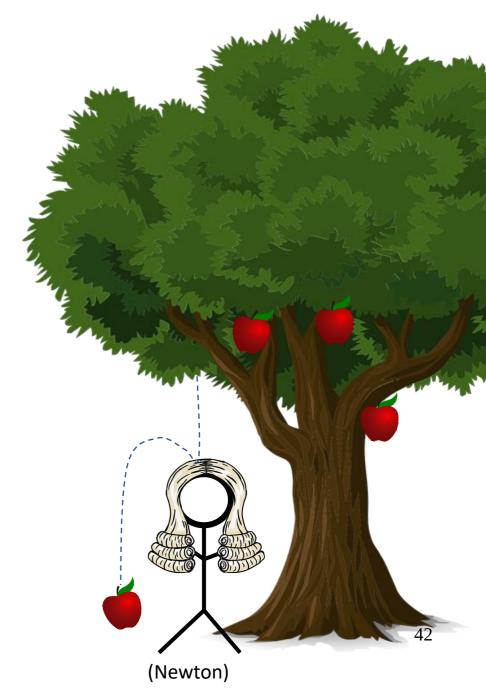
Building (better) nuclear models

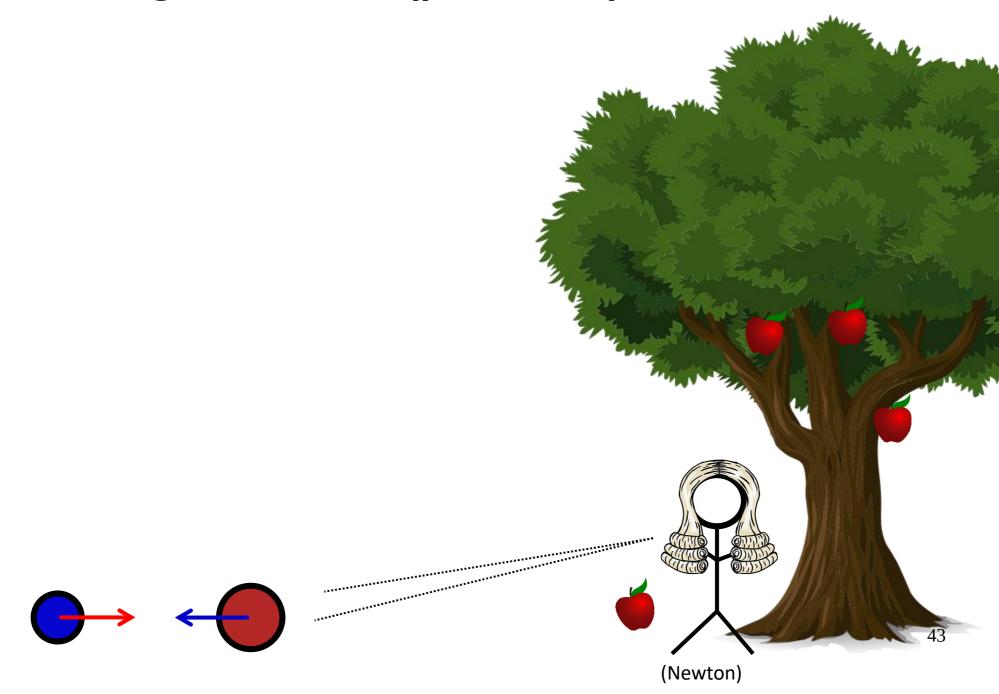
Challenges (Hands-On Session)

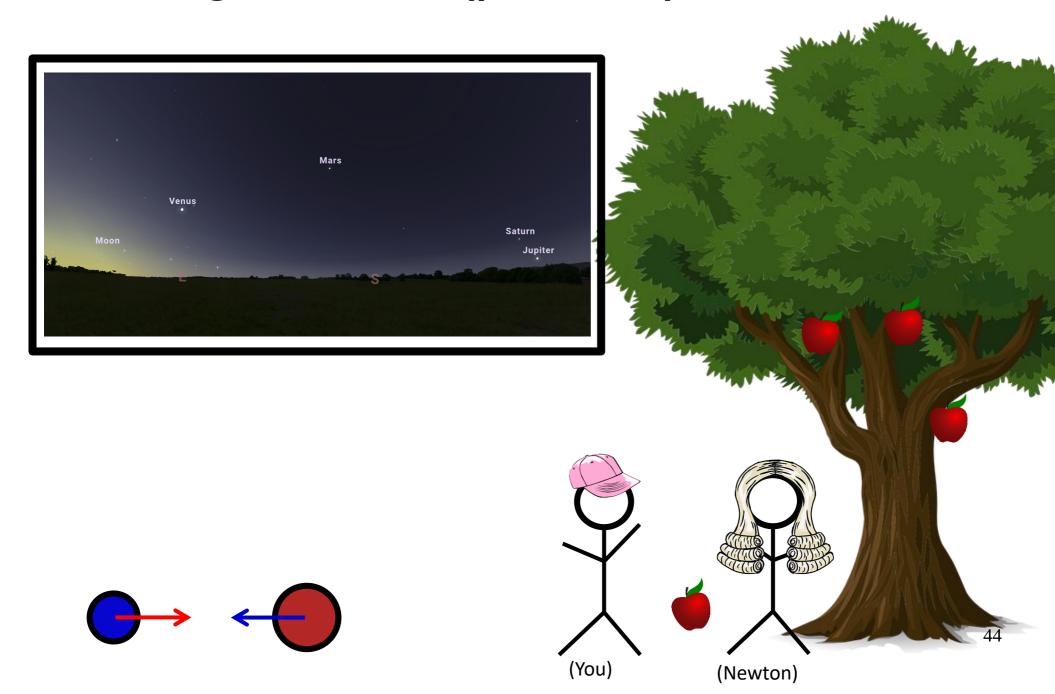
Questions?





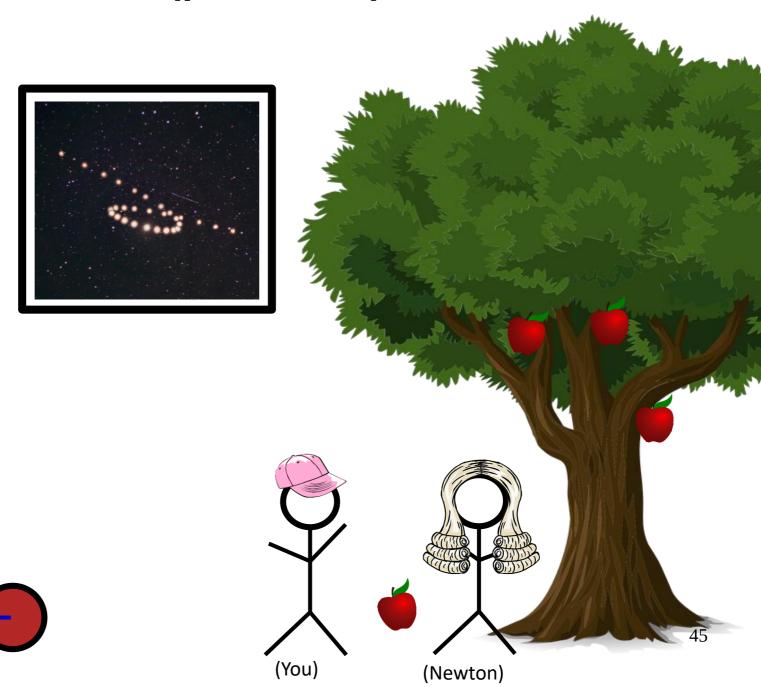


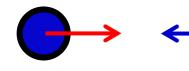




Behaviors:

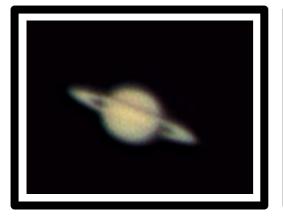
•Trajectories





Behaviors:

- •Trajectories
- Structure

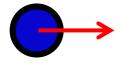


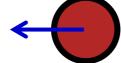




(Newton)

(You)

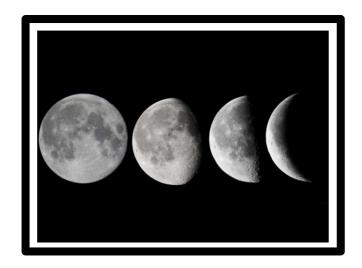


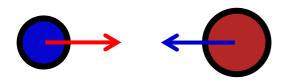


Building models (planets)

Behaviors:

- •Trajectories
- Structure
- Brightness







Building models (planets)

Behaviors:

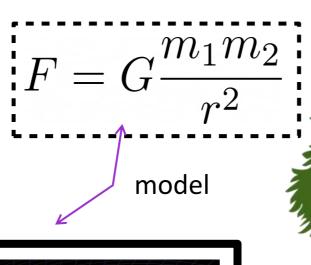
- Trajectories
- Structure
- Brightness

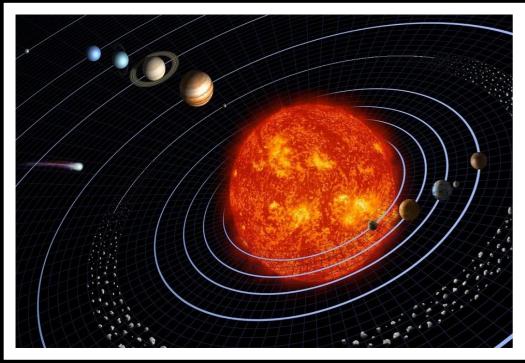


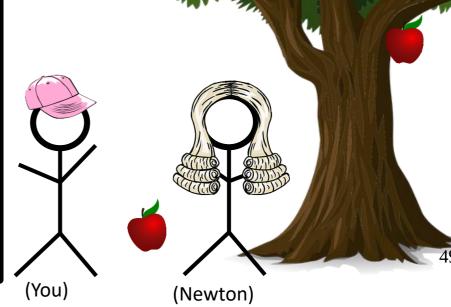


Behaviors:

- Trajectories
- Structure
- Brightness







Behaviors:



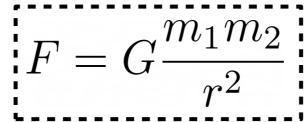
•Trajectories



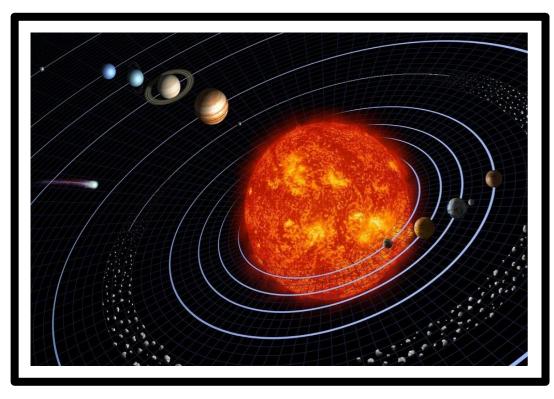
Structure

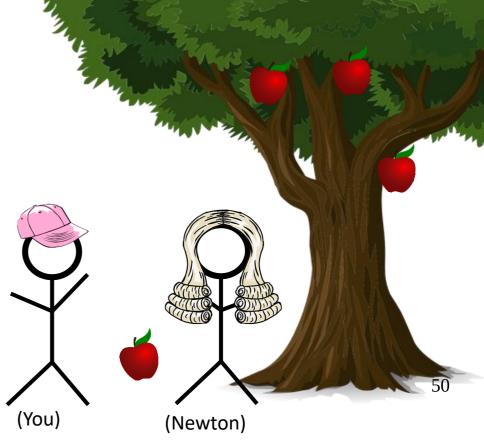


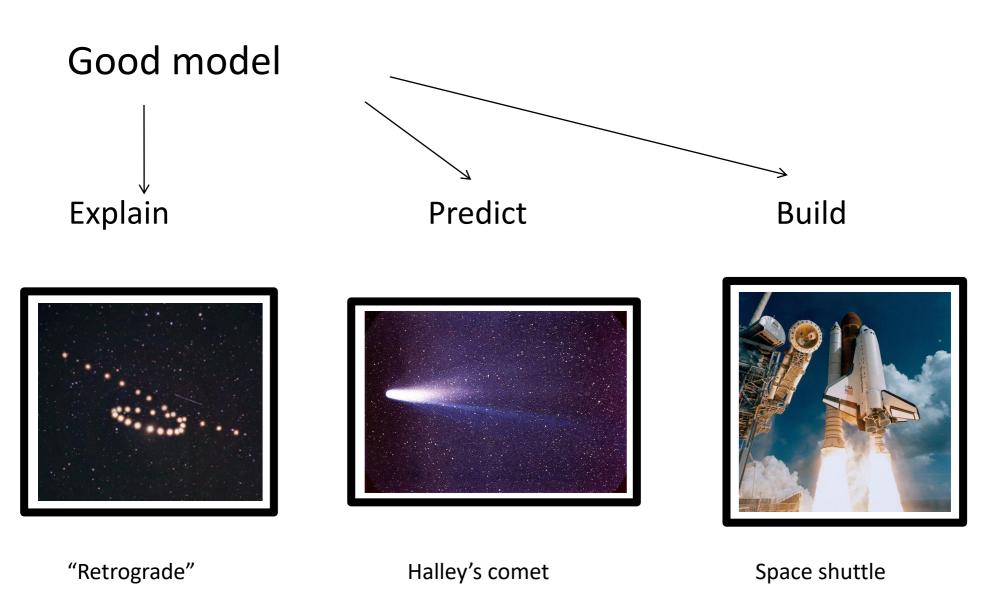
Brightness



Good model







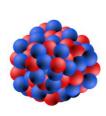
XXI century

Building models (nuclear)

Behaviors:

Binding energy

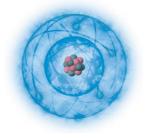
(energy "debt")

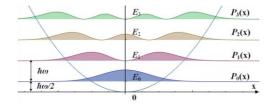




Structure

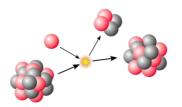
(arrangement of nucleons)



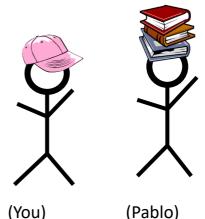


Reactions

(smashing nuclei)

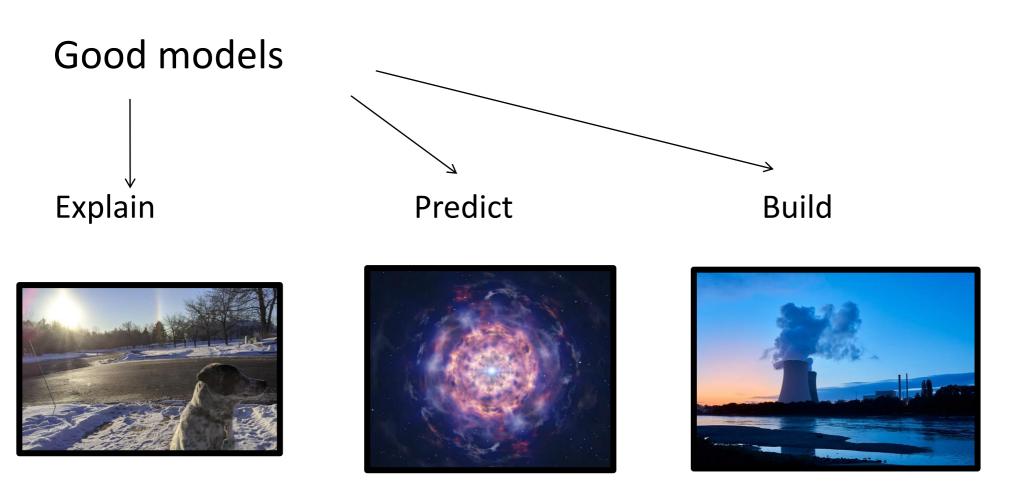








Building models (nuclear)



Burning Sun

Kilonova after merger

Nuclear energy

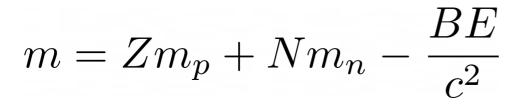
→ Energy needed to break it apart

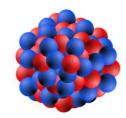
$$m = Zm_p + Nm_n - \frac{BE}{c^2}$$





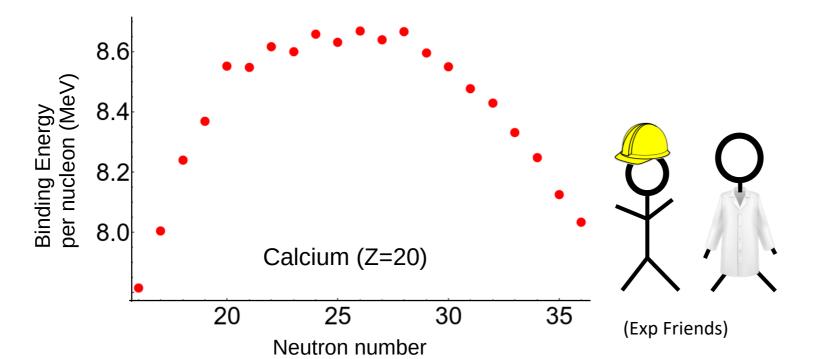
Energy needed to break it apart





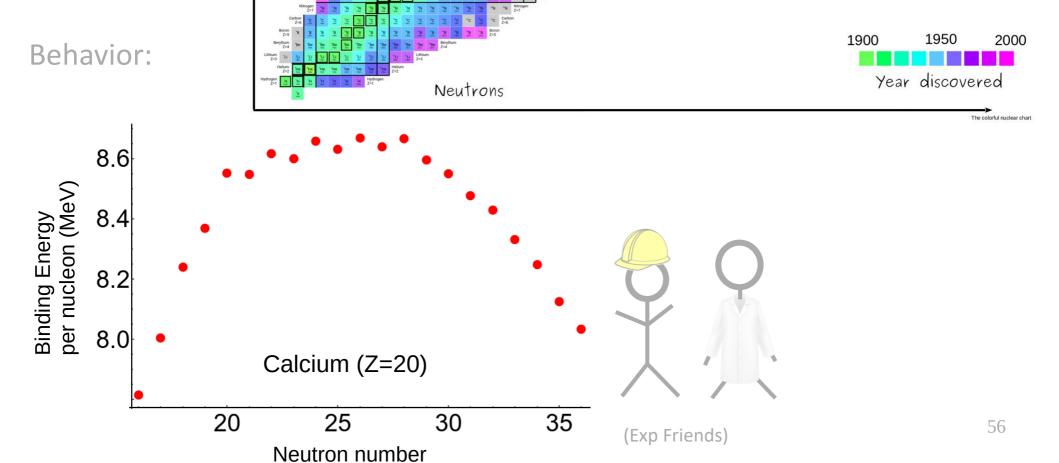


Behavior:

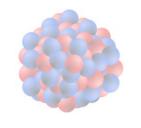




$$m = Zm_p$$



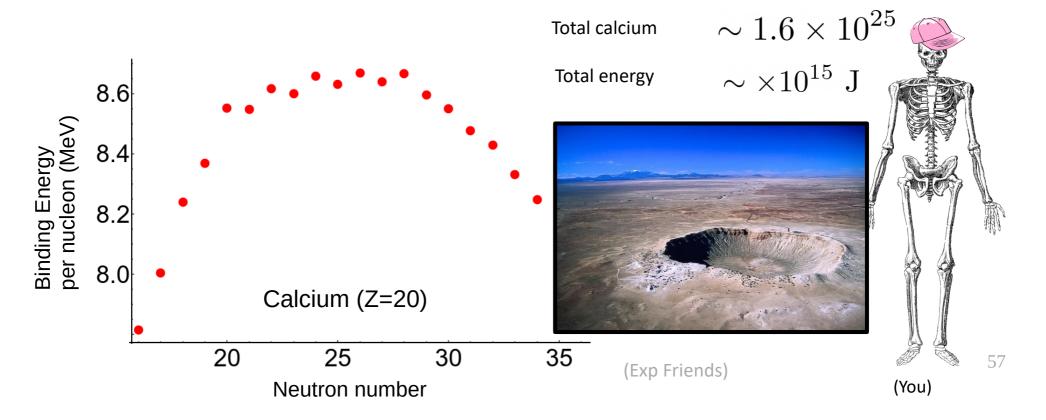
Energy needed to break it apart

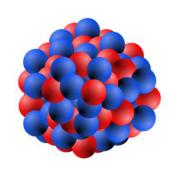


 $m_{\cdot} = Z_{\cdot} m_{\cdot \cdot \cdot} + V_{\cdot} m_{\cdot \cdot \cdot} - \frac{DL}{C}$

 \approx ($0.09\approx1/11$) \times impact energy forming Meteor Crater, Arizona (\approx 1 \times 10 16 J)

≈ energy released by a hurricane in 1 second (≈6×10¹⁴ J)

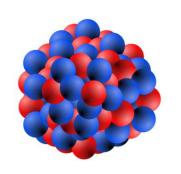




Liquid drop model



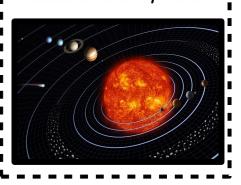
$$BE(N, Z) =$$



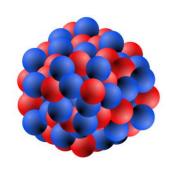
Liquid drop model



$$F = G \frac{m_1 m_2}{r^2}$$



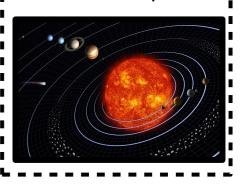
$$BE(N, Z) =$$



Liquid drop model



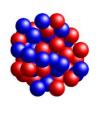
$$F = G \frac{m_1 m_2}{r^2}$$



$$BE(N, Z) =$$

More nucleons



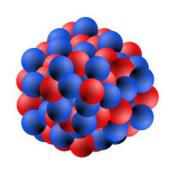




BE

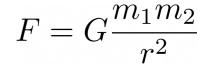


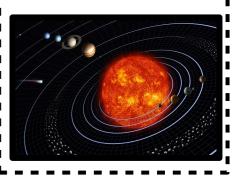




Liquid drop model



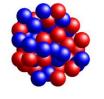




$$BE(N, Z) = a_V(N + Z)$$

More nucleons



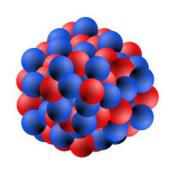




BE

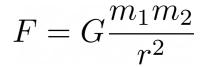






Liquid drop model





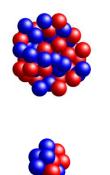


$$BE(N,Z) = a_V(N+Z)$$

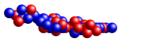
More nucleons

BE

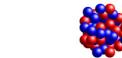
More surface



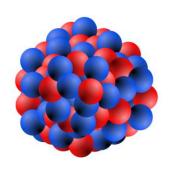






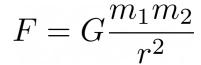


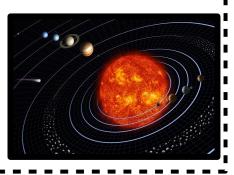




Liquid drop model



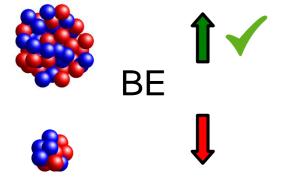


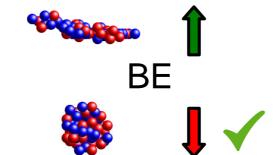


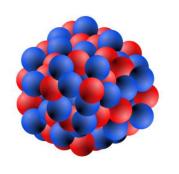
$$BE(N, Z) = a_V(N + Z) - a_S(N + Z)^{2/3}$$

More nucleons

More surface

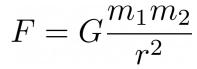






Liquid drop model





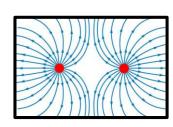


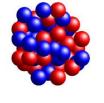
$$BE(N, Z) = a_V(N + Z) - a_S(N + Z)^{2/3}$$

More nucleons

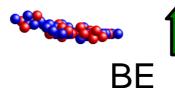
More surface

More protons



















BE



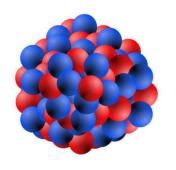






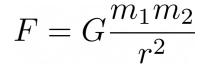


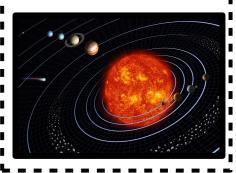




Liquid drop model





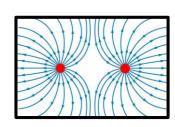


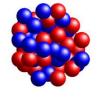
$$BE(N, Z) = a_V(N + Z) - a_S(N + Z)^{2/3} - a_C \frac{Z^2}{(N + Z)^{1/3}}$$

More nucleons

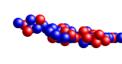
More surface

More protons



















BE



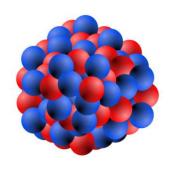






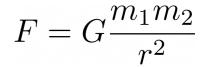






Liquid drop model







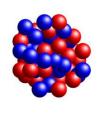
$$BE(N, Z) = a_V(N + Z) - a_S(N + Z)^{2/3} - a_C \frac{Z^2}{(N + Z)^{1/3}}$$

More nucleons

More surface

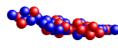
More protons

More asymmetry



























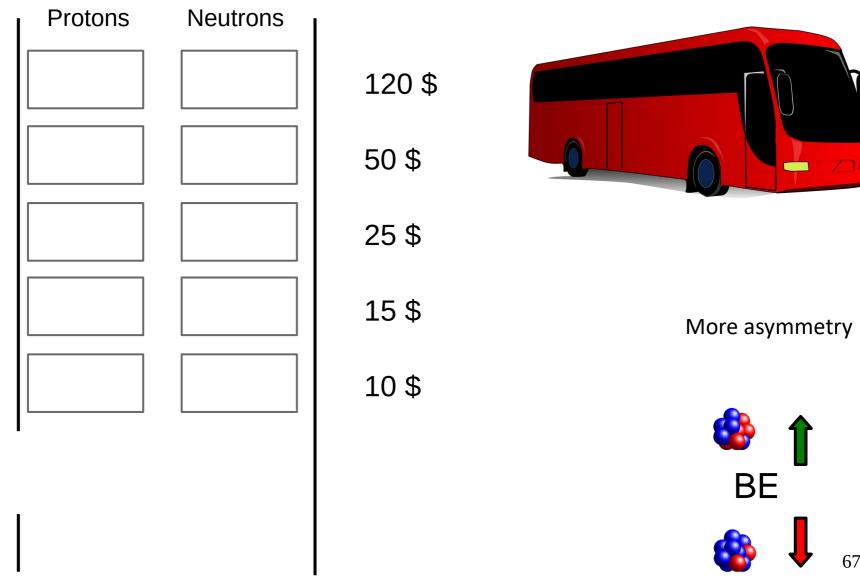


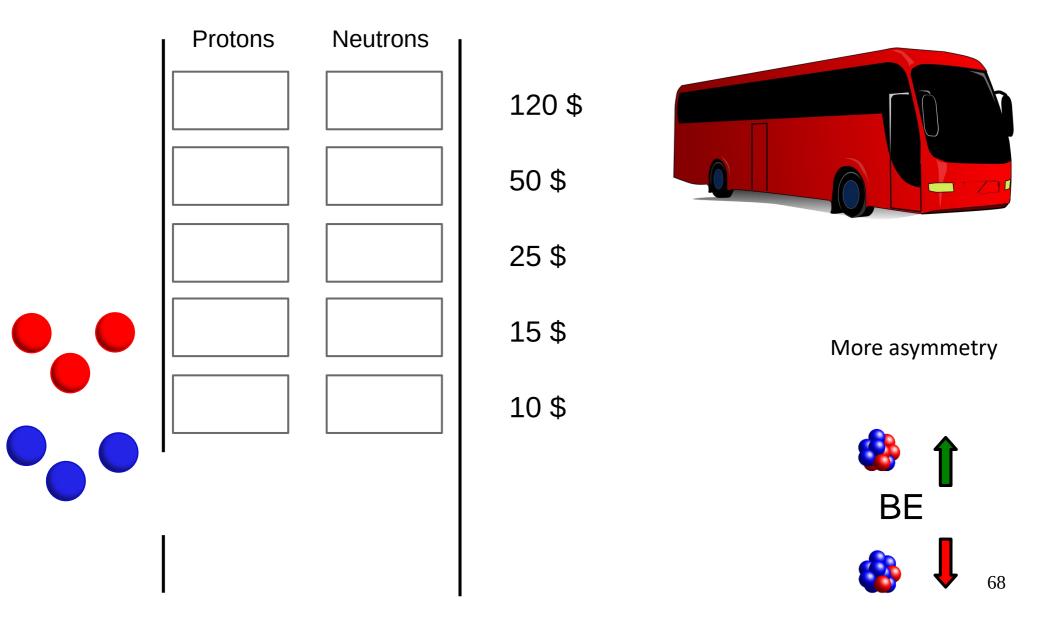


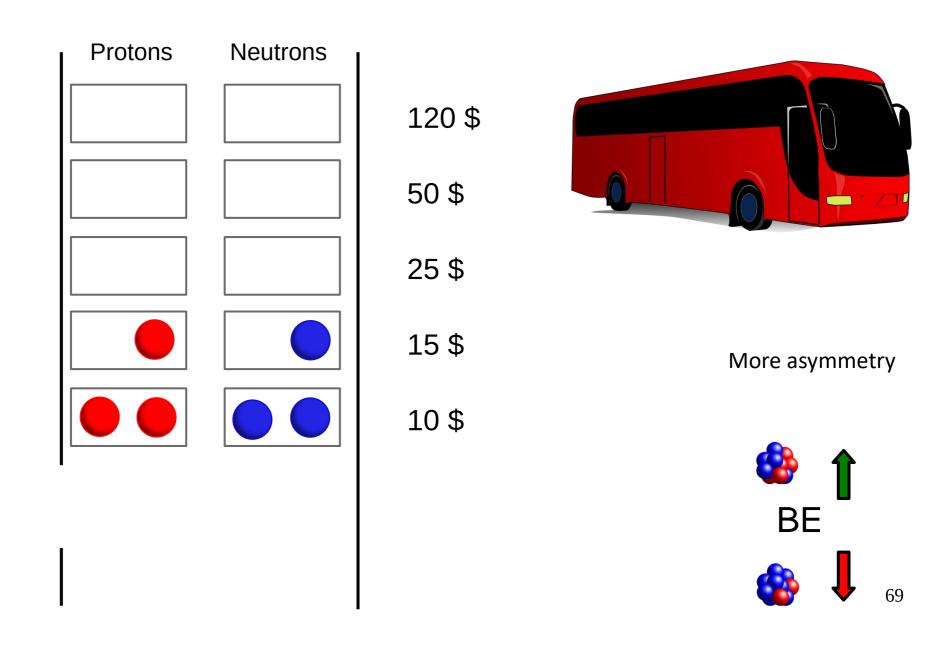


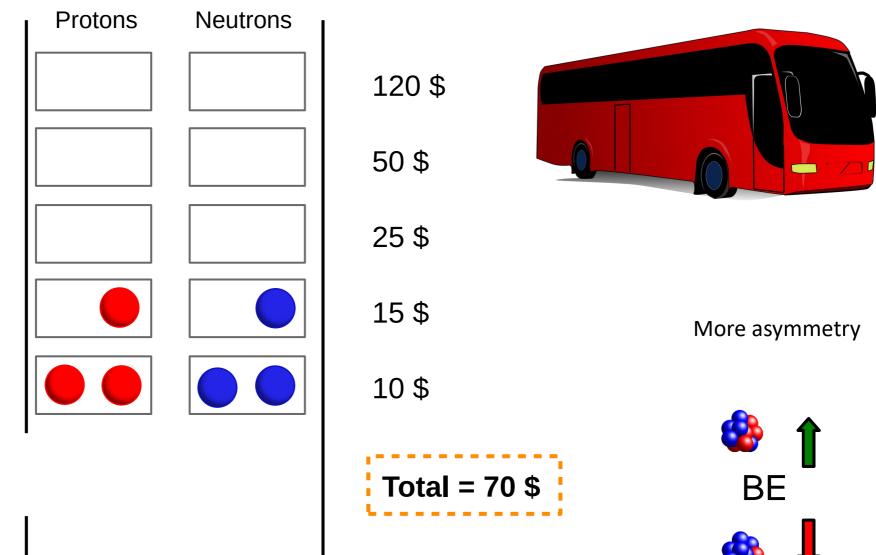


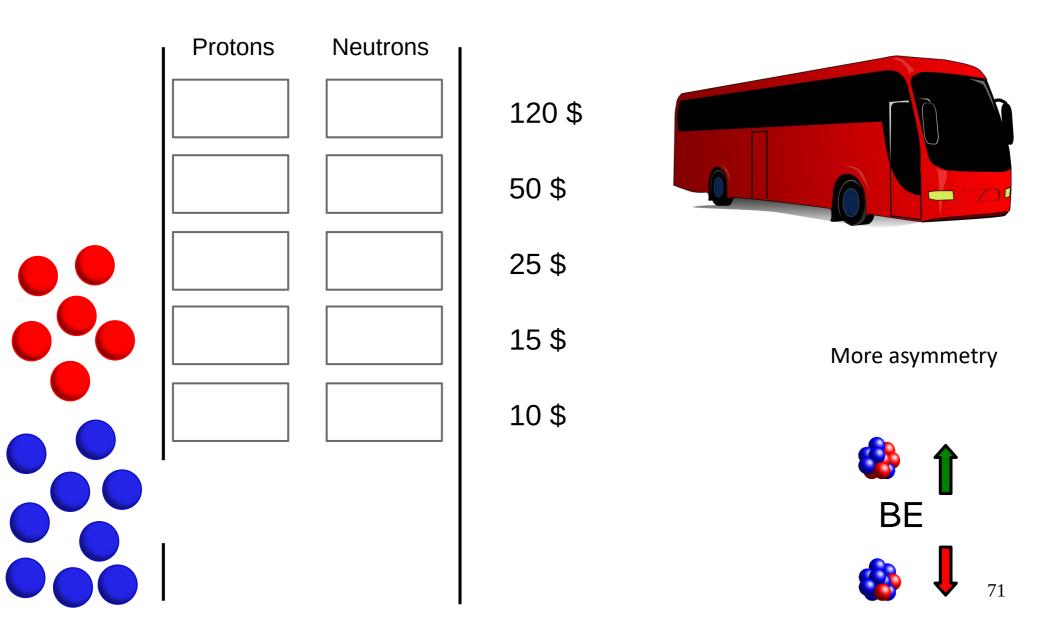


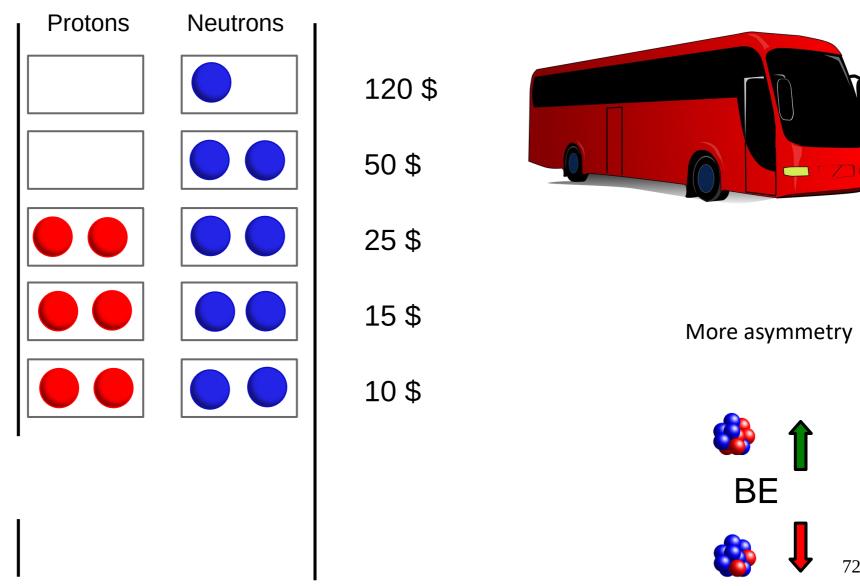




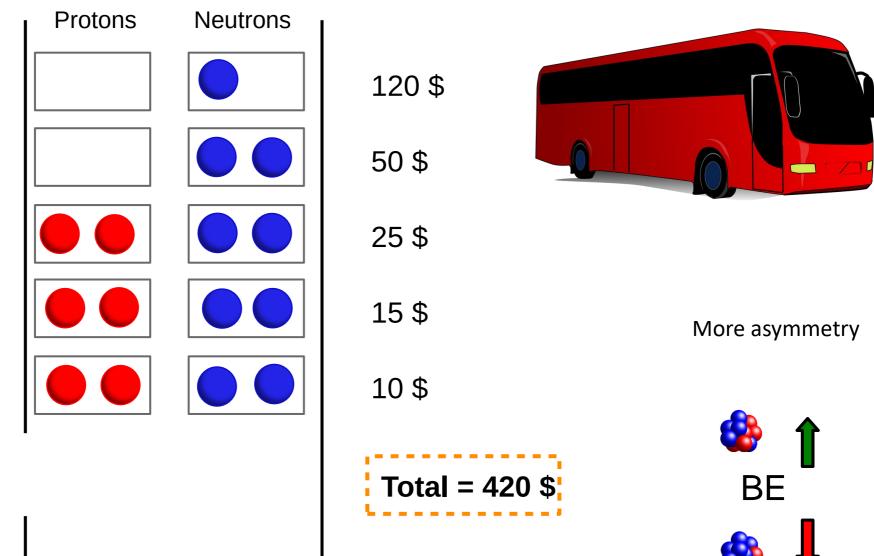




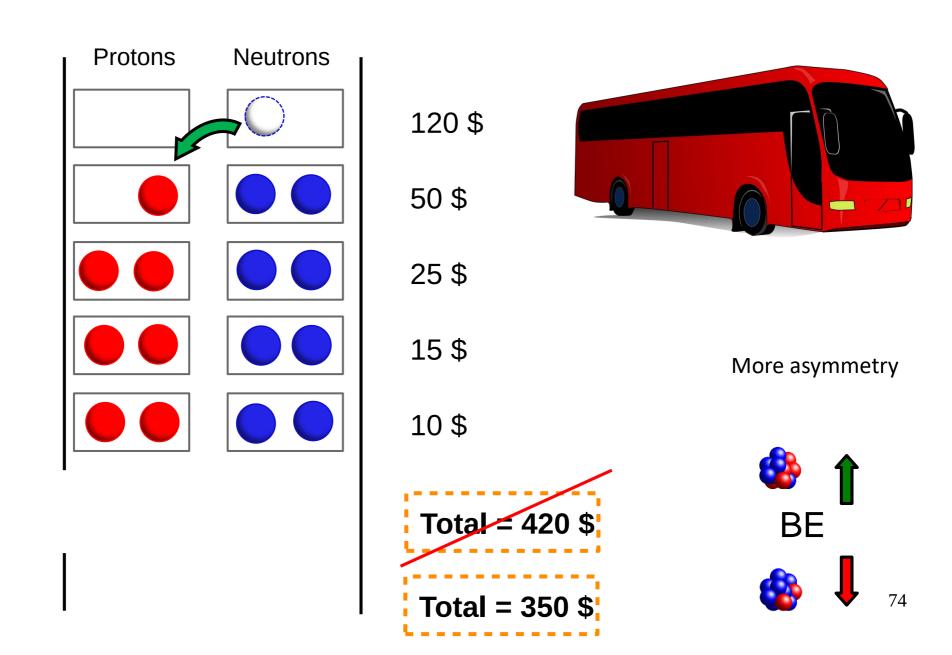




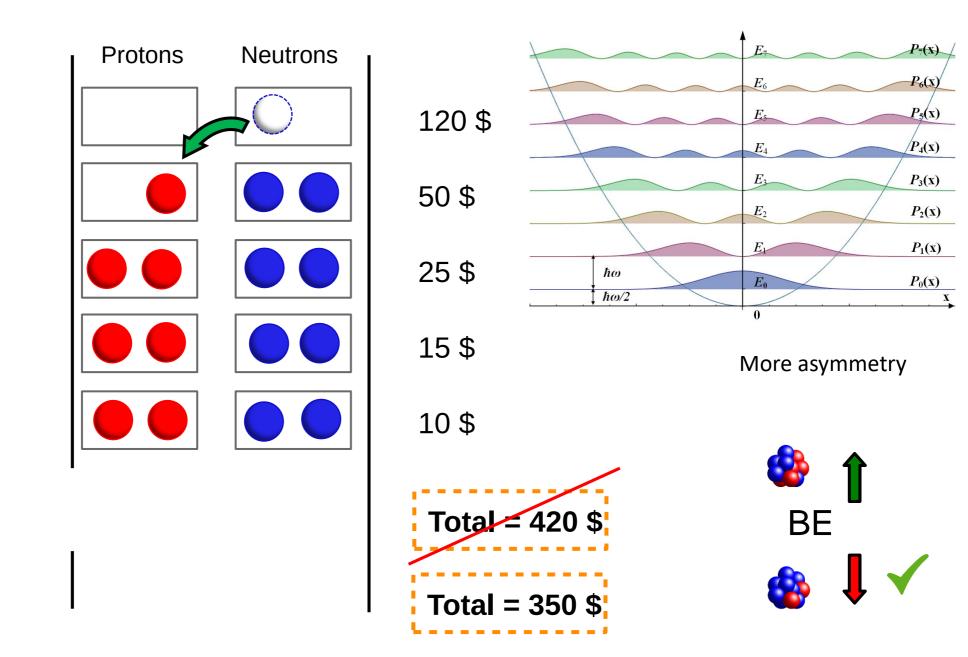
Binding energy (Asymmetry parenthesis)

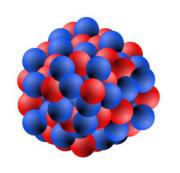


Binding energy (Asymmetry parenthesis)



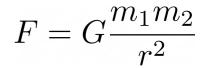
Binding energy (Asymmetry parenthesis)

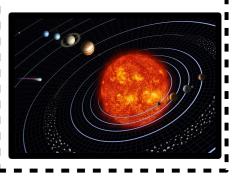




Liquid drop model







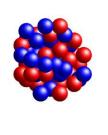
$$BE(N,Z) = a_V(N+Z) - a_S(N+Z)^{2/3} - a_C \frac{Z^2}{(N+Z)^{1/3}} - a_A \frac{(N-Z)^2}{N+Z}$$

More nucleons

More surface

More protons

More asymmetry



BE

















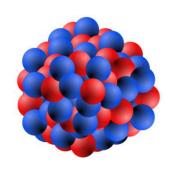








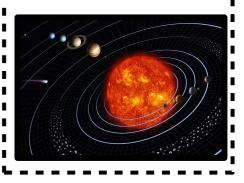




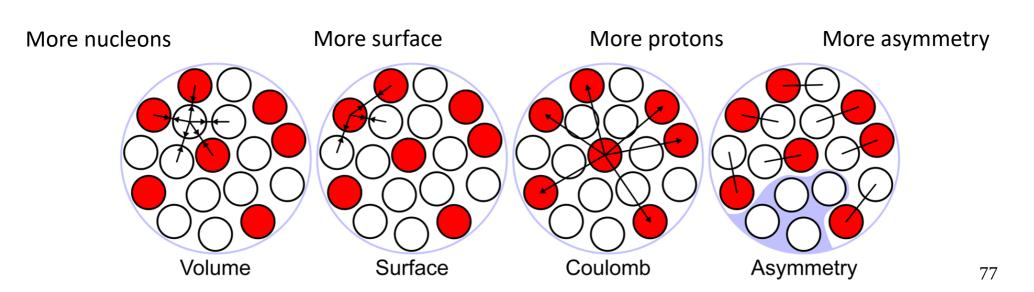
Liquid drop model



$$F = G \frac{m_1 m_2}{r^2}$$



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Liquid drop model

Mean squared error: 0.02 Variance score: 0.96

Mean absolute error: 0.07

[14.01172846 13.28609536 0.57346032 16.98655754]

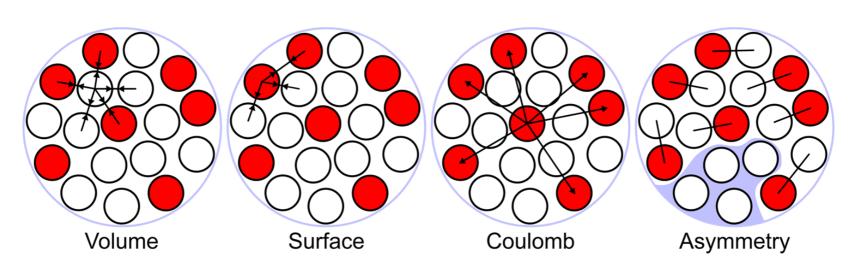
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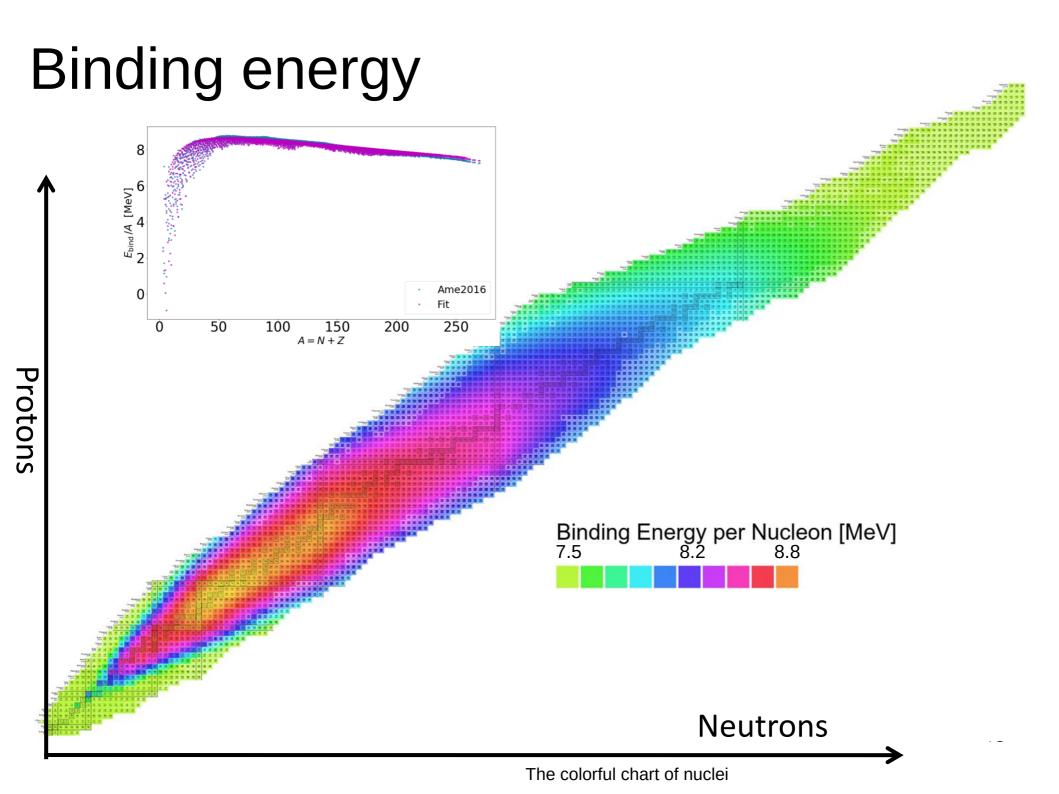
More nucleons

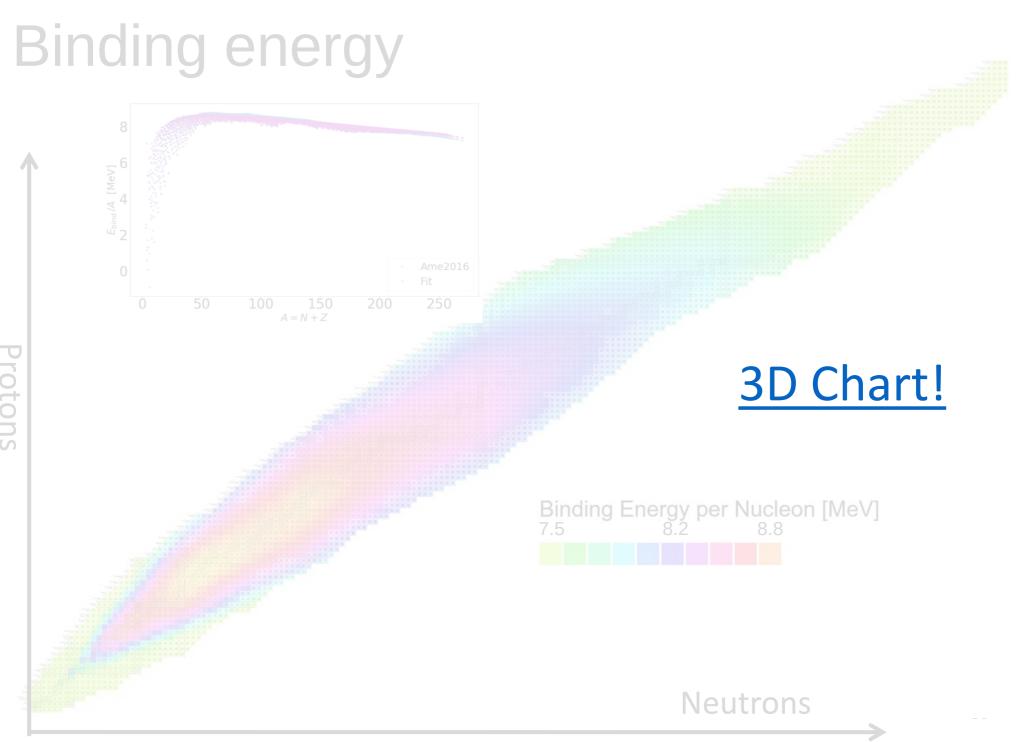
More surface

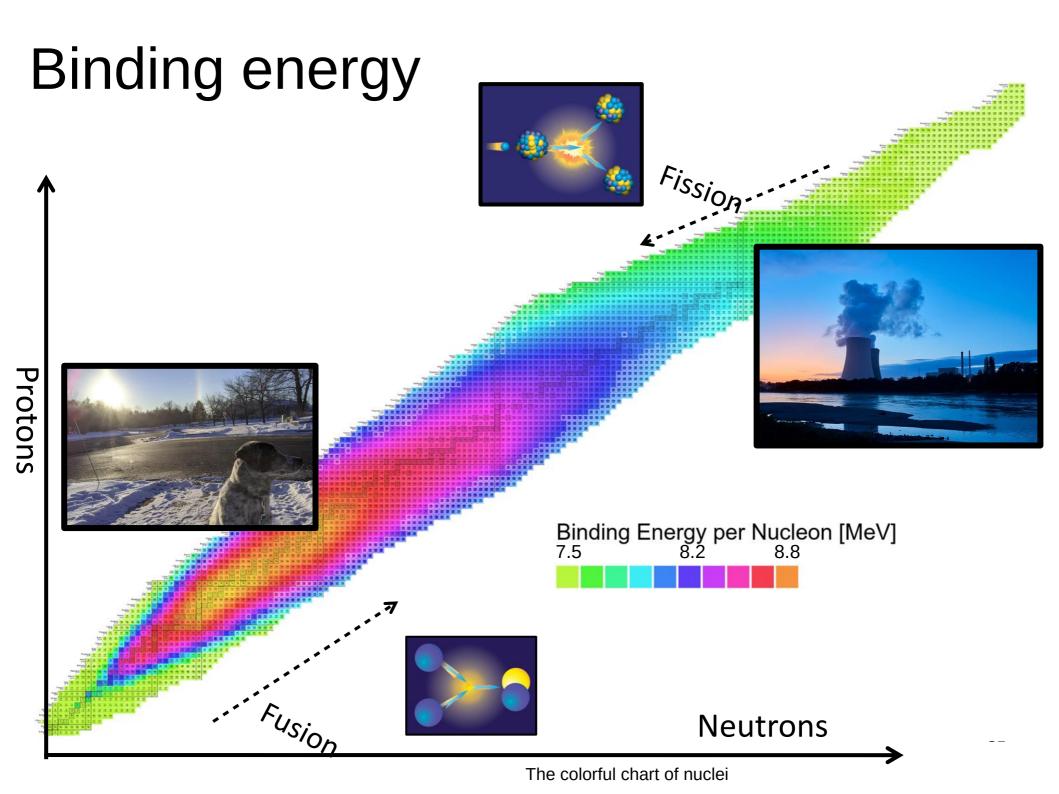
More protons

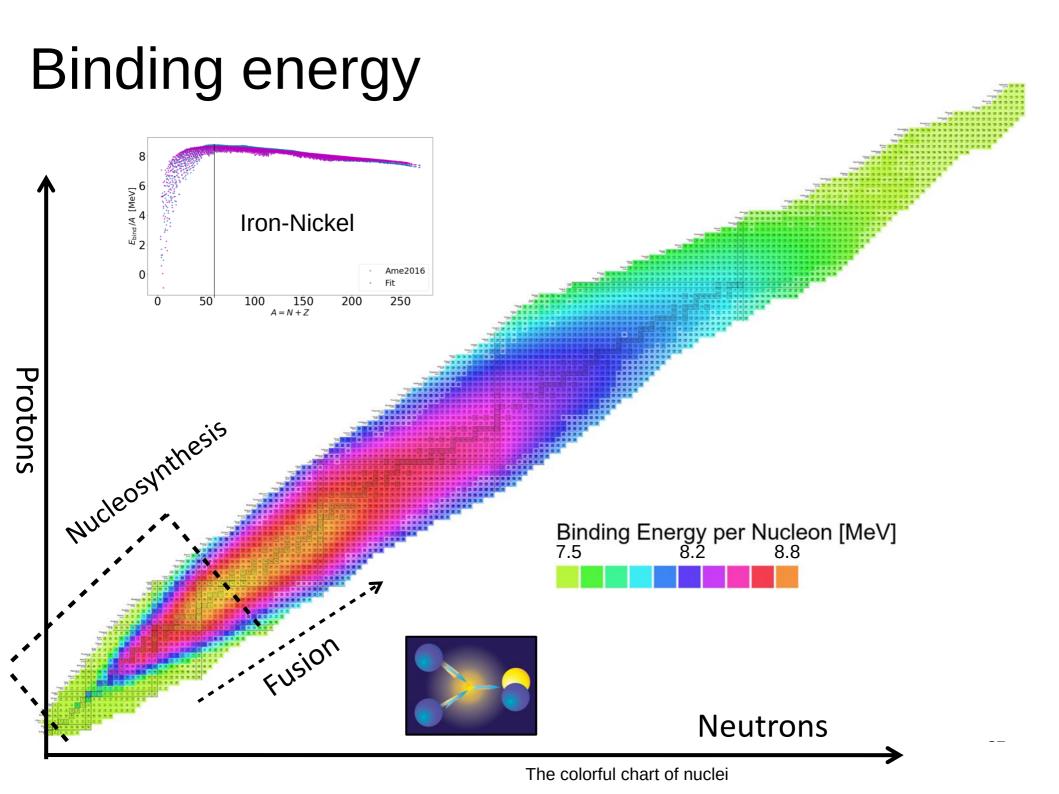
More asymmetry

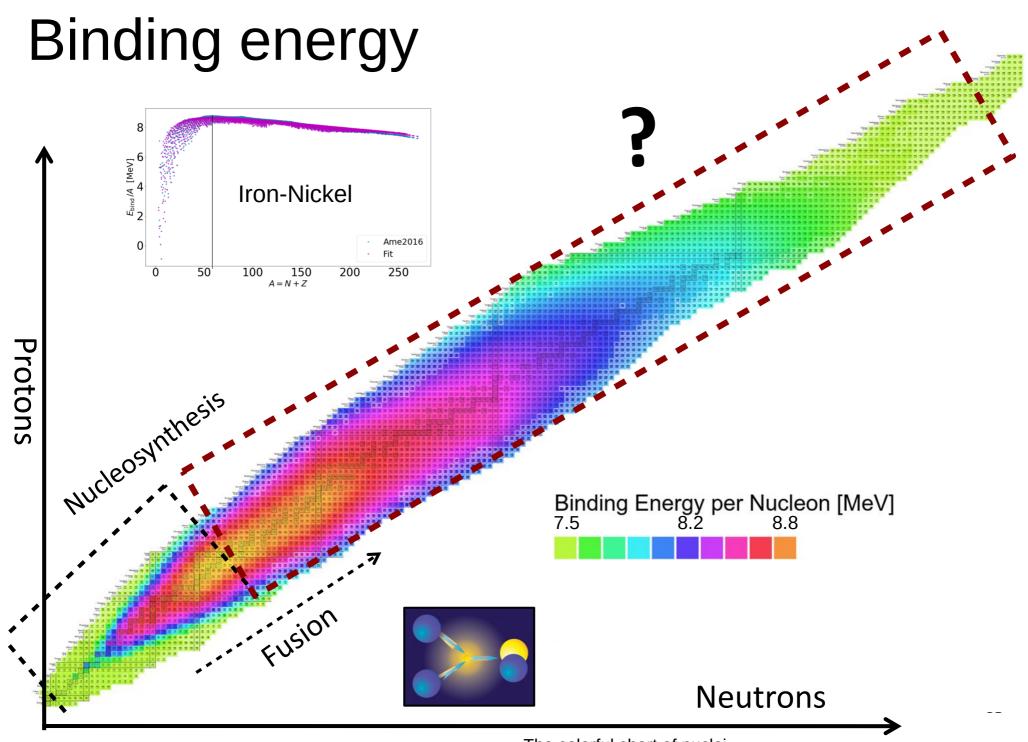


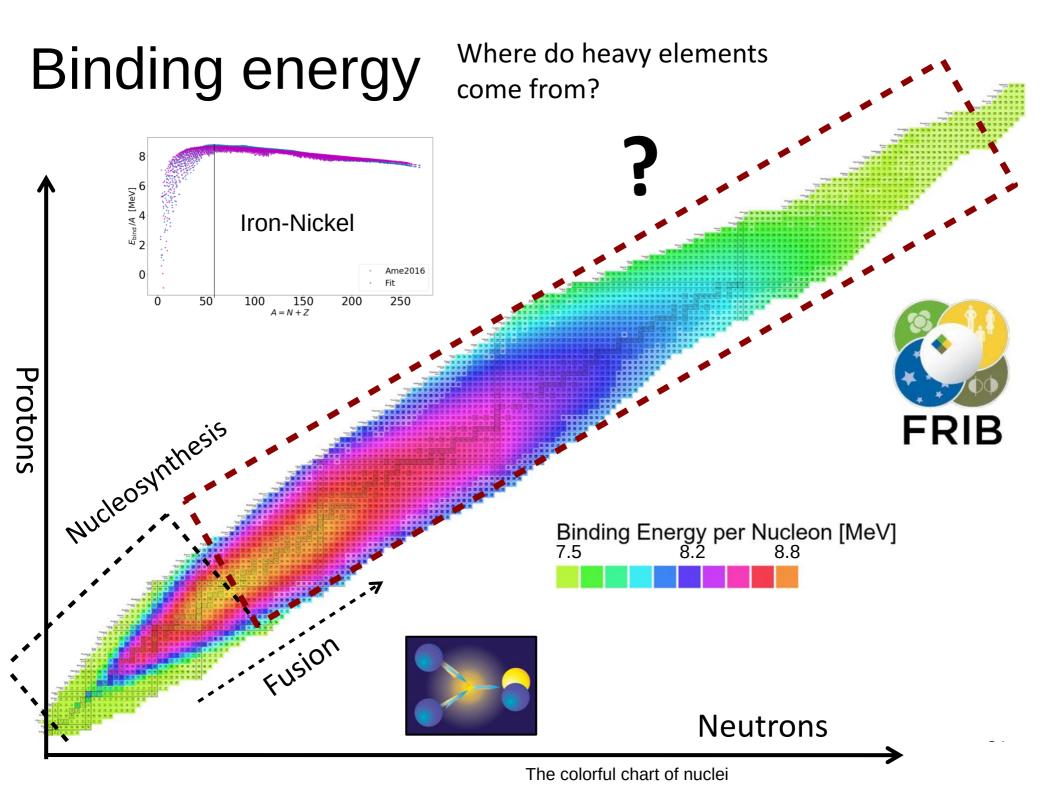


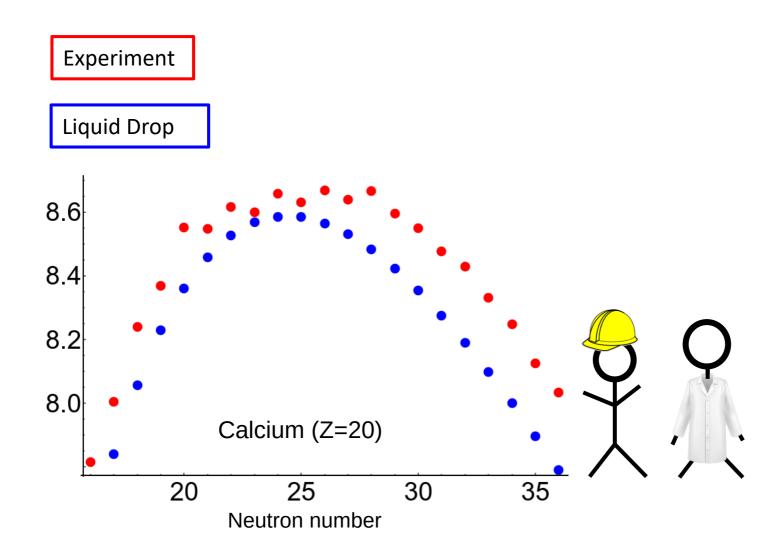


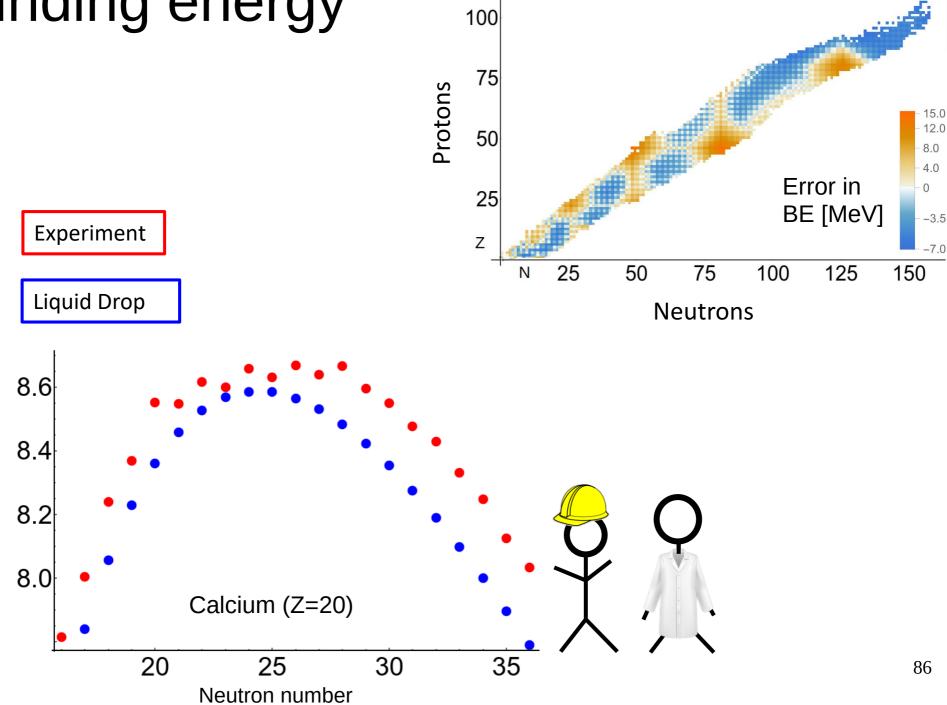


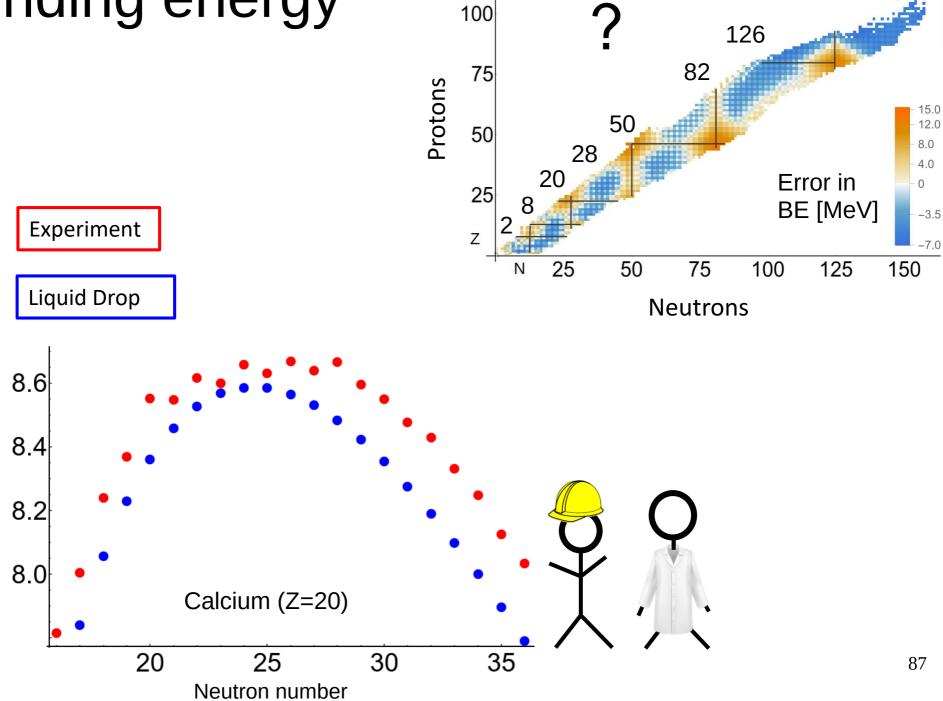




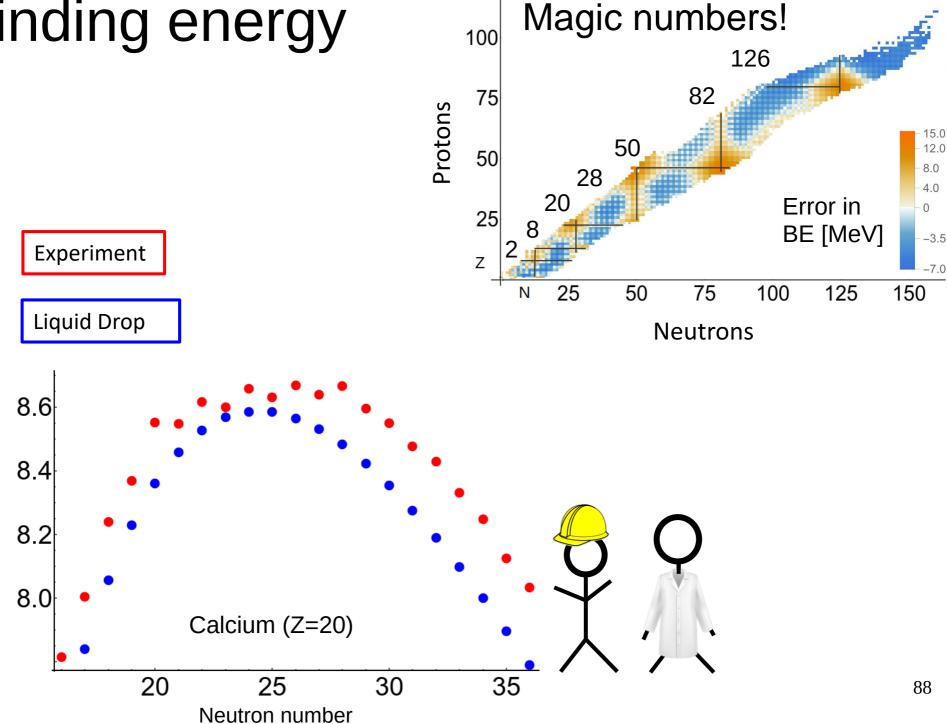








Rinding I



For today

Who am 1?

Why theory?

Building models

Building a (simple) nuclear mode

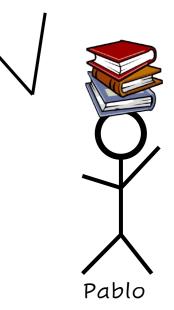
Quantum mechanics



Building (better) nuclear models

Challenges (Hands-On Session)

Questions?



"I think I can safely say that nobody understands quantum mechanics."

Richard Feynman

"I think I can safely say that nobody understands quantum mechanics."

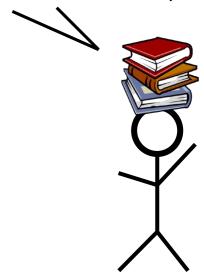
two things we need today



1) Everything comes in "quanta"

two things we need today

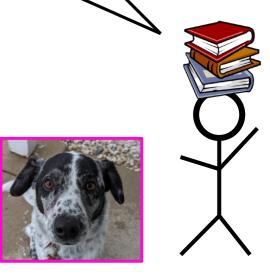




1) Everything comes in "quanta"

2) Schrodinger equation* describes the dynamics of the system

two things we need today

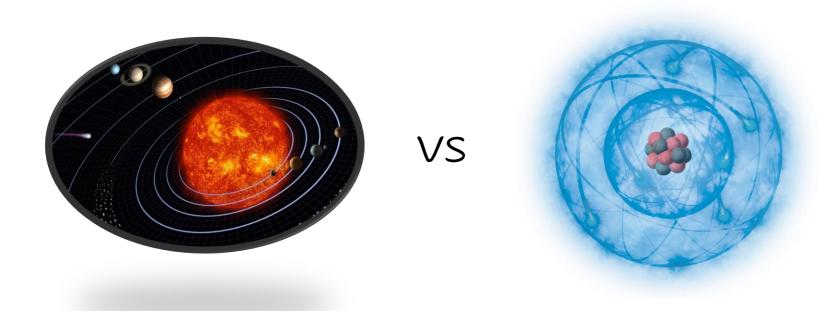






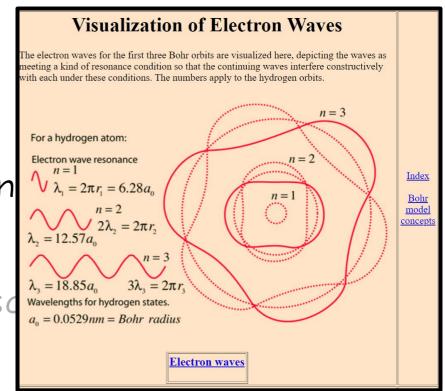
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1) Everything comes in "quan

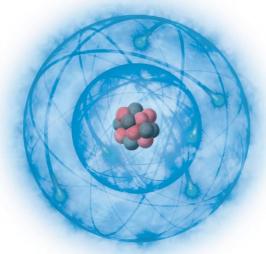
2) Schrodinger equation* desc dynamics of the system



http://hyperphysics.phy-astr.gsu.edu/hbase/ewav.html

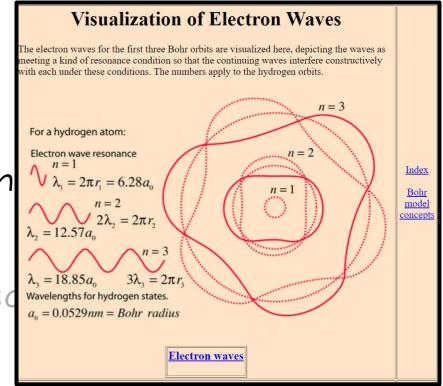


VS

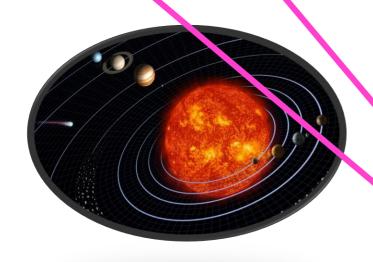


1) Everything comes in "quan

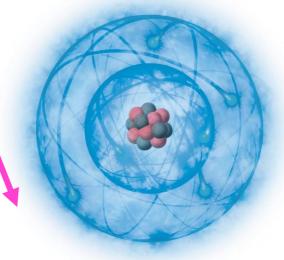
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VS

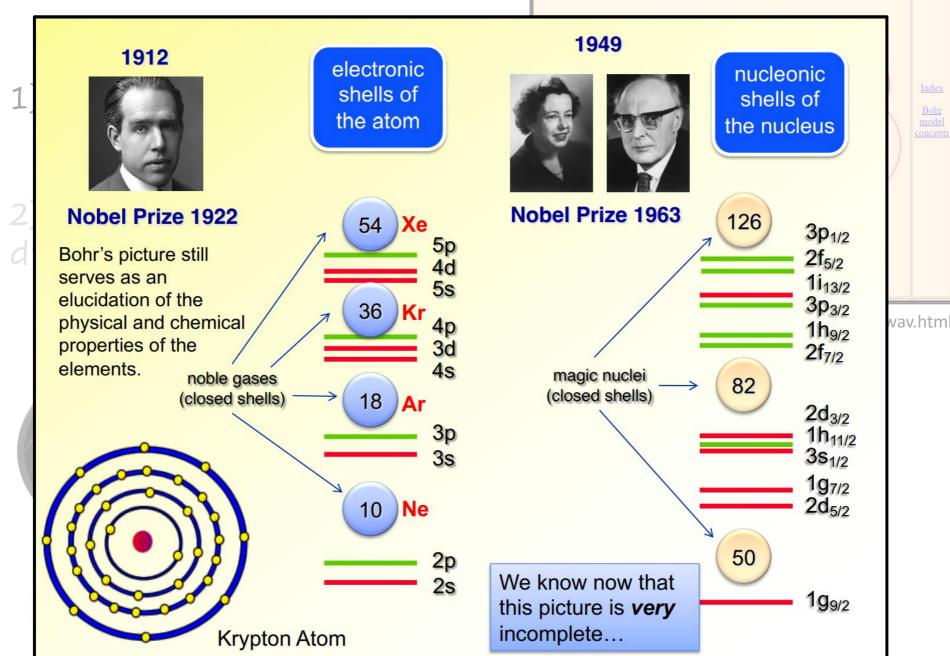


Pablo: don't forget the rope

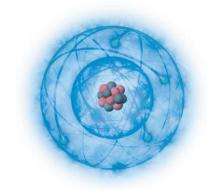
Thanks Tibor for the rope!!

Visualization of Electron Waves

The electron waves for the first three Bohr orbits are visualized here, depicting the waves as meeting a kind of resonance condition so that the continuing waves interfere constructively with each under these conditions. The numbers apply to the hydrogen orbits.



Slide made by Witek Nazarewicz



1) Everything comes in "quanta"

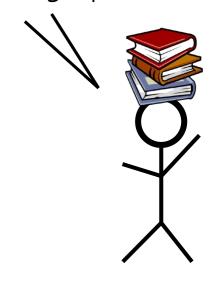
2) Schrodinger equation* describes the dynamics of the system

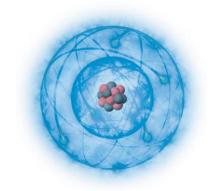


Nuclei looks more like an onion than like grapes

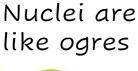


Nucleus





- 1) Everything comes in "quanta"
- 2) Schrodinger equation* describes the dynamics of the system



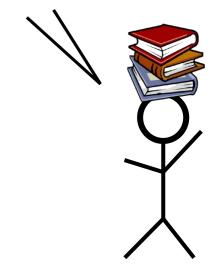


Not-nucleus

Nuclei looks more like an onion than like grapes



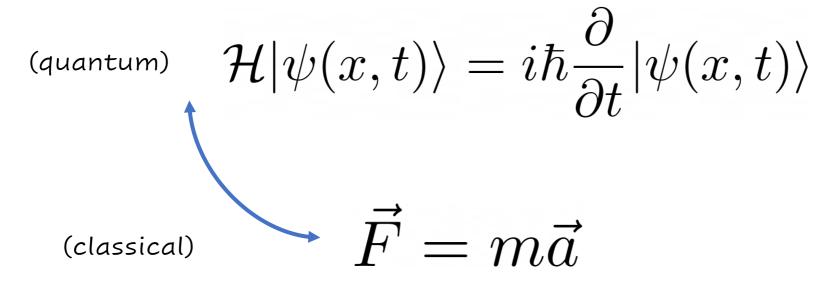
Nucleus



- 1) Everything comes in "quanta"
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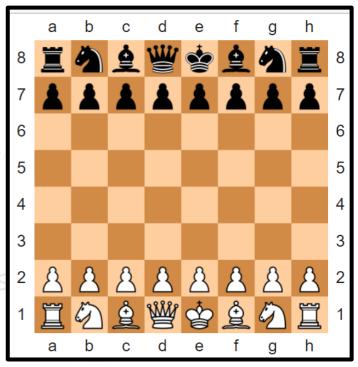
$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

- 1) Everything comes in "quanta"
- 2) Schrodinger equation* describes the dynamics of the system



1) Everything comes in "quantum

 Schrodinger equation* describes dynamics of the system

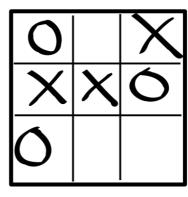


Chess

(quantum) $\mathcal{H}|\psi(x,t)
angle=i\hbarrac{\partial}{\partial t}|\psi(x,t)$

(classical)





Tic tac toe

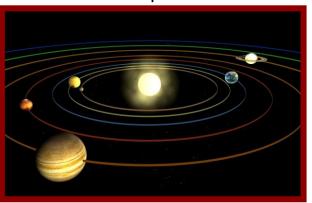
Think of it as the rules of the game



1) Everything co

$$F = G \frac{m_1 m_2}{r^2}$$

Solar System Video - The Best Planet Video for Educational Purposes



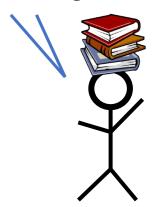
 Schrodinger equation* describes the dynamics of the system

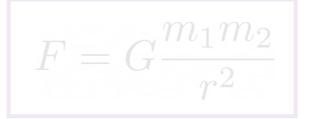
(quantum)
$$\mathcal{H}|\psi(x,t)
angle=i\hbarrac{\partial}{\partial t}|\psi(x,t)
angle$$

(classical)

$$\vec{F} = m\vec{a}$$

Think of it as the rules of the game







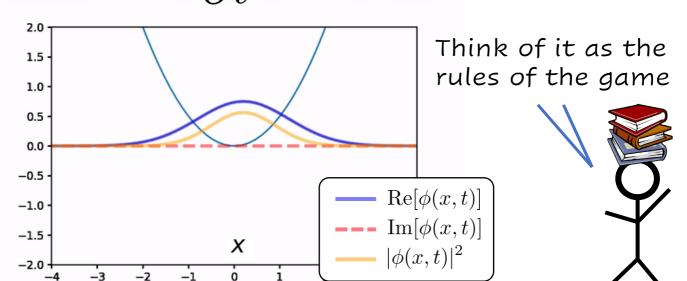
2) Schrodinger equation* describes the dynamics of the system

(quantum)

$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x^2$$

Harmonic Oscillator

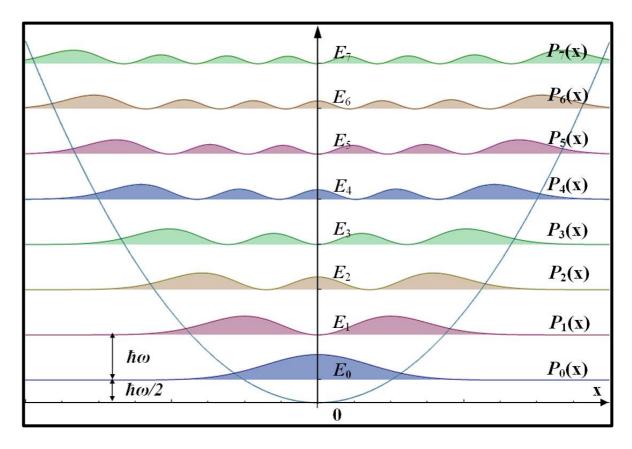


Spectrum

$$E_n=\hbar\omegaig(n+rac{1}{2}ig)$$

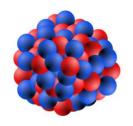
$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x^2$$

Harmonic Oscillator



$$\mathcal{H}|\psi(x)\rangle = E|\psi(x)\rangle$$

Can we model the nucleus with this?

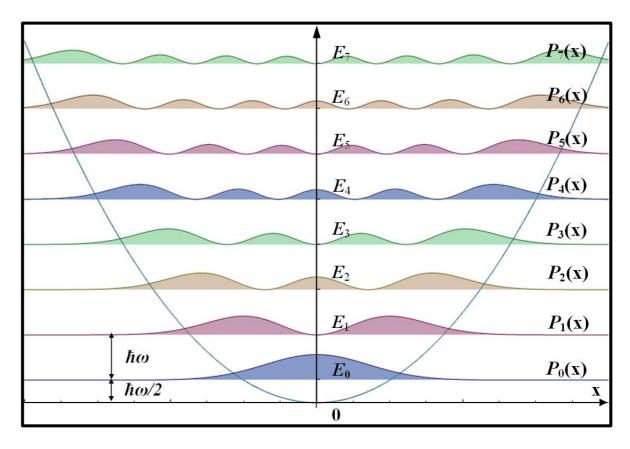


Spectrum

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Harmonic Oscillator



$$\mathcal{H}|\psi(x)\rangle = E|\psi(x)\rangle$$

Can we model the nucleus with this?

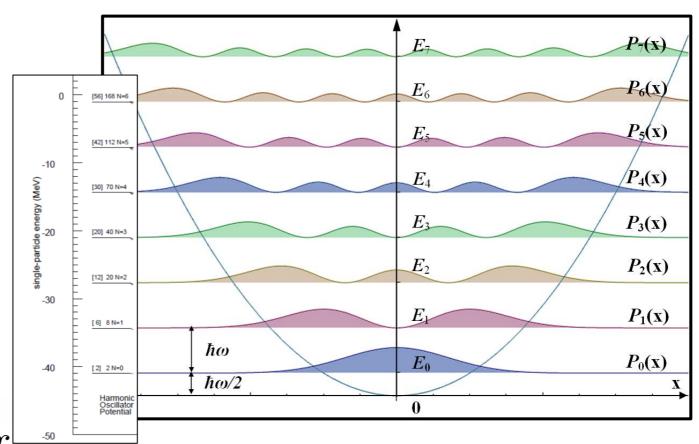


Spectrum

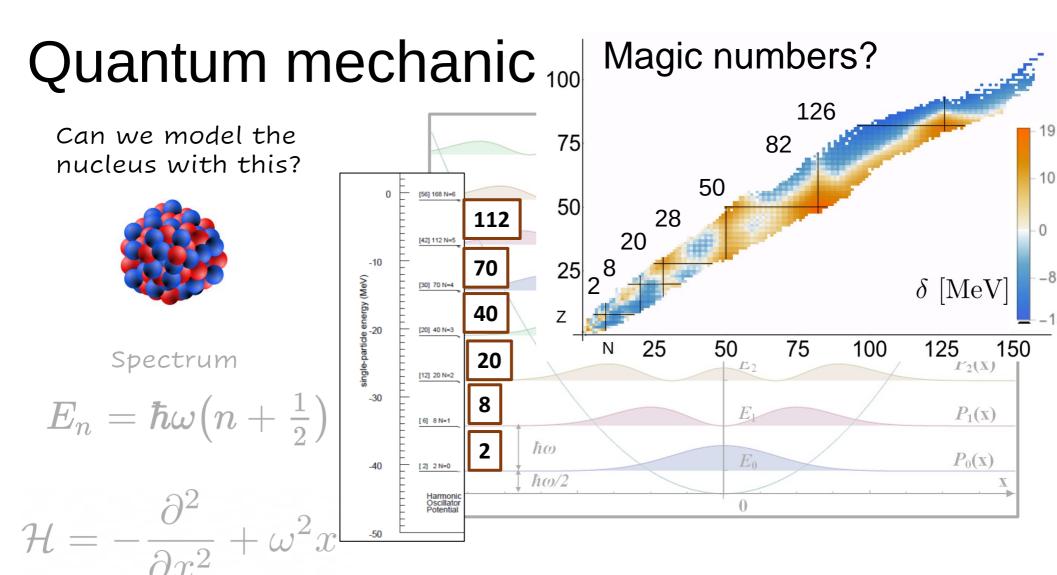
$$E_n=\hbar\omegaig(n+rac{1}{2}ig)$$

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x$$

Harmonic Oscillator

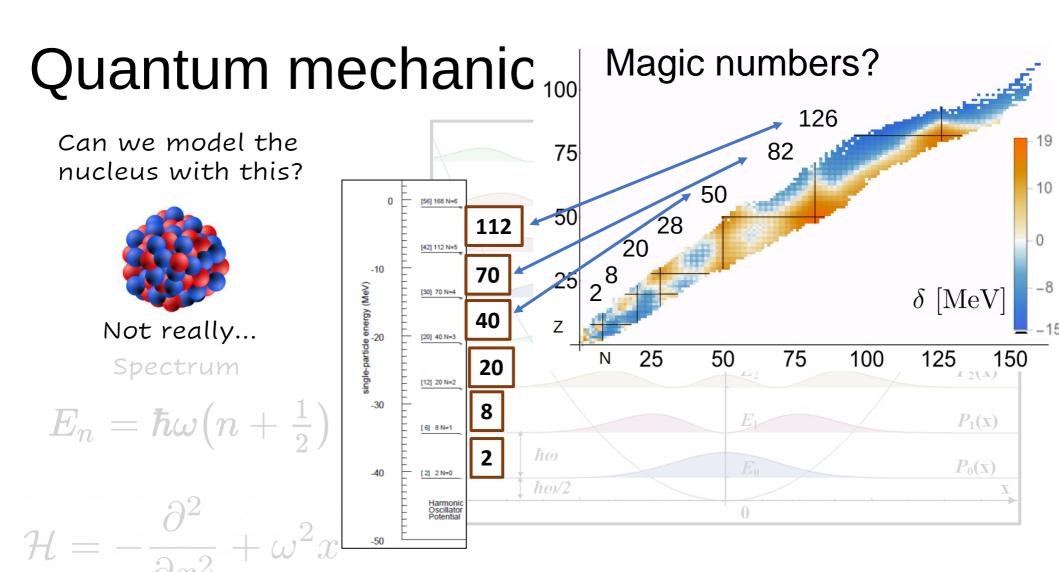


$$\mathcal{H}|\psi(x)\rangle = E|\psi(x)\rangle$$



Harmonic Oscillator

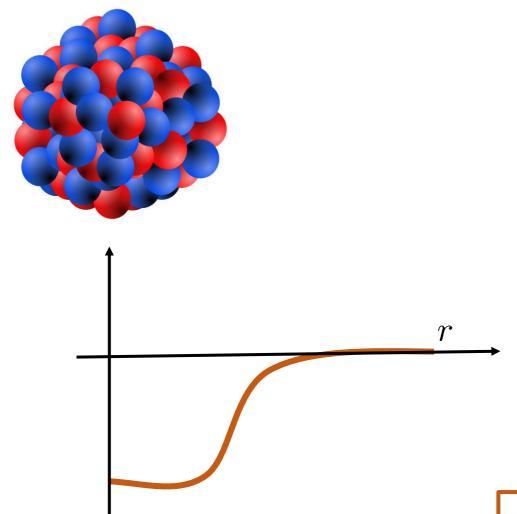
$$\mathcal{H}|\psi(x)\rangle = E|\psi(x)\rangle$$

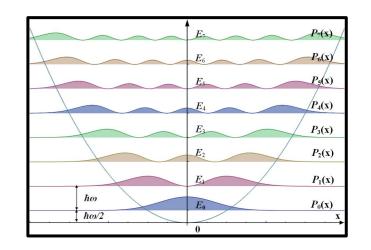


Harmonic Oscillator Time-independent

$$\mathcal{H}|\psi(x)\rangle = E|\psi(x)\rangle$$

Quantum mechanics



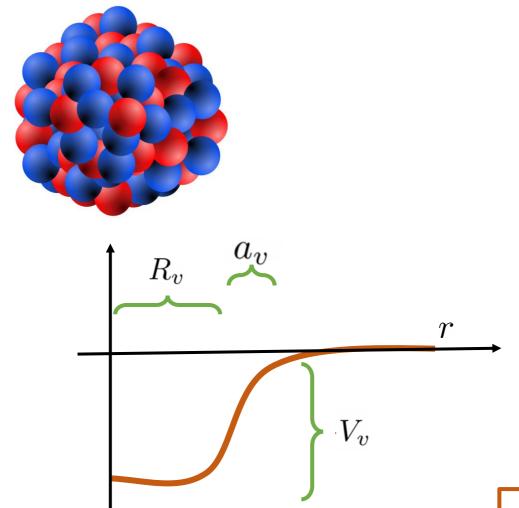


$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x^2$$

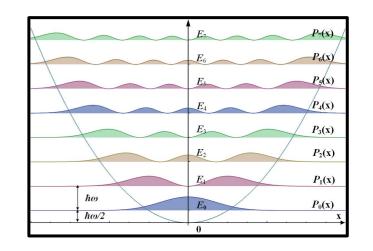
$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + V(r)$$

$$-V_v \left[1 + \exp\left(\frac{r - R_v}{a_v}\right) \right]$$

Quantum mechanics



Woods-Saxon potential

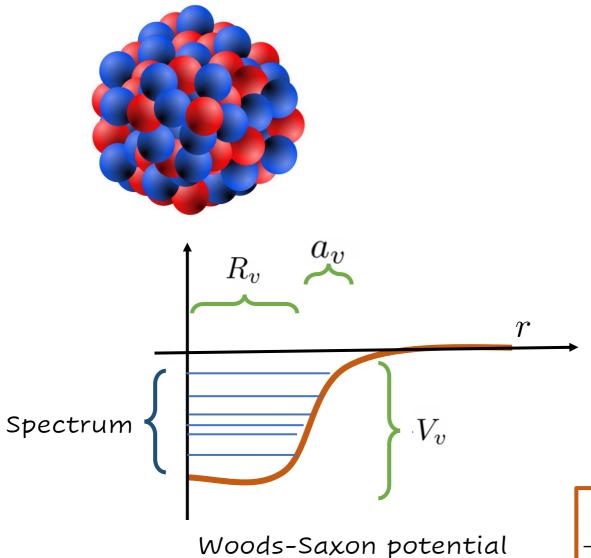


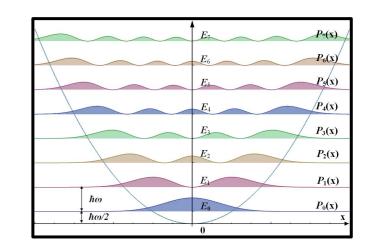
$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x^2$$

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + V(r)$$

$$-V_v \left[1 + \exp\left(\frac{r - R_v}{a_v}\right) \right]$$

Quantum mechanics





$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \omega^2 x^2$$

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + V(r)$$

$$-V_v \left[1 + \exp\left(\frac{r - R_v}{a_v}\right) \right]$$

 $P_7(\mathbf{x})$ Quantum mechanies $P_6(\mathbf{x})$ Neutron Single-Particle Energies Magic numbers! [16] 180 0j15 [8] 164 1g7 [2] 156 3s1 100 [2] 168 3s [10] 166 2d 0 [56] 168 N=6 126 6] 154 2d5 [18] 156 1g [12] 148 Oi11 [10] 136 1g9 75 82 112 [26] 138 Oi 126 [2] 126 2p1 [6] 124 1f5 10 50 [4] 118 2p3 [42] 112 N=5 [6] 112 2p [14] 114 Ói13 50 [14] 106 1f [10] 100 Oh9 28 8] 90 1f7 -10 **70** 0 20 [22] 92 0h single-partide energy (MeV) [12] 82 0h11 25 [30] 70 N=4 [2] 70 2s1 [4] 68 1d3 -8 [2] 70 2s $\delta \, [{\rm MeV}]$ [10] 68 1d [6] 64 1d5 [8] 58 Og7 40 Z 50 [18] 58 Og [20] 40 N=3 25 75 50 100 125 150 N [10] 50 0g9 [6] 40 1p [4] 38 1p3 [6] 34 0f5 20 [14] 34 01 [12] 20 N= [8] 28 Of7 [2] 20 1s [2] 20 1s1 -30 8 [4] 18 0d3 [10] 18 0d [6] 14 Od5 Spectrum [6] 8 N=1 8 [2] 8 0p1 [4] 6 0p3 [6] 8 Op -40 [2] 2 N=0 [2] 2 0s [2] 2 0s1 Woods-Saxon potent Woods-Saxon Plus Spin-Orbit Potential Woods-Saxon Harmonic Oscillator Potential Potential

-50

 $P_7(\mathbf{x})$ Quantum mechanics $P_6(\mathbf{x})$ **Neutron Single-Particle Energies** Magic numbers! [16] 180 0j15 [8] 164 1g7 100 [2] 168 3s [10] 166 2d 2] 156 3s1 0 126 [56] 168 N=6 6] 154 2d5 [18] 156 1g [12] 148 Oi11 [10] 136 1g9 75 82 112 [26] 138 Oi 126 [2] 126 2p1 [6] 124 1f5 10 50 [4] 118 2p3 [42] 112 N=5 [6] 112 2p [14] 114 Ói13 50 [14] 106 1f [10] 100 Oh9 28 8] 90 1f7 -10 **70** 0 20 [22] 92 0h single-partide energy (MeV) [12] 82 0h11 25 [30] 70 N=4 2] 70 2s1 [2] 70 2s $\delta \, [{\rm MeV}]$ 4] 68 1d3 [10] 68 1d [6] 64 1d5 [8] 58 Og7 40 Z 50 [18] 58 Og [20] 40 N=3 25 75 50 100 125 150 N [10] 50 0g9 [6] 40 1p [4] 38 1p3 [6] 34 0f5 20 [14] 34 01 [12] 20 N= [8] 28 Of7 [2] 20 1s [2] 20 1s1 -30 8 4] 18 Od3 [10] 18 0d [6] 14 Od5 Spectrum [6] 8 N=1 8

-40

-50

[2] 2 N=0

Harmonic

Oscillator

Potential

[2] 8 0p1 [4] 6 0p3

[2] 2 0s1

Woods-Saxon Plus Spin-Orbit Potential

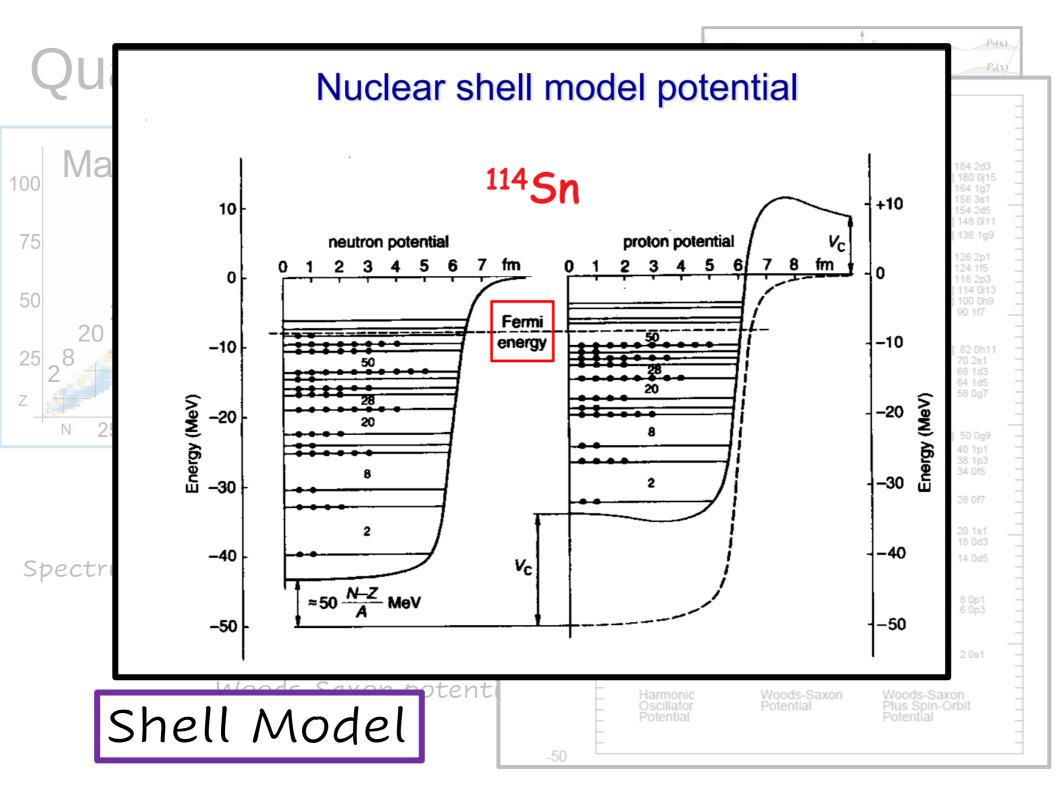
[6] 8 Op

[2] 2 0s

Woods-Saxon

Potential

Shell Model



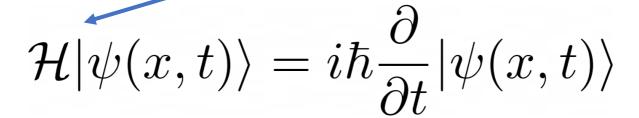
$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

Rules of the game (we don't have them)

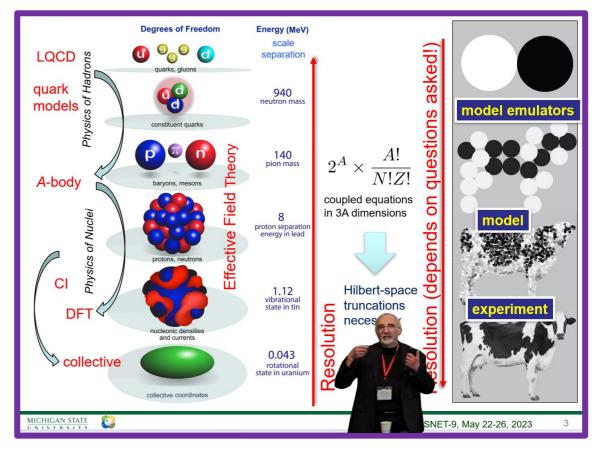
$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$



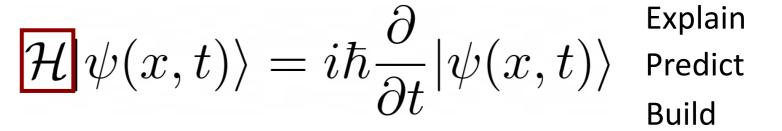
Rules of the game (we don't have them)



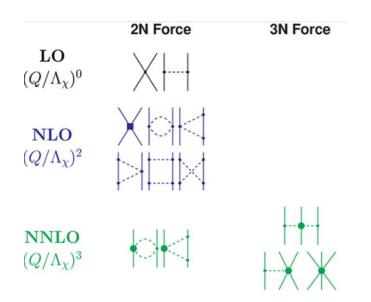




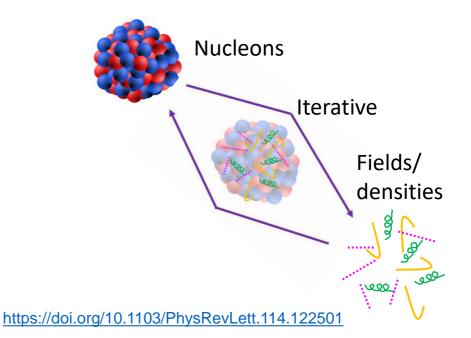
Each model is a new set of guessed rules



Chiral Effective Field Theory



Density Functional Theory



https://doi.org/10.3389/fphy.2020.00057

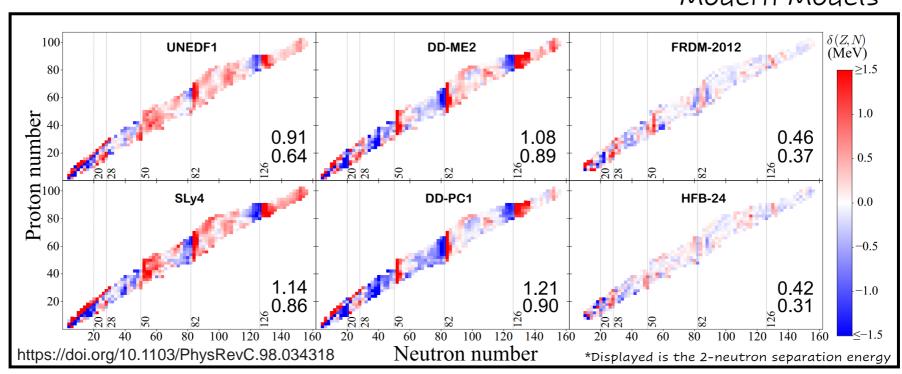
Each model is a new set of guessed rules

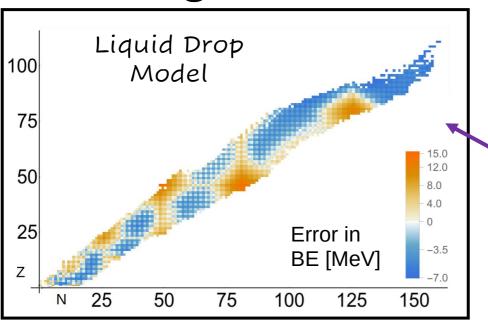


Nuclear Masses*



Modern Models

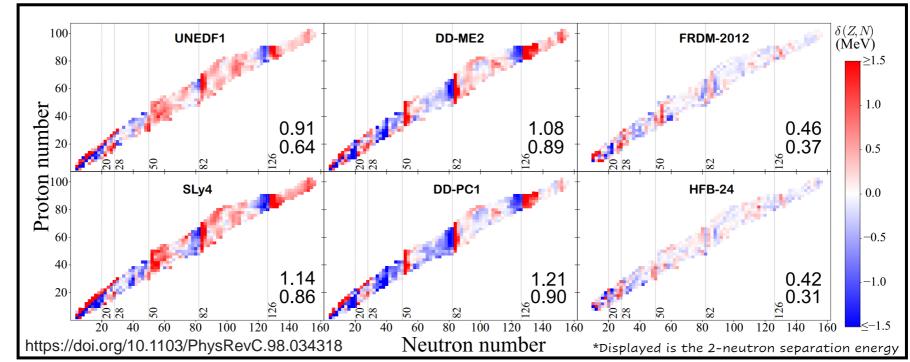




Each model is a new set of guessed rules

Nuclear Masses*

Modern Models

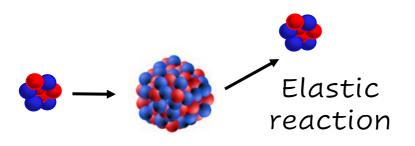


Building better models: Reactions

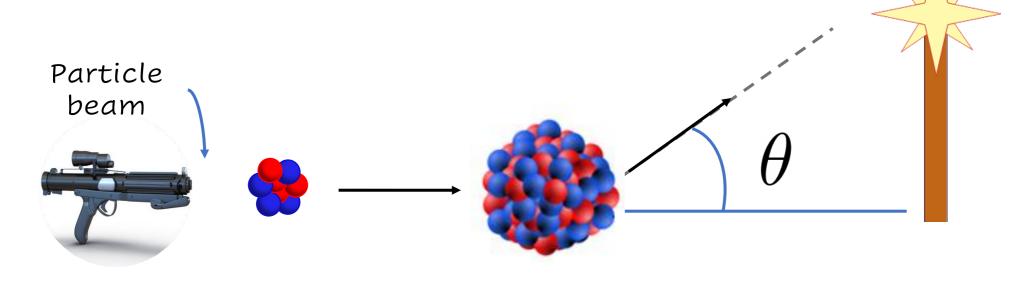
Particle beam θ

Building better models: Reactions

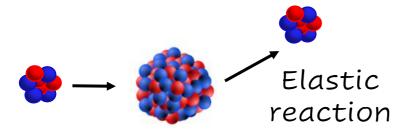
Particle beam θ

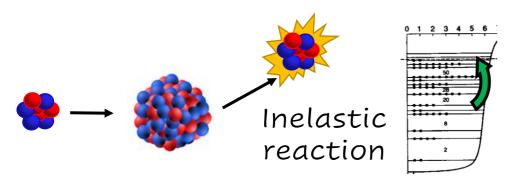


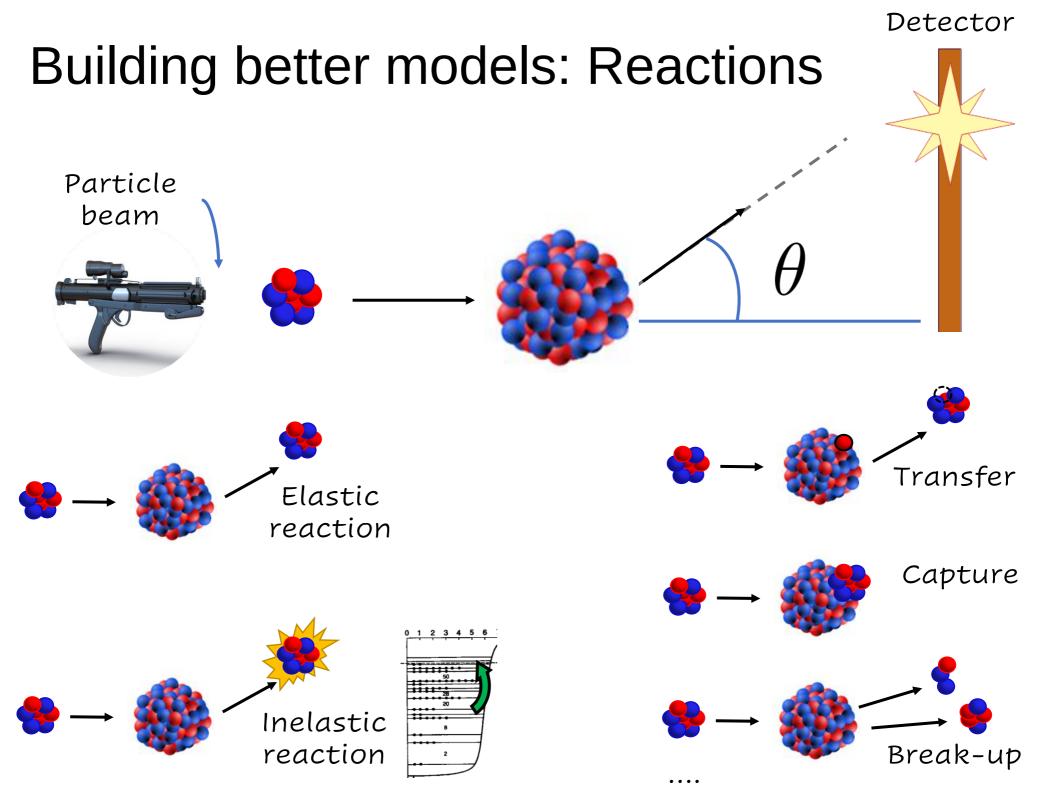
Building better models: Reactions



Detector







Building better models: Reactions

Particle beam All this gives us hints about the rules of the game

$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$



Elastic reaction

ransjer

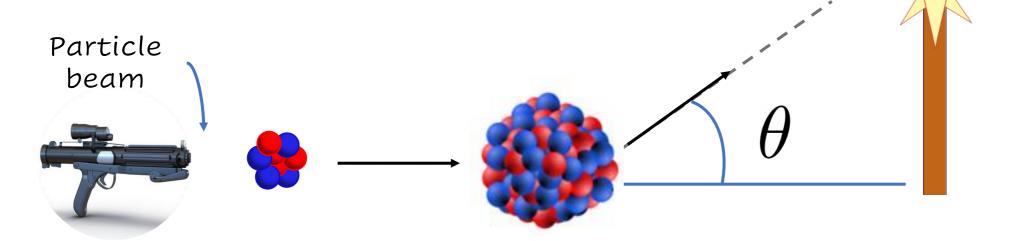
Capture



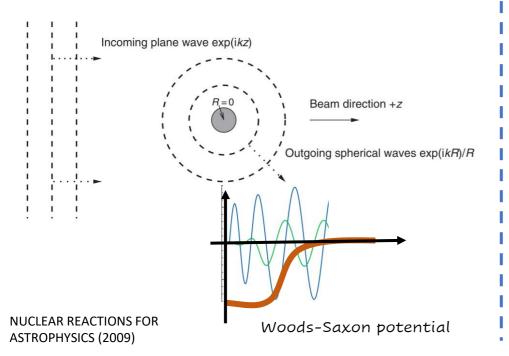




Building better models: Reactions



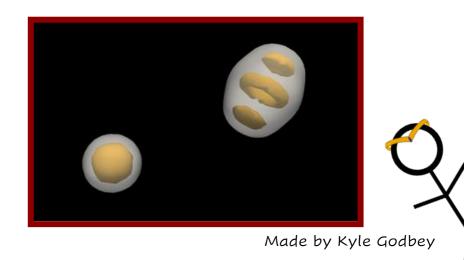
Optical Potentials

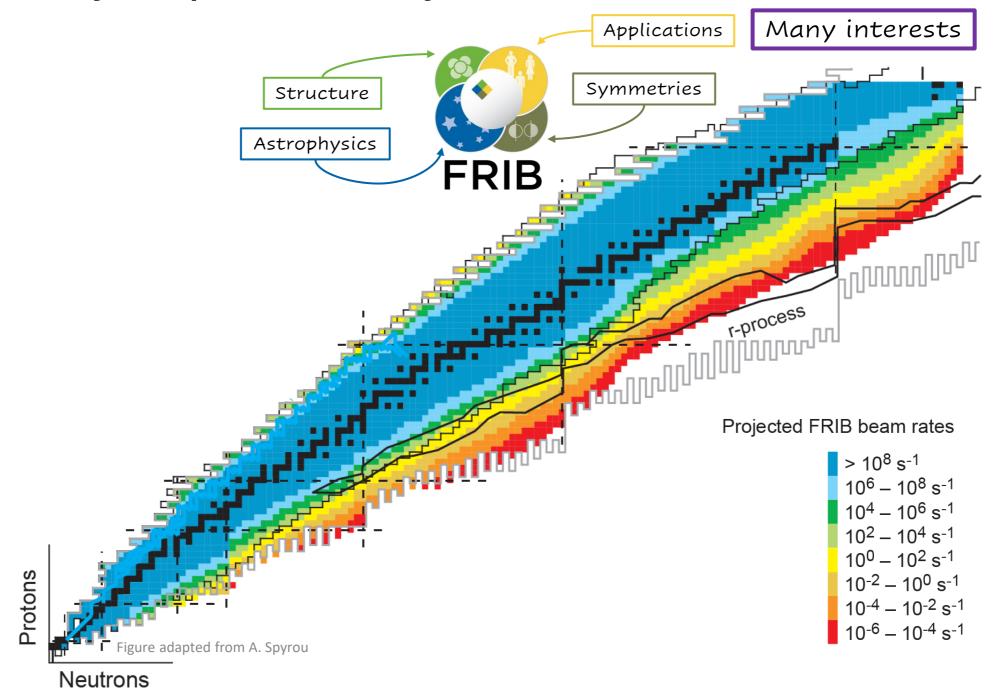


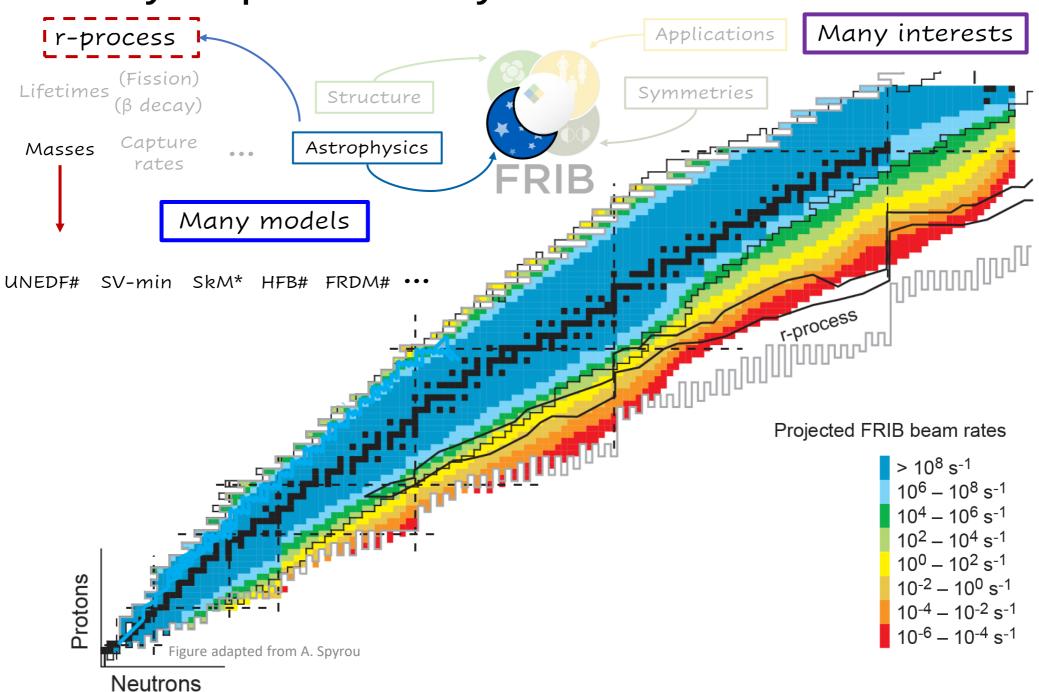
Time-dependent Density Functional Theory

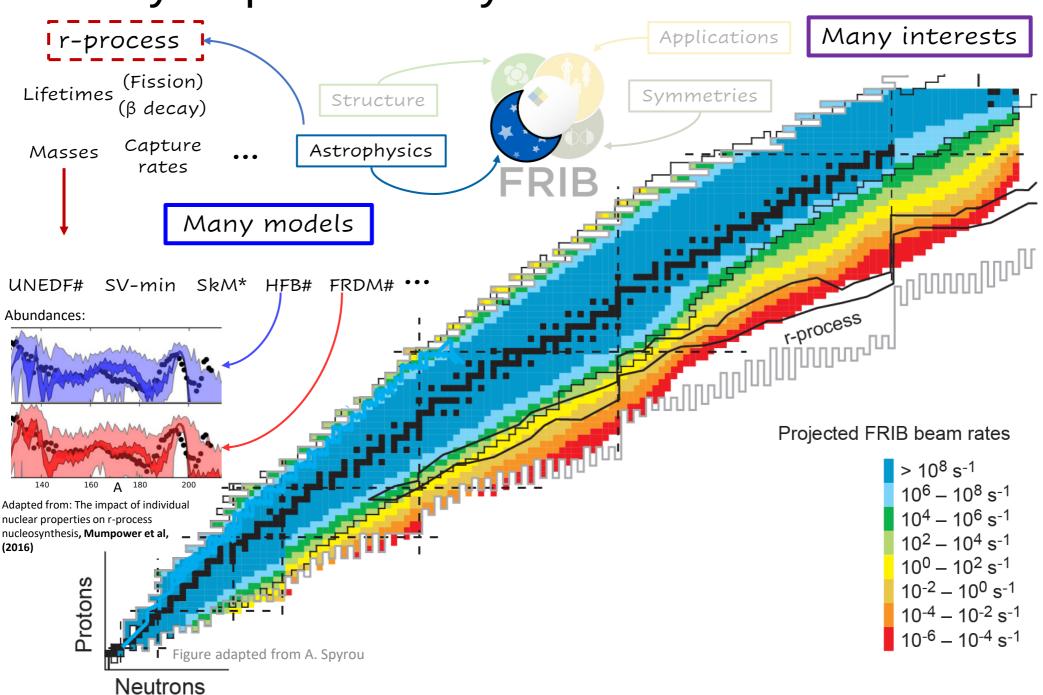
$$\mathcal{H}|\psi(x,t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(x,t)\rangle$$

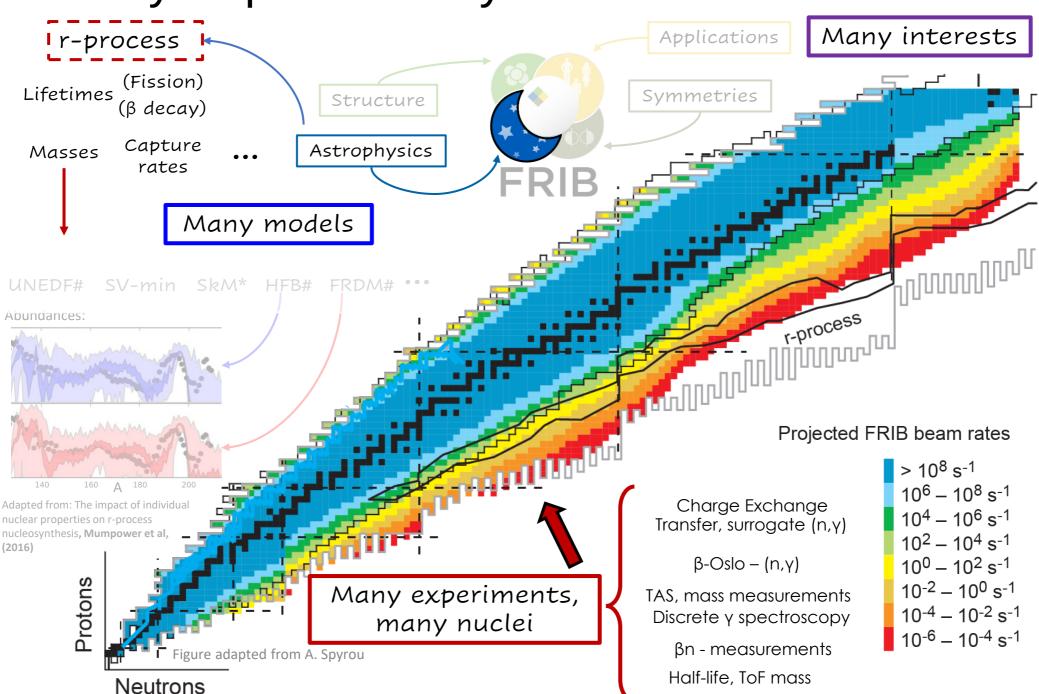
Detector

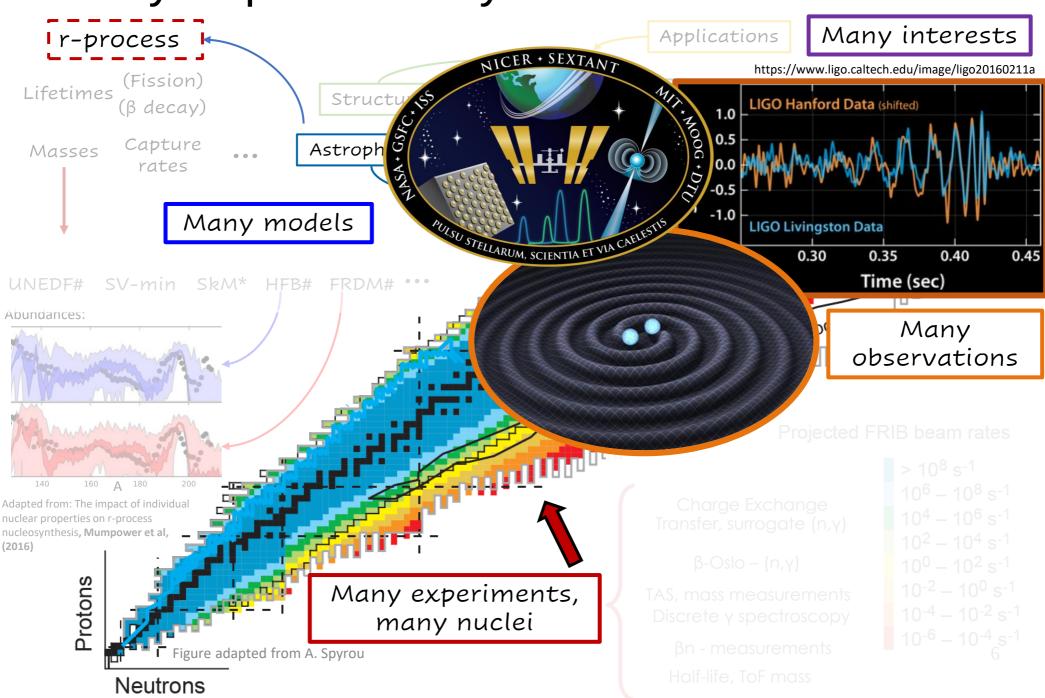




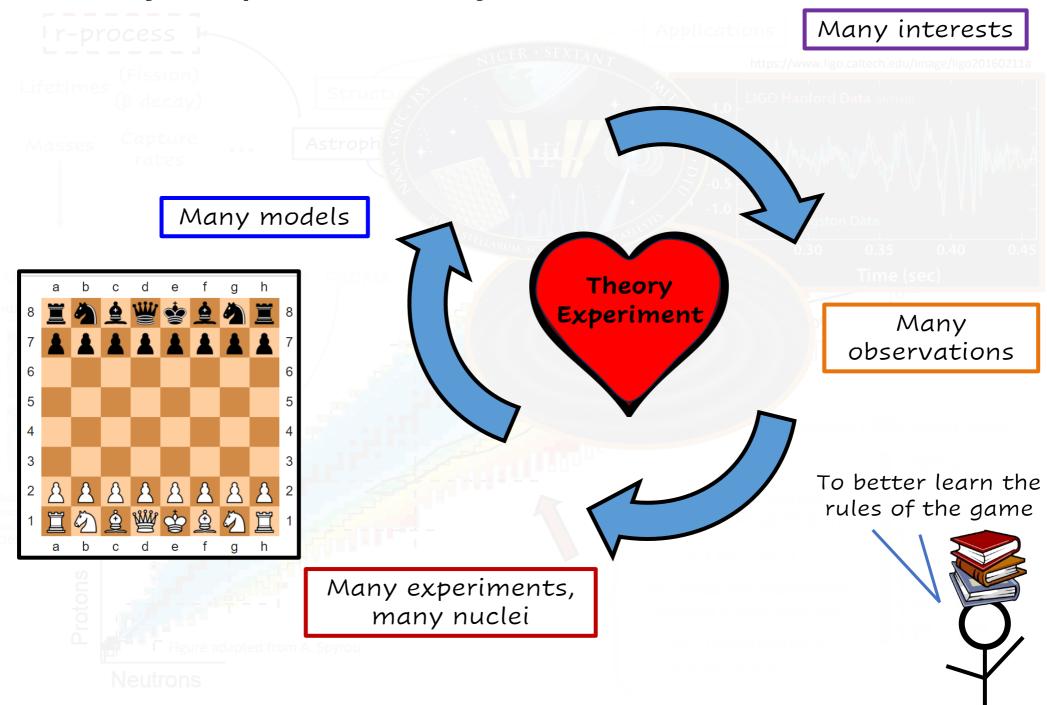








Many interests Many models Theory Experiment Many observations Many experiments, many nuclei



For today

Who am 1?

Why theory?

Building models

Building a (simple) nuclear mode

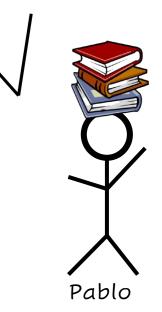
Quantum mechanics

Building (better) nuclear models

Challenges (Hands-On Session)



Questions?



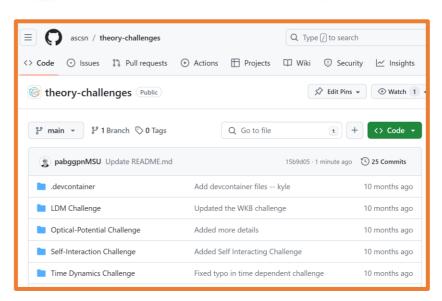
Hand-on session set-up



Advanced Scientific Computing and Statistics Network



https://github.com/ascsn/theory-challenges

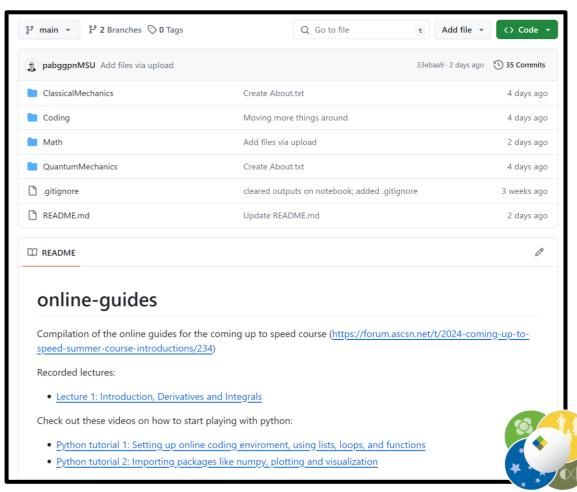


Starting up with Python





Link to the videos



Online guides with video-lectures and python notebooks!

Math Classical Mechanics Python Quantum Mechanics



Liquid Drop Model 🖈 🛨





Reaction cross sections \bigstar



Time Dynamics 🛨



Self Interaction *



Proton emitters lifetimes 🗙 🛨



Single particle spectrum 🖈 🖈







Calibrating the Liquid Drop Model Challenge





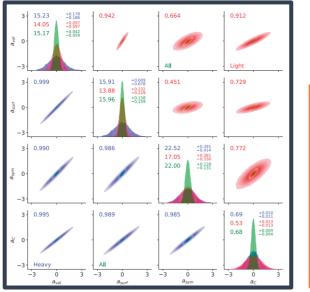
The purpose of this challenge is for you to calibrate the Liquid Drop Model https://en.wikipedia.org/wiki/Semi-empirical_mass_formula and compare the results of a "black box" calibration vs a principled Bayesian one.

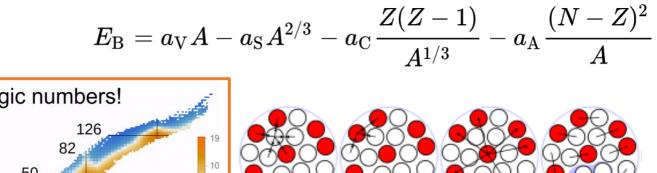
Your task is to:

- Import the data from the AME 2016 table (included in the github). We are only using nuclei above A=16 to avoid light nuclei where the LDM fails particularly. Perform a curve fit using the built in functions from python (https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.curve fit.html) and take note of the reported uncertainties in the parameters.
- Make a plot of the residuals and estimate the model error on its best fit.
- Make a model calibration using the Bayesian formalism that is defined in the acompaning file "# Guided Example Bayesian calibration". For the error, use your estimation from the previous point (the model error in this case is much smaller than the actual experimental uncertainties).
- Plot the corner plot posterior as well as the model values on the Binding Energy per nucleon for the Calcium chain up to 60Ca including the available experimental data.
- What would be the results if you have used in the calibration the Binding Energy per nucleon instead of the total Binding Energy?
- Bonus: Find the experimental error in the masses and repeat the calibration using only experimental errors. This should give a good demonstration on the dangers of not taking into account model errors.

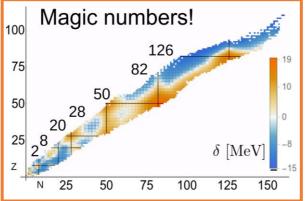


Asymmetry





Surface



Reaction Cross Section Challenge 🖈 🖈

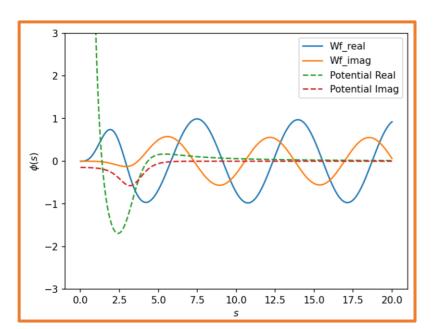


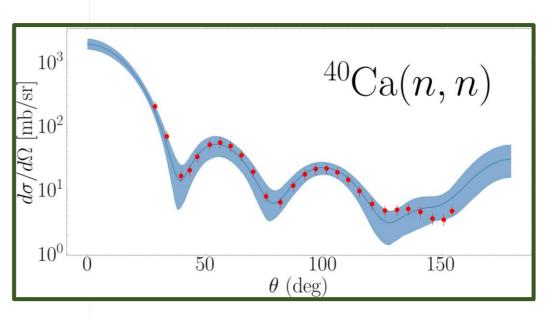
Notebook adapted from the ROSE challenges made by Daniel Odell and Pablo Giuliani: https://indico.cern.ch/event/1223721/contributions/5394829/. Functions for calculating the wave-function solutions and phaseshifts adapted from the ROSE github: https://github.com/odell/rose

The purpose of this challenge is to extract information of a nucleus through the scattering cross section of particles that interact with it (in this case, neutrons). We will use an optical potential to model such interaction.

The acompanying re-scaled Schrodinger equation is:

$$\left[-rac{d^2}{ds^2}+rac{\ell(\ell+1)}{s^2}+U(s,\omega,k)-1
ight]\phi(s)=0 \ ,$$





Time Dynamics Challenge



This challenge is about computing the time evolution of a quantum system. We will focus on the harmonic oscillator for this first exploration (you could try a self interacting particle after you finish this challenge). Our Hamiltonian is:

$$H=-rac{\partial^2}{\partial x^2}+lpha x^2$$

Let us drop the numerical constants to simplify notation ($\hbar = 1$).

The evolution of a quantum mechanical wave function is described through Schrodinger equation as:

$$H\ket{\phi(t,x)}=irac{\partial}{\partial t}\ket{\phi(t,x)},$$

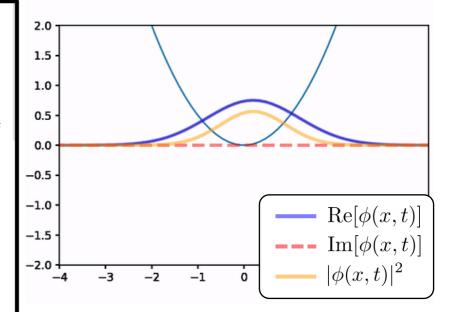
which results in the evolution operator from an initial state:

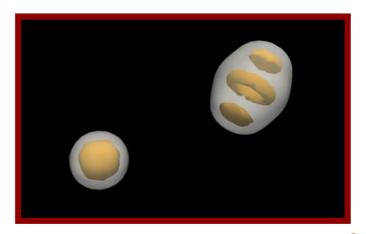
$$|\phi(t,x)\rangle = e^{-iHt}|\phi(0,x)\rangle.$$

To solve the problem numerically, the evolution operator is usually expanded in its Taylor approximation and a finite time step Δt is taken:

$$|\phi(\Delta t,x)
anglepprox ig(1+(-iH\Delta t)+rac{1}{2}(-iH\Delta t)^2+...ig)|\phi(0,x)
angle.$$

By taking small steps Δt , we can leave the expansion up to a small order (even linear in Δt) and arrive at the final time by successively applying the approximated evolution operator.





$$^{48}\text{Ca} + ^{249}\text{Bk}$$



Self Interaction challenge



The purpose of this challenge is for you to build a solver for a self interacting particle:

$$H\phi(x) = \lambda\phi(x),$$

with

$$H=-rac{\partial^2}{\partial x^2}+\kappa x^2+q
ho(x),$$

where the density is defined as:

$$\rho(x) = |\phi(x)|^2,$$

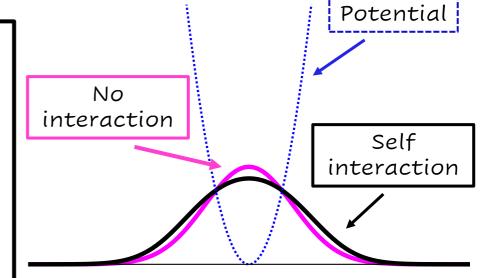
and the wave-function is normalized:

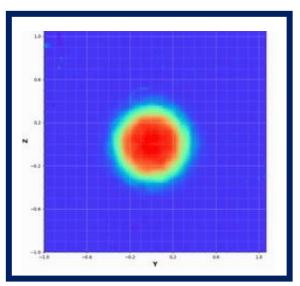
$$\int |\phi(x)|^2 dx = 1$$

With parameters $\alpha = \{\kappa, q\}$. This is the 1D Gross-Pitaevskii equation describing approximately the low-energy properties of dilute Bose-Einstein condensates. We will use it as a proxy for the non-linear Density Functional Theory equations. Check out

https://journals.aps.org/prc/abstract/10.1103/PhysRevC.106.054322 for a cool emulator on it.

Note that H depends on ϕ , this is a tricky problem to solve. One approach is to solve it first for q=0 (no self-interaction), obtain the wave function ϕ , create the density $\rho(x)$, plug it back into H and solve it again, repeating until the system converges. One recomendation is to mix the new solutions slowly to avoid instabilities: when updating the new density $\rho(x)$ to mix it with the previous one, around 85% and 15% old with new.





40Ca nucleus vibrating

Calculating life time of proton emitters \bigstar



The purpose of this challenge is for you to calculate, and compare with experimental data, the life time of proton decays for several proton emitter nuclei. We will follow the directions of the accompanying file: "WKB-protons.pdf" prepared by Witek Nazarewicz as part of his nuclear structure class.

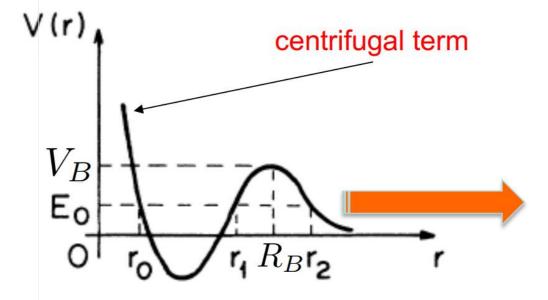
Your task is to:

• Solve questions 1 and 2 of the attached pdf. Consider that making integrals is easy if you discretize the "x" space and replace them by dot products (ask for help if you don't know how to do this)

Lifetimes

Nucleus	Q_p (keV)	Orbit	$t_{1/2}^{\mathrm{exp}}$
$^{109}_{53}\mathrm{I}_{56}$	829 ± 4	$1d_{5/2}$	$(100 \pm 5) \mu s$
¹¹² ₅₅ Cs ₅₇	823 ± 7	$1d_{5/2}$	$(500 \pm 100) \ \mu s$
¹¹³ ₅₅ Cs ₅₈	977 ± 4	$1d_{5/2}$	$(17 \pm 2) \mu s$
$^{146}_{69}\mathrm{Tm}_{77}$	1140 ± 5	$0h_{11/2}$	$(235 \pm 27) \text{ ms}$
	1210 ± 5	$0h_{11/2}$	$(72 \pm 23) \text{ ms}$
$^{147}_{69}\mathrm{Tm}_{78}$	1071 ± 3	$0h_{11/2}$	$(2.7^{+2.4}_{-0.9})$ s
	1132 ± 4	$1d_{3/2}$	$(360 \pm 40) \mu s$
$^{150}_{71}\mathrm{Lu}_{79}$	1283 ± 4	$0h_{11/2}$	(40^{+30}_{-20}) ms

$$\Gamma = S_p \mathcal{N} \frac{\hbar^2}{4\mu} \exp\left\{-2 \int_{r_1}^{r_2} |k(r)| dr\right\}$$



Woods-Saxon spectrum challenge

The purpose of this challenge is for you to build the single particle spectrum of a Woods-Saxon potential with a spin-orbit term. Our Hamiltonian is:

$$\left[-rac{\hbar^2}{2m}rac{d^2}{dr^2}+rac{\hbar^2}{2m}rac{\ell(\ell+1)}{r^2}+V_{ ext{eff}}(r,lpha)-E
ight]\phi(r)=0 \ ,$$

where the effective potential is:

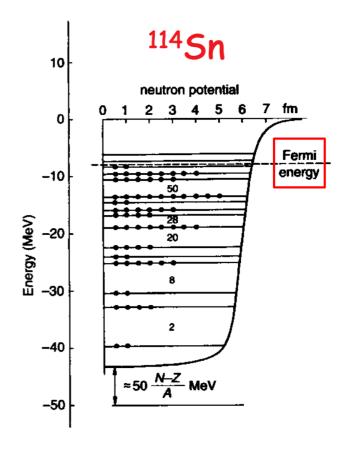
$$V_{
m eff}(r,lpha) = V_{
m WS}(r) + (ec{\ell}\cdotec{s})V_{
m SO}(r)$$

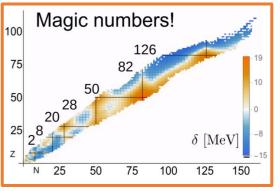
where the Woods-Saxon term is defined as:

$$V_{
m WS}(r,lpha) = V \Big[1 + \exp\Big(rac{r-R}{a}\Big) \Big]^{-1},$$

and the spin orbit is:

$$V_{
m SO}(r,lpha) = V_{
m SO} r_0^2 rac{1}{r} rac{d}{dr} \Big[1 + \exp\Big(rac{r-R}{a}\Big) \Big]^{-1},$$





https://forum.ascsn.net/



https://github.com/ascsn/theory-challenges

