Lecture 5: *Nuclear Structure 3*

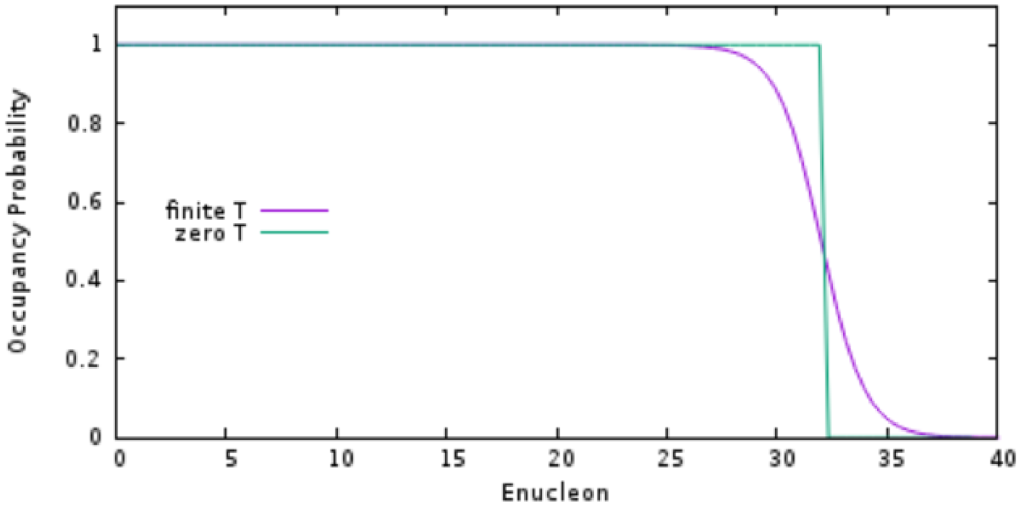
- Fermi Gas Model
  - Microscopic approach
  - Thermodynamic approach
- Nuclear level density

The nucleus as a Fermi gas

- To now we've focused on nuclear properties for cases where a few degrees of freedom dominate
    - E.g. a single uncoupled nucleon in a spherical well (shell model)
    - E.g. a collective rotation or vibration of nucleons in the nucleus (collective model)
    - E.g. a single uncoupled nucleon in a deformed well along with a collective rotation (Nilsson model)
- However, a typical nucleus has many nucleons and therefore many degrees of freedom
- These will become important in particular for highly-excited nuclei, since many degrees of freedom will then be relevant
- As such, we can understand some nuclear properties from the viewpoints of statistical mechanics and thermodynamics
- Since our neutrons and protons are spin-$^1/_2$ particles, they're fermions and so Fermi-Dirac statistics will apply
- Protons and neutrons are treated as two independent systems of fermions
- The approach of treating a nucleus as a fluid of fermions is known as the Fermi gas model

Nuclear properties from a microscopic picture

- Our nucleons are fermions (i.e. they obey Pauli exclusion) and are confined to a fixed volume by the potential they collectively generate
- Therefore, the nucleons will fill the available single-particle levels, upward in energy from the lowest level until we run out of nucleons
- At zero temperature, the nucleons fill all levels up to the Fermi energy, E_F, which we can find by finding the properties of the highest filled level

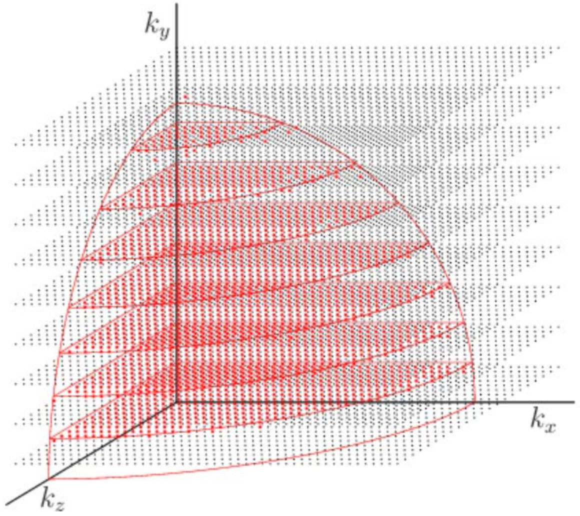


- Nucleons confined to a rectangular box with side-lengths $L_x = L_y = L_z = L$ will each occupy an orbital that corresponds to one solution to the Schrödinger equation for a standing wave in a box, $\psi(x, y, z) = C\sin(k_x x)\sin(k_y y)\sin(k_z z)$, where the wave number components k_i correspond to the principal quantum number n_i via $k_i = \frac{n_i \pi}{L}$
- Each single-particle level corresponds to a unique combination of n_x, n_y, n_z, which can be assigned to a single lattice point in $\boldsymbol{k}$-space
- Since allowed values of n_i are integers, the spacing between each lattice point is $\frac{\pi}{L}$

Nuclear properties from a microscopic picture

- The number of unique combinations of n_x, n_y, n_z with wave number $k_0 = \sqrt{k_x^2 + k_y^2 + k_z^2}$ less than some wave number k_f is approximated by the volume of an octant of a sphere

$$N_{levels} = \frac{1}{8}\frac{4\pi}{3}n_f^3 = \frac{1}{8}\frac{4\pi}{3}\left(\frac{k_f L}{\pi}\right)^3$$



L. van Dommelen, Quantum Mechanics for Engineers (2012)

- Since our nucleons will fill all available levels up the Fermi level, "N_{levels}" corresponds to how many of a type of nucleon our nucleus has, i.e. $N_{levels} = Z$ for our proton gas and $N_{levels} = N$ for our neutron gas
- The length of the "box" is just the nuclear radius $L = R = r_0 A^{1/3} fm$
- Therefore, the Fermi wave numbers for our protons and neutrons are

$$k_{f,protons} = \frac{\pi}{r_0}\left(\frac{2Z}{3\pi A}\right)^{1/3} \quad , k_{f,neutrons} = \frac{\pi}{r_0}\left(\frac{2N}{3\pi A}\right)^{1/3}$$, where the Fermi energy $E_f = \frac{p_f^2}{2m} = \frac{\hbar^2 k_f^2}{2m}$

- Using $r_0 \approx 1.2\ fm, m \approx 931.5 MeV/c^2$, and $\hbar c \approx 197 MeV\ fm$,

$$E_{F,p} \approx 51\left(\frac{Z}{A}\right)^{2/3} MeV \text{ and } E_{F,n} \approx 51\left(\frac{N}{A}\right)^{2/3}$$ …so, for $Z = N$, $E_F \approx 32MeV$

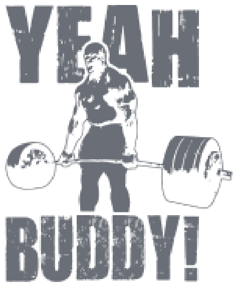
This corresponds to a Lorentz factor of γ≈1.02, so our non-relativistic treatment seems safe.

- The average kinetic energy $\langle E_{KE}\rangle = \frac{\int_0^{p_F} E_{KE} p^2 dp}{\int_0^{p_F} p^2 dp} = \frac{3}{5}\frac{p_f^2}{2m} = \frac{3}{5}E_f \approx 20MeV$, for $Z = N$

Estimating nuclear properties from microscopic system properties

- Consider the average kinetic energy of our nucleons, $\langle E_{KE} \rangle \approx 30.6 \left(\frac{Z\ or\ N}{A}\right)^{2/3} MeV$
  - The de Broglie wavelength $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{\sqrt{2mE}}$
  - For $m \approx 931.5 MeV/c^2$ and $\hbar c \approx 197 MeV\ fm$, $\lambda \approx \frac{5.15}{(Z\ or\ N)^{1/3}} A^{\frac{1}{3}}$
    - so for $Z = N = \frac{A}{2}$, $\lambda \approx 4.1 fm$
  - Compare to the heaviest stable $Z = N$ isotope, ^{40}Ca
    - $R\left({}^{40}Ca\right) \approx 1.2(40)^{1/3} fm = 4.1 fm$

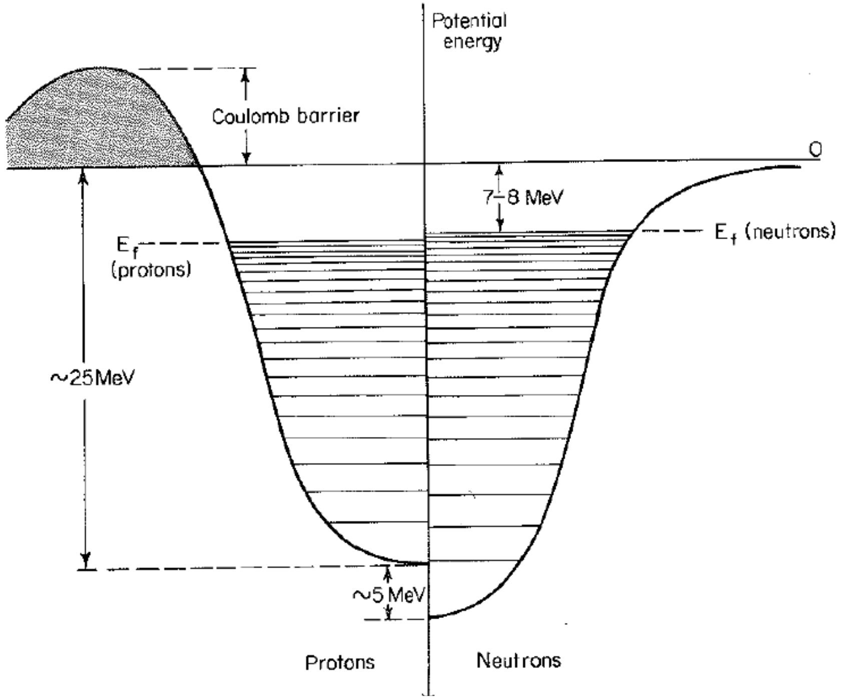
- Now consider the total kinetic energy of the nucleons
  - We can estimate the total kinetic energy as: $E_{KE} = Z\langle E_{KE,Z} \rangle + N\langle E_{KE,N} \rangle$
  - From the virial theorem (2*KE=n*PE, where V(r)~r^n. For a potential $V(r) \propto r^2$, like a harmonic oscillator), $E_{PE} = E_{KE}$
  - So an estimate for the binding energy per nucleon is $\frac{\text{BE}}{\text{A}} = \frac{E_{PE}}{A} = 30.6 \frac{Z^{5/3} + N^{5/3}}{A^{5/3}}$
    - For Z, N corresponding to most stable nuclides, this gives: $\frac{BE}{A} \approx 19 MeV$
    - Compare to the bulk-binding term of the SEMF, $a_v A$, where $a_v \approx 15 MeV$

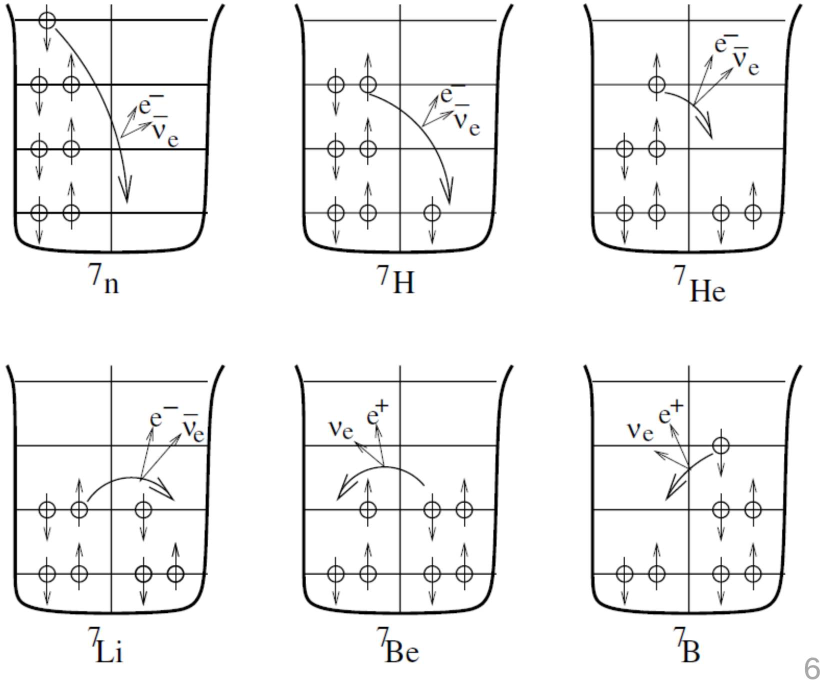


Implications of the Fermi levels

- Protons and neutrons each fill available levels up to their respective Fermi levels
- For each case, the Fermi level must be $\sim 8\ MeV$ below the top of the potential well, since $\mathrm{BE/A} \sim 8 MeV$ for stable nuclides
- For $N = Z, E_F \approx 32 MeV$, so the potential well depth is $V_0 \approx E_F + BE/A \approx 40 MeV$
- However, protons suffer from Coulomb repulsion, and so their potential well depth is somewhat more shallow
- As such, it takes fewer protons to fill single-particle levels up to the same binding energy
- If there is a mismatch in the neutron and proton Fermi levels (which is greater than $M_n - (M_p + M_e)$), then it is energetically favorable for a neutron to transmute into a proton *or vice versa*
- By expanding our estimate on the previous slide for BE in terms of $N - Z$, it turns out $BE \approx \frac{3}{5} E_F + \frac{4}{3} E_F \frac{\left(Z - \frac{A}{2}\right)^2}{A}$, revealing the asymmetry term from the SEMF
- This estimates $a_a \approx 43$, where the SEMF fit yields $a_a \approx 90$

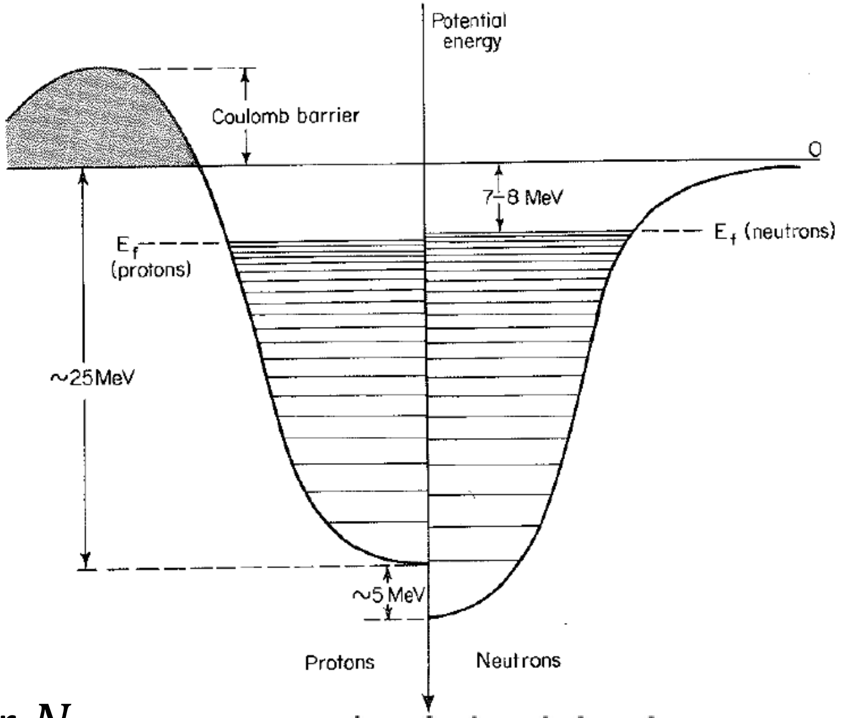
G. Harvey, Introduction to Nuclear Physics and Chemistry (1962)





Basdevant, Rich, & Spiro, Fundamentals in Nuclear Physics (2005)

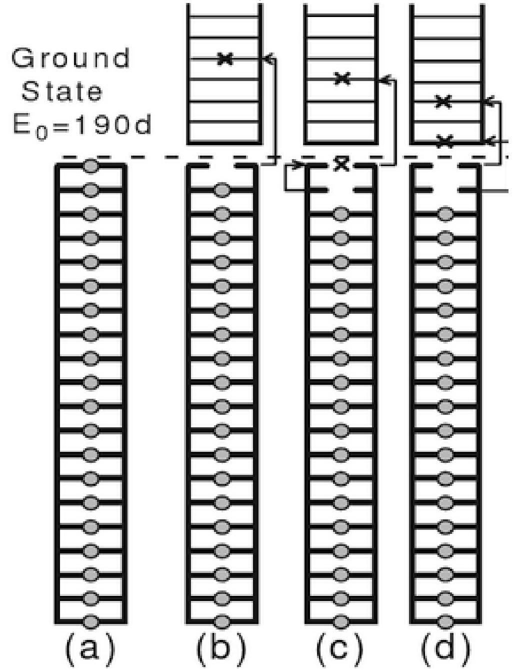
Single-particle and nuclear levels



- Note that in our single-particle level diagram, the level spacing decreases as the level energy increases
- This is a consequence of the fact that $N_{levels}(k) = \frac{1}{8}\frac{4\pi}{3}\left(\frac{kL}{\pi}\right)^3$ and so the spacing between single particle energies $\varepsilon = \frac{\hbar^2 k^2}{2m}$ goes as $\left(\frac{dN_{level}}{d\varepsilon}\right)^{-1} \propto \varepsilon^{-1/2}$
- The actual excitation energy E_x of a nucleus is determined by the sum of single-particle energies
- The number of ways to achieve E_x for various combinations of ε of our N fermions is a problem of combinatorics
- For the approximation of constant single-particle level spacing d, the excitation energy is some integer multiple M of the level spacing
- To find the number of ways we can arrange our N fermions to achieve M, we have the problem from number theory finding the partitions of integers
- The approximate solution (G.Hardy & S.Ramanujan, Proc. London Math. Soc. (**1918**)) for the number of partitions (a.k.a. density of nuclear states) at an excitation energy $U = Md$ is

$$p_N(M) \approx \frac{\exp\left(\pi\sqrt{\frac{2}{3}M}\right)}{\sqrt{48}M} \text{ for } N \geq M$$

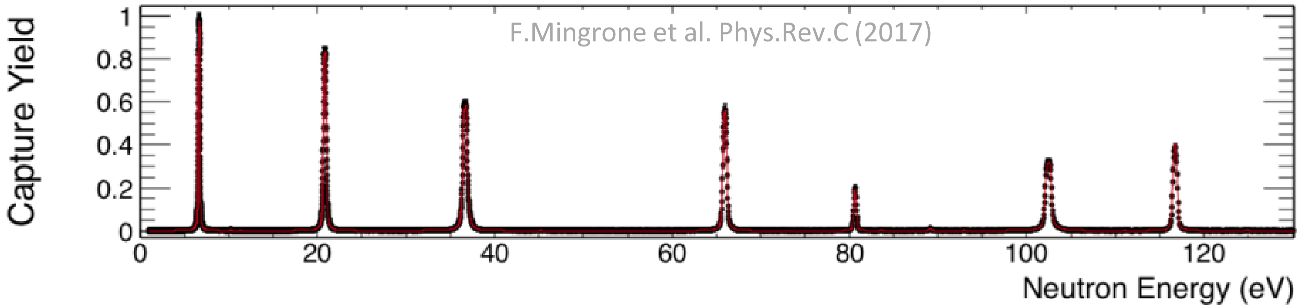
We'll see this mirrors the solution to the far more popular thermodynamic approach



A. Cole, Statistical Models for Nuclear Decay (2000)

Microscopic-based state density estimate: ^{238}U

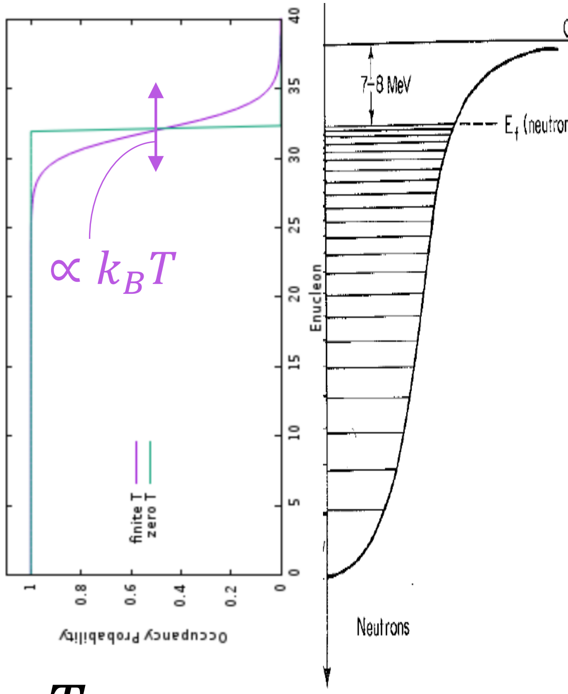
- The single-particle spacing at the Fermi level will roughly be the same as the binding energy penalty for violating $N = Z$, since if we started at *N=Z*, adding another nucleon would, via Pauli exclusion, fill the next single-particle level
- We derived the SEMF asymmetry term from the Fermi gas model to be $a_a f_a(A) = \frac{4}{3}E_F \frac{\left(Z - \frac{A}{2}\right)^2}{A}$, so rewriting in terms of $N - Z$, $a_a f_a(A) = \frac{2}{3}E_F \frac{(N-Z)^2}{A}$
- i.e. the single-particle energy level spacing will be $d \approx \frac{2}{3}\frac{E_F}{A}$ …which, for ^{238}U, $d \approx 0.103 MeV$
- At the excitation energy required to unbind a neutron from ^{238}U, the neutron separation energy, $U \approx 6MeV$, so $M \approx 60$
- Our predicted number of partitions is then $p_N(M) \approx 200{,}000 MeV^{-1}$
- Looking at neutron-capture on ^{238}U, the neutron-resonance spacing can be used as a measure of the nuclear state density
- We see $\sim$1 resonance per $20eV$, so $\sim 5 \times 10^4$ levels per MeV



Connection to thermodynamics

- Statistical mechanics links microscopic descriptions of systems with many possible states to macroscopic thermodynamic descriptions, where the key link is the entropy S
- In the microscopic picture, it describes how many configurations are available to a system, g
  $S = k_B \ln(g)$ (which you can confirm by checking out Boltzmann's tombstone)
- In the macroscopic picture, it is related to the internal energy E, pressure P, volume V, chemical potential μ, particle number N, and temperature T, by the fundamental thermodynamic relation:
  $dE = TdS - PdV + \mu dN$
- Here, N and V aren't changing, so $dS = \frac{dE}{T}$, i.e. $S(E) = \int \frac{dE}{T(E^*)} + constant$
- To obtain the relationship between T and E^*, recall that E^* is just a sum of the single-particle energies ε of the fermions excited by T
- The number of fermions excited near the Fermi surface due to T is proportional to the $k_B T$, but also to the density of single-particle levels in that energy region $\frac{dN_{level}}{d(k_B T)} \equiv a$
- So the number of excited fermions is $N_{exc.} \approx a k_B T$
- Each fermion will roughly have the classical thermal excitation energy $\varepsilon \approx k_B T$
- So the excitation energy is $E^* = \sum \varepsilon_i \approx N_{exc.}\varepsilon \approx a k_B^2 T^2$, meaning $T \approx \frac{1}{k_B}\sqrt{E^*/a}$

See V.Weisskopf, Phys. Rev. (1937) or Bohr & Mottelson for fancier arguments



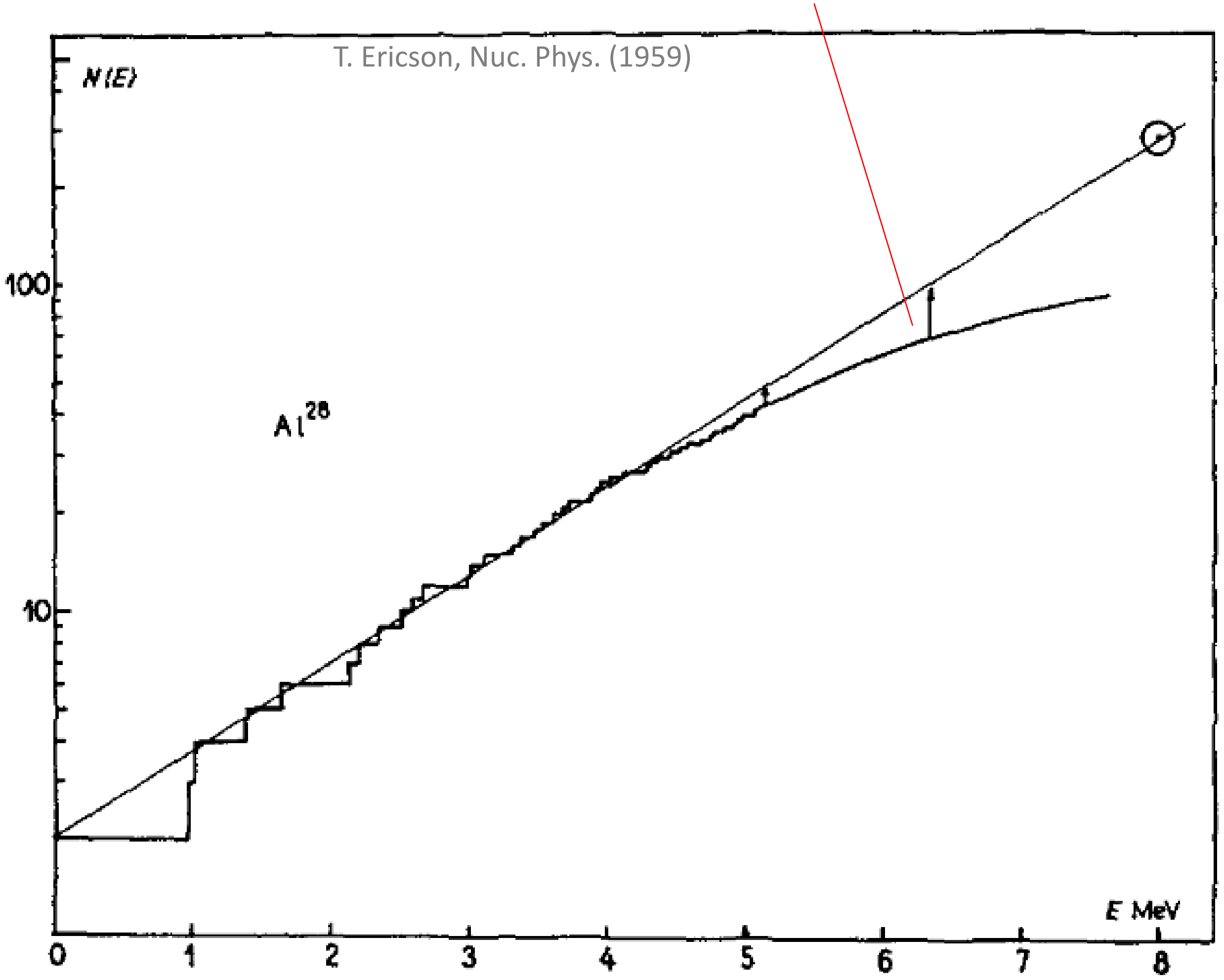
This is the "nuclear temperature"

Connection to thermodynamics

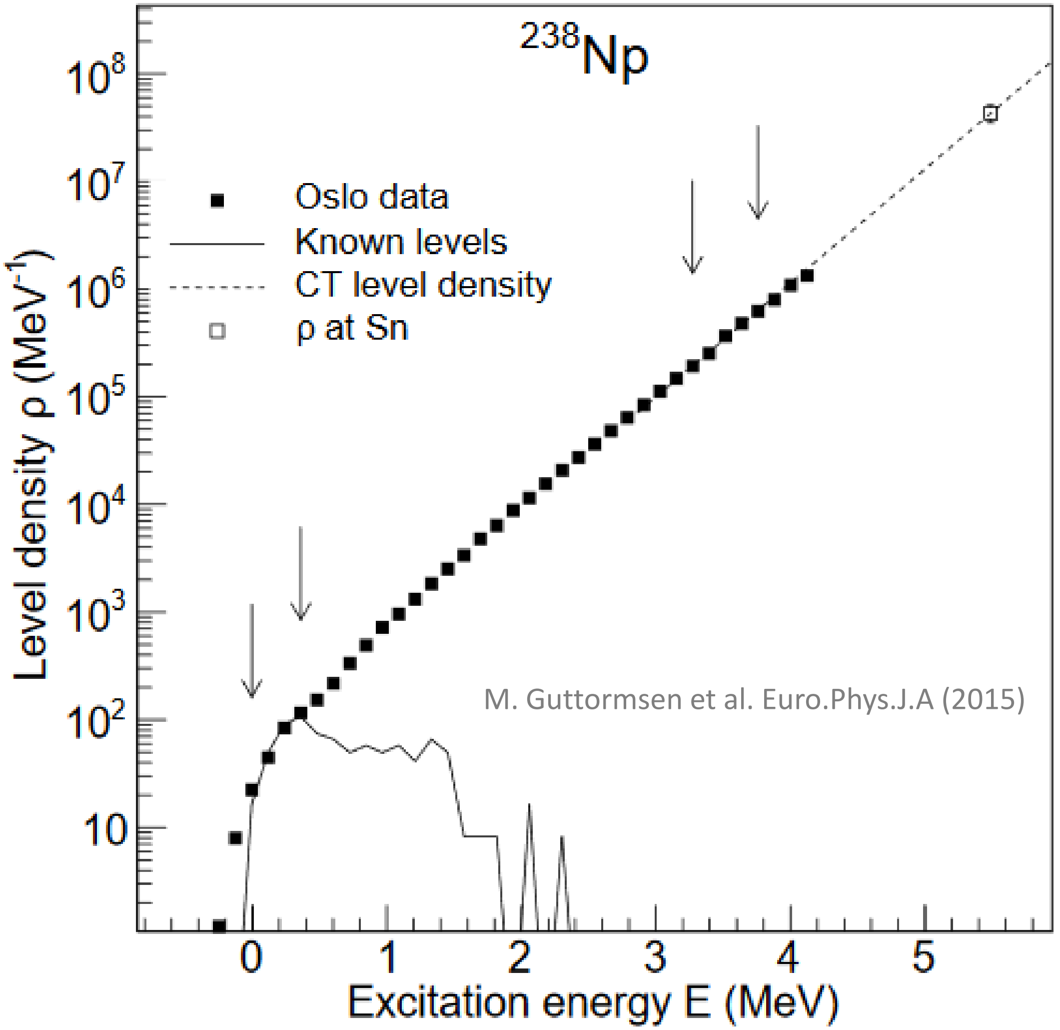
- Now we can solve for our entropy: $S(E) = \int \frac{dE}{T(E^*)} + constant \approx \int k_B \sqrt{\frac{a}{E^*}} dE + constant$
- Since a zero-temperature system has zero entropy, $S(E) \approx k_B 2\sqrt{aE^*}$
- Recall from the microscopic picture, $S = k_B \ln(g)$
- So, the number of accessible configurations (a.k.a. nuclear states) for our system is $g \approx \exp\left(2\sqrt{aE^*}\right)$
- The density of states is going to be proportional to the total number of states $\left(\frac{d}{dx}e^x = e^x\right)$
- So, the state density $\rho(E^*) = C \exp\left(2\sqrt{aE^*}\right)$, where C is a constant
- A more careful treatment using partition functions and other statistical mechanics tools yields: $\rho(E^*) = \frac{\sqrt{\pi}}{12a^{1/4}E^{*5/4}} \exp\left(2\sqrt{aE^*}\right)$ H. Bethe, Phys. Rev. (1936)
- Going back to our estimate for ^{238}U and using $a = 1/d$ and $E^* = S_n$, we get $\rho \approx 3 \times 10^4 MeV^{-1}$
- In practice, C and a are usually fit to data
- C in particular isn't so relevant, since we can normalize $\rho(E^*)$ to the region at low excitation energy where individual levels can be counted and ideally also to $\rho(E^* = S_n)$

Experimental results confirm the exponential behavior of $\rho(E^*)$

One challenge in comparing to counts of discrete states is knowing if your measurement missed any levels

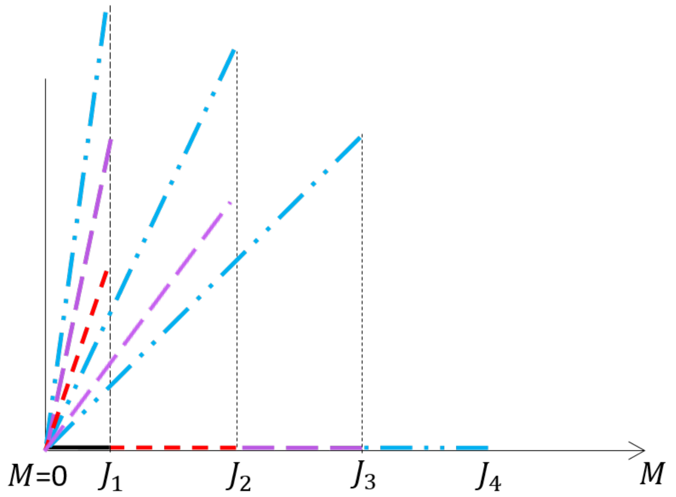


Techniques which are sensitive to the integrated number of levels can overcome this …though with assistance from models



From state density to level density

- Often times we're not interested only in the number of states near a given excitation energy, but rather the density of nuclear levels with some spin J, $\rho(E^*, J)$
- To do this, we can use a sort of neat trick that takes advantage of the fact that the density of levels with a given J is related to the density of levels with the projection $J_z = M$
- Say we have states of several different J and we want to tally-up how many have a given spin projection M
- We see that only states with $J \geq M$ can have the projection M
- Thus the count of states with $M = J + 1$ will only be missing the states that have spin J
- Therefore, $\rho(E^*, J) = \rho(E^*, J = M) - \rho(E^*, J = M + 1)$



- The momentum projection M of a state will be the sum of the momentum projections for the individual nucleons $M = \sum m_i$, where there are $2j_i + 1$ possible values of m_i
- $-j_i \leq m_i \leq j_i$ will be equally probable, so M will essentially be a random combination $(\langle M \rangle = 0)$
- Via the central limit theorem, we therefore expect the probability a state to have a given M is:

$$P(M)|_J = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-J^2}{2\sigma^2}\right)$$ and, logically, $\rho(E^*, J = M) = P(M)|_J * \rho(E^*)$

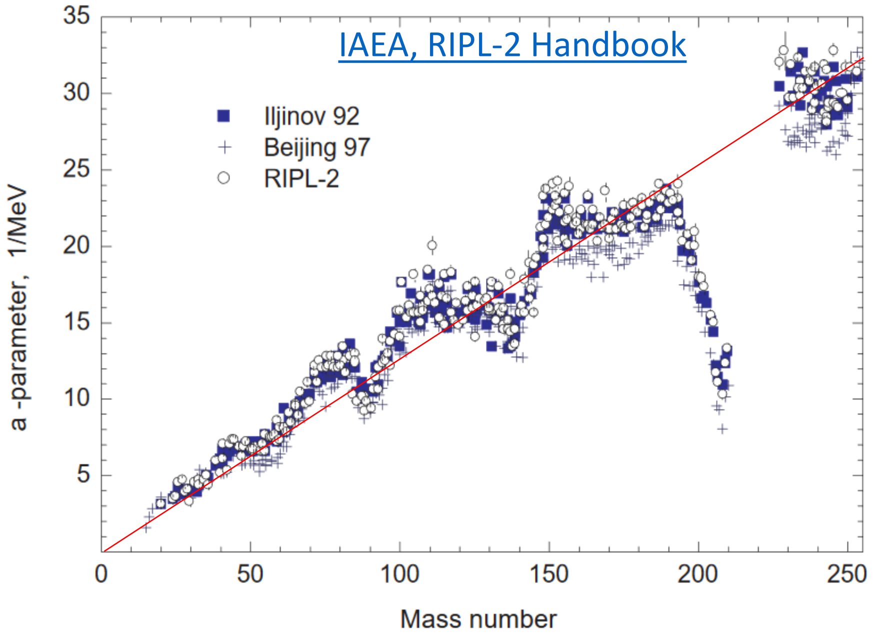
From state density to level density

an alternative approach approximates ρ(E,J=M) – ρ(E*,J=M+1) ≈ ∂ρ(E*,M)/∂M and gets the same result

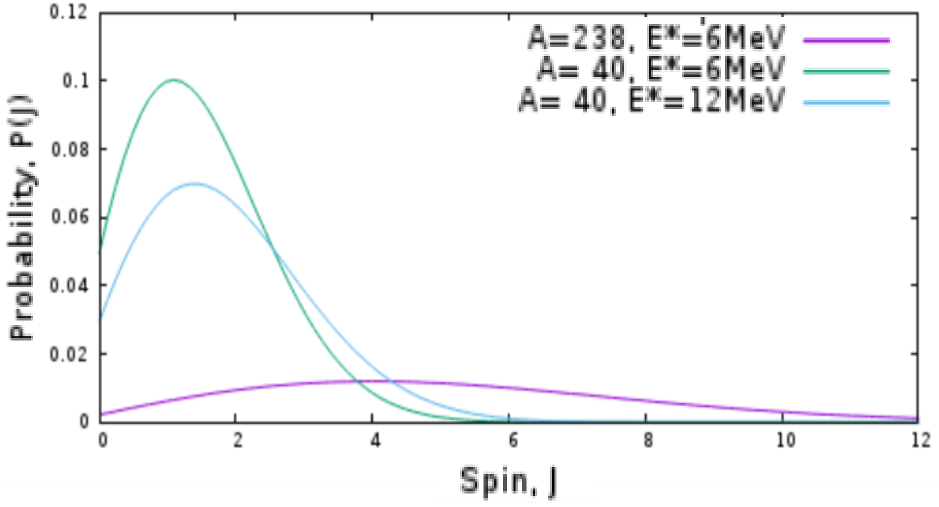
- As such, our level density $\rho(E^*,J) = \rho(E^*,J=M) - \rho(E^*,J=M+1)$ is
$$\rho(E^*,J) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(\frac{-J^2}{2\sigma^2}\right)\rho(E^*) - \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(\frac{-(J+1)^2}{2\sigma^2}\right)\rho(E^*)$$
- It turns out (See, e.g. Chapter 2: Statistical Models for Nuclear Decay (A.L. Cole)), this is approximately equal to:
$$\rho(E^*,J) \approx \rho(E^*)\frac{2J+1}{2\sigma^2}\exp\left(\frac{-\left(J+\frac{1}{2}\right)^2}{2\sigma^2}\right) = \rho(E^*)P(J)$$
- The level-density is the state-density adjusted for the distribution of nuclear spin states, the "spin-distribution"
- As an aside, an important and often overlooked point is that we assumed states with a given J, M were degenerate in energy and therefore we're assuming spherical nuclei.
- The variance of the spin distribution, σ^2 is known as the *spin-cutoff parameter* and it obviously impacts our results a great deal *[Often just σ is referred to as the spin-cutoff parameter, so beware]*
- A common approach to estimating σ^2 is to consider the nucleus as a rigid rotating body
- If we assume an ensemble of nuclei each have some energy E due to the nuclear temperature $T \approx \frac{1}{k_B}\sqrt{E^*/a}$ and that E expressed rotationally, then $P(E) \propto \exp\left(\frac{E_{rot}}{k_B T}\right) \propto P(J)$
- Recalling from last time that $E_{rot} = \frac{\hbar^2 J(J+1)}{2I}$, we see that in this approximation $\sigma^2 = \frac{I k_B T}{\hbar^2}$

σ^2 and the spin distribution

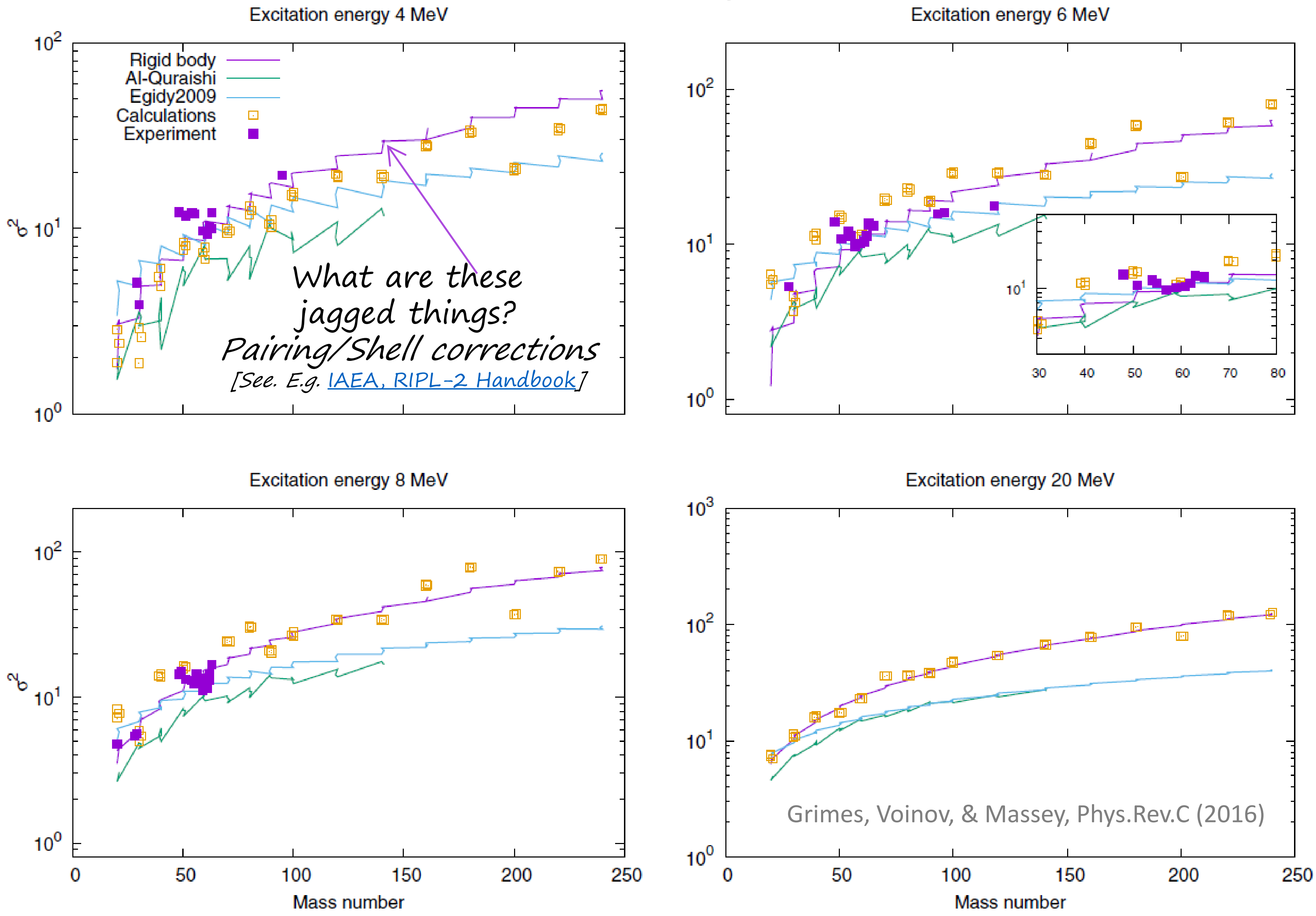
- Having found $\sigma^2 = \frac{Ik_BT}{\hbar^2}$, now we need to estimate the moment of inertia I
- Since we assumed a spherical nucleus earlier to justify the degeneracy of E^* in M, we'll double-down and use I for a rigid sphere: $I = \frac{2}{5}MR^2$
- Using this and the previously derived formula for the nuclear temperature $T \approx \frac{1}{k_B}\sqrt{E^*/a}$, and the standard estimate for the nuclear radius $R = r_0 A^{1/3}$: $\sigma^2 = \frac{2Mr_0^2A^{2/3}}{5\hbar^2}\sqrt{\frac{E^*}{a}}$
- Using $M = Am_u \approx \left(931.5\, {}^{MeV}/_{c^2}\right)$A, $\hbar c \approx 197 MeV\ fm, r_0 \approx 1.2 fm$: $\sigma^2 \approx 0.014A^{5/3}\sqrt{\frac{E^*}{a}}$
- It turns out, fits to neutron resonances yield $a \approx {}^{A}/_{8}\, MeV^{-1}$
- Therefore, $\sigma^2 \approx 0.0509A^{7/6}\sqrt{E^*}$



Implied spin distributions

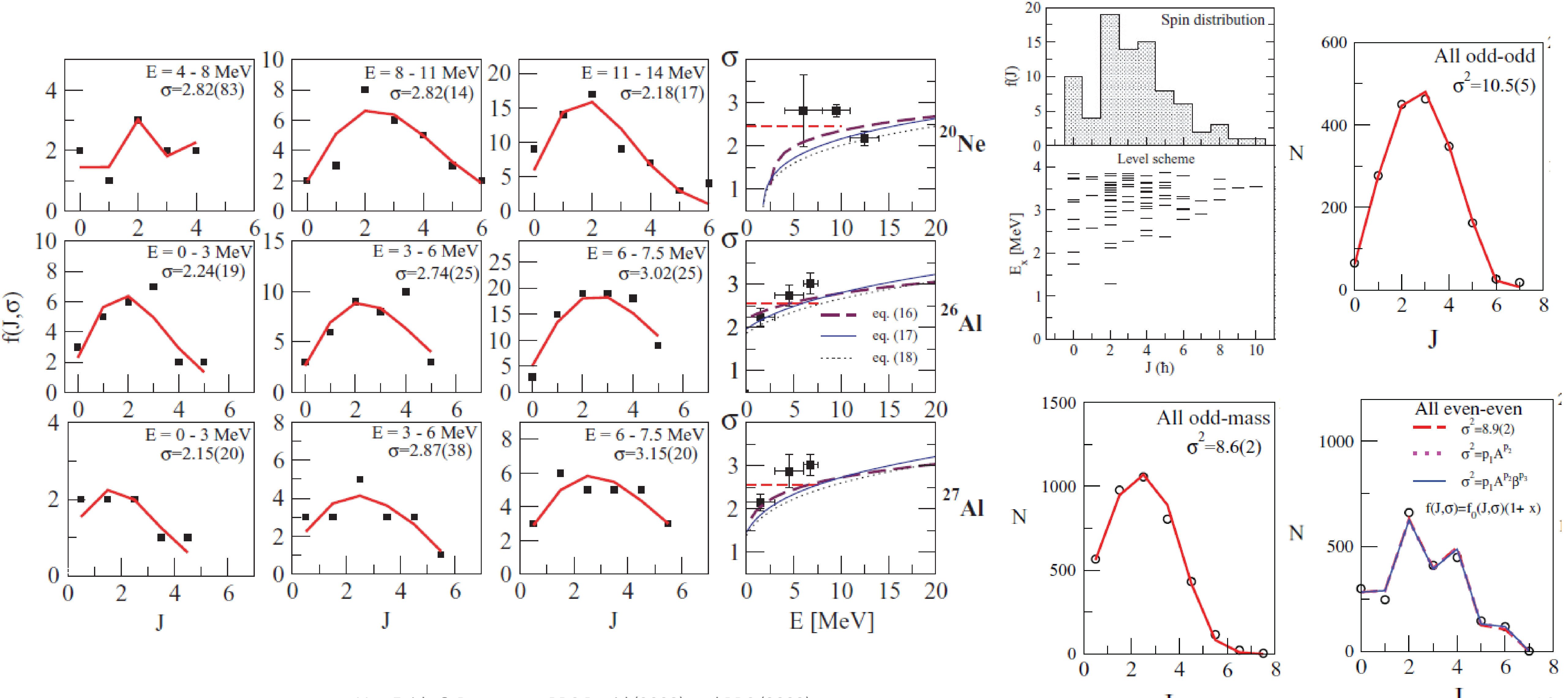


Experimental results show $\sigma^2_{rigid\ body}$ does pretty ok



Spin distributions are predicted reasonably well

… though σ^2 appears to have a weaker dependence on A and E^*



Von Egidy & Bucurescu, PRC Rapid (2008) and PRC (2009)

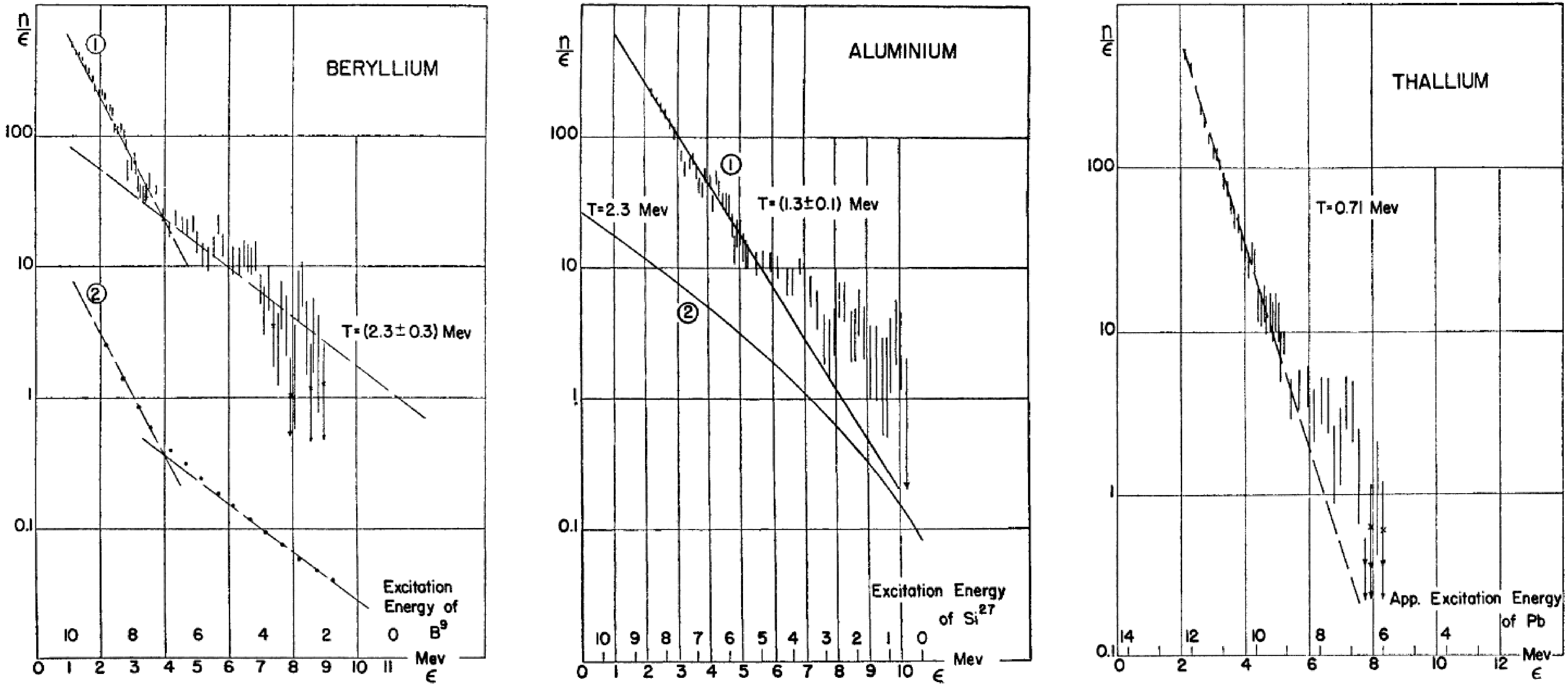
FERMI GAS MODEL II: REVENGE OF THE LOW-T EFFECTS

Not all that long ago in this very same Galaxy, some perceptive physicists noticed there was a disturbance in the level density at low excitation energies.

Two ~~warring~~ collegial factions came up with separate approaches to remedy the issue and restore correct level density predictions to the Galaxy …

Early experiments showed different behavior for $\rho(E^*)$ at low E^*

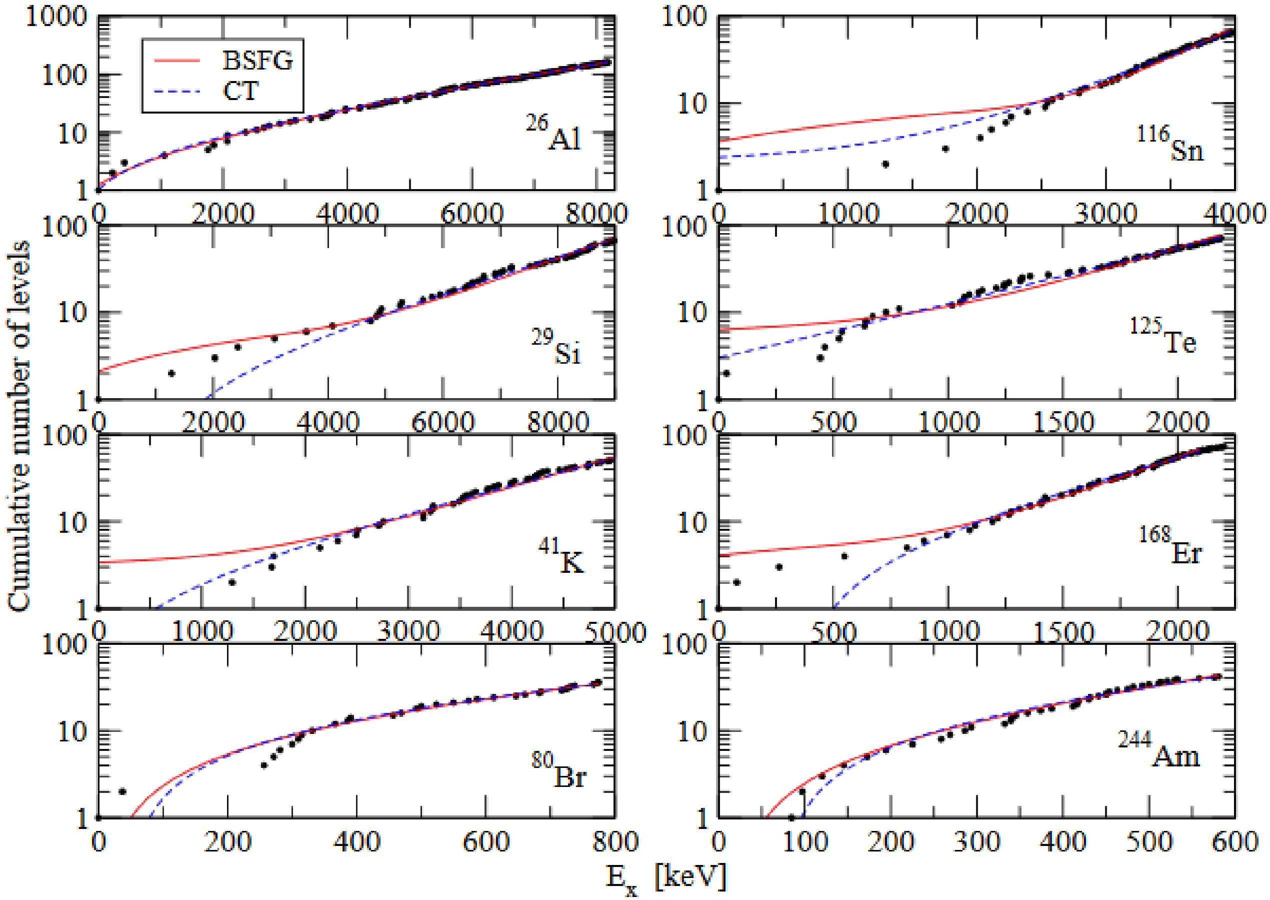
P.Gugelot, Phys. Rev. (1951)



Level density at low excitation energy

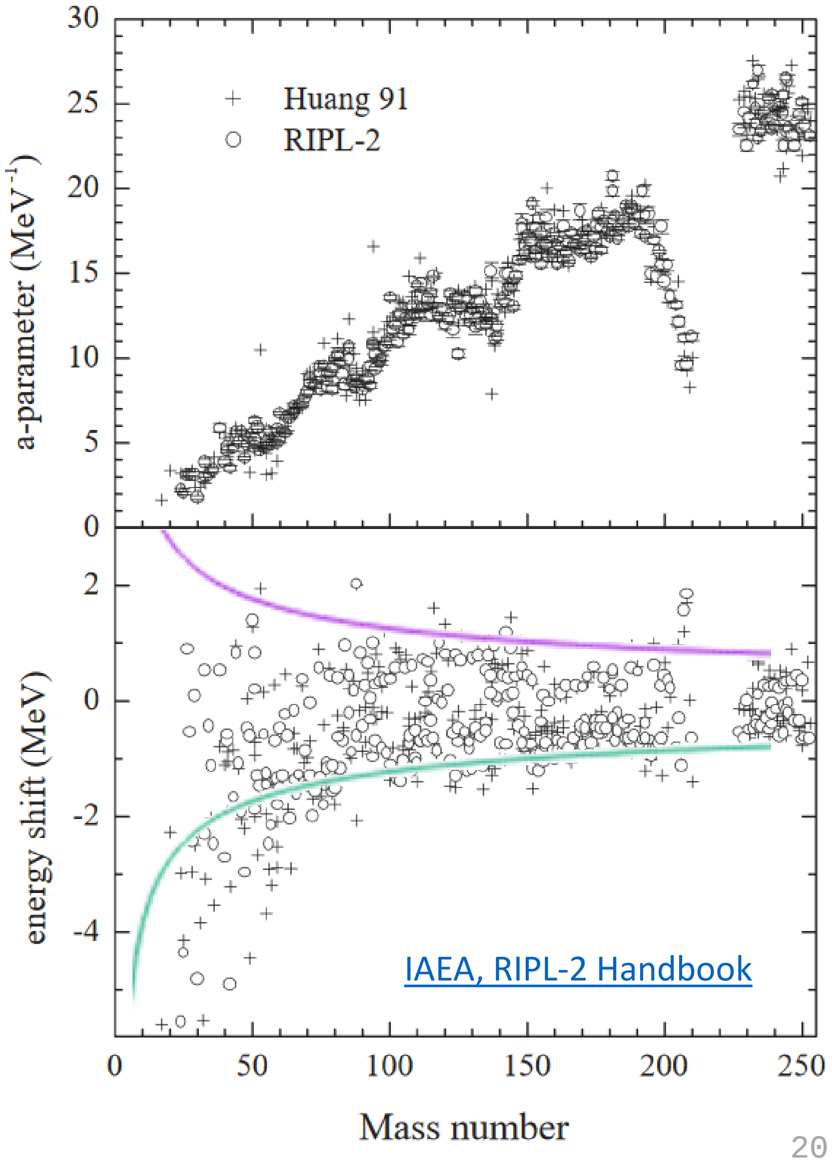
- Two different approaches are commonly used fix $\rho(E^*)$ predictions for low E^*
  1. Back-shifted Fermi Gas Model:
     - Shifts the "ground state" from which E^* is calculated and correct for nucleon pairing
  2. Constant Temperature + Fermi Gas Model:
     - Uses a separate functional form for $\rho(E^*)$ below some threshold in E^*, still also shifting the ground state
- Neither is necessarily better than the other, though recent literature seems to favor CT

Von Egidy & Bucurescu, J.Phys.Conf.Ser (2012)



Back-shifted Fermi gas model

- We became so enamored with our beautiful shiny new Fermi gas model that we forgot all of the lessons from our newly abandoned shell model
- Nucleons form pairs and those pairs cost some energy to break and having an unpaired nucleon penalizes nuclear binding
- As such, it costs less energy to form excited states for nuclei with odd nucleons (the more the better [i.e. odd-Z and odd-N]) and it costs more energy to form excited states for nuclei with no odd nucleons
- This cost is the pairing energy from the liquid-drop model
  $\Delta_{BSFG} \approx i a_{par} \left(\sqrt{A}\right)^{-1}$ …where it turns out $a_{par} \approx 12$
  and, recall, $i_{even-even} = +1, i_{odd-odd} = -1, i_{odd-even} = 0$
- All that needs to be done is to substitute
  E^* for a corrected energy $U = E^* - \Delta_{BSFG}$
- Empirically, an additional "backshift" δ is subtracted as well
- For regions where data are available,
  the level density at the Fermi surface a, Δ_{BSFG}, and δ are allowed to vary and are fit to the data

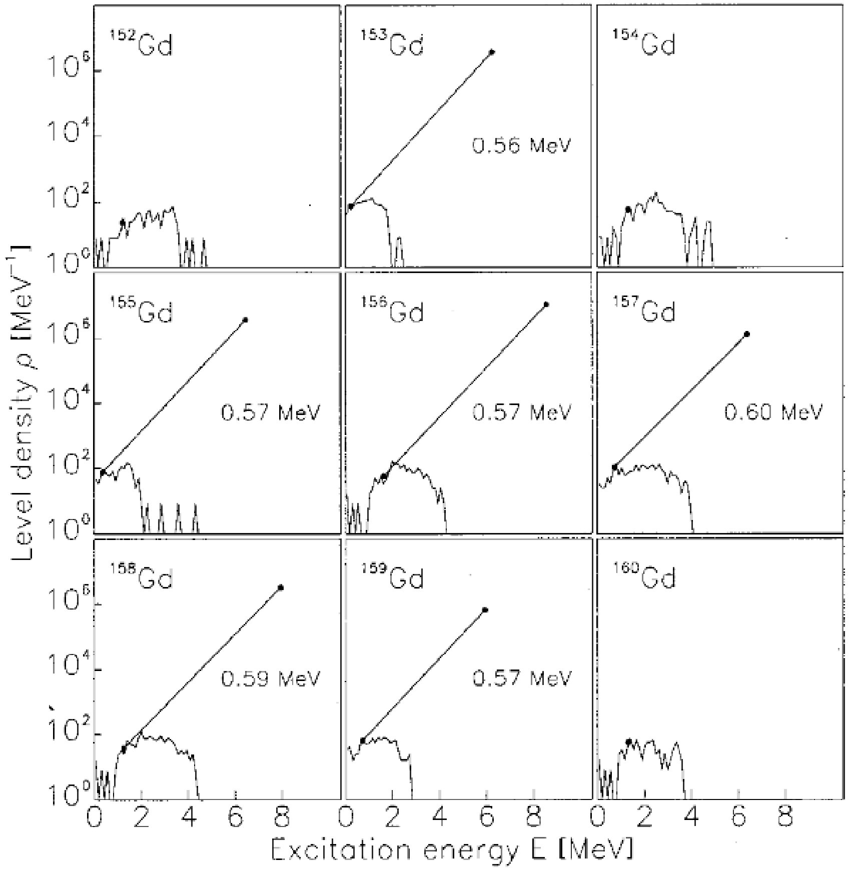


Constant-temperature + Fermi Gas Model

a.k.a. "Gilbert and Cameron Model", because Gilbert & Cameron, Can.J.Phys. (1965)

- Looking at the same phenomenon in a different way, we can take a thermodynamic approach
- Recall the number of accessible configurations $g(E^*) \propto \exp\left(\sqrt{aE^*}\right)$ and $T \approx \frac{1}{k_B}\sqrt{E^*/a}$, so $g(E^*) \propto \exp\left(\frac{E^*}{T}\right)$
- Therefore, the change in $g(E^*)$ as a function of E^* is $\frac{\partial g}{\partial E^*} = \rho(E^*) \propto \frac{1}{T}\exp\left(\frac{E^*}{T}\right)$
- Since $\frac{1}{T} = \frac{\partial S(E^*)}{\partial E^*} = \frac{\partial k_B \ln(g)}{\partial E^*} \propto \frac{\partial \ln(\rho(E^*))}{\partial E^*}$, we see constant T means $\ln(\rho(E^*))$ is linear in E^*, hence the model name
- The interpretation (M.Guttormsen et al. PRC **63** (2001)) is that energy goes into breaking Cooper pairs of nucleons, leaving the temperature constant, until some energy, above which the Fermi gas model is more suitable
- As before, we use the correction $U = E^* - \Delta$, but we neglect the backshift for pairing δ, since the CT is already accounting for pairing

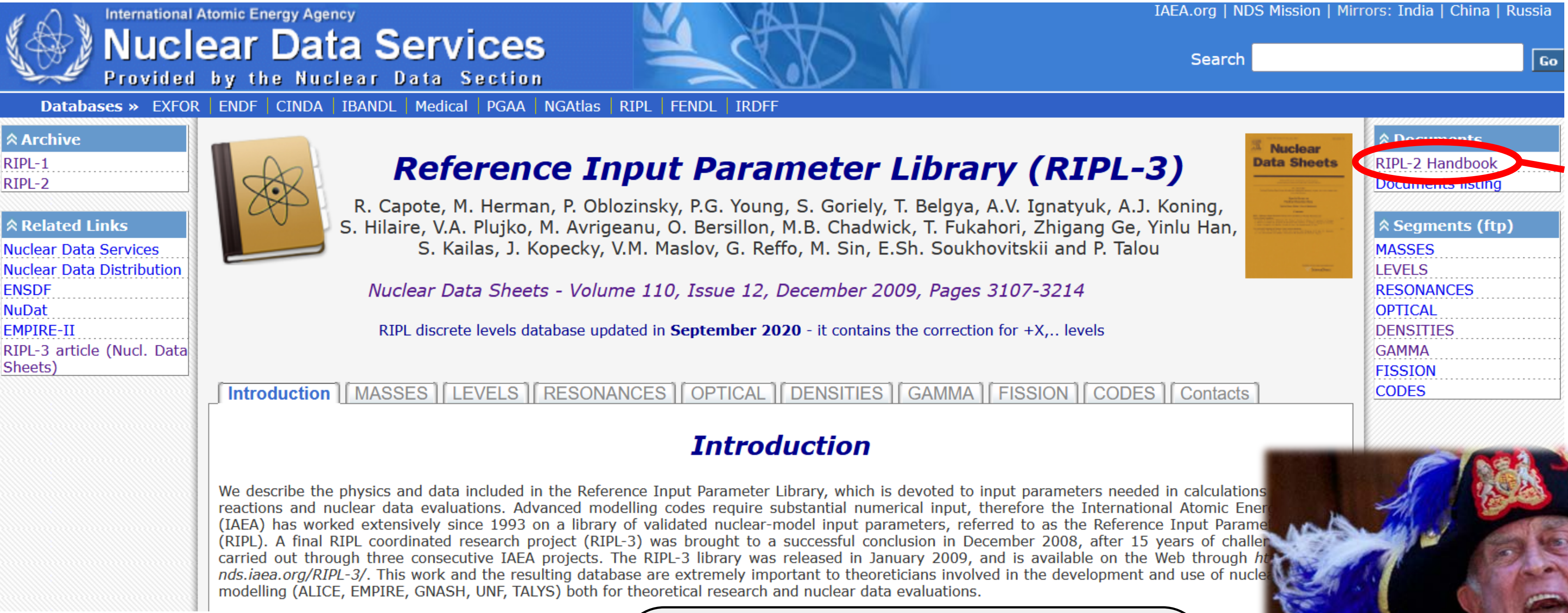
M.Guttormsen et al. PRC **63** (2001)



Note: Sometimes CT is used all by itself, as it does a pretty good job up to moderate excitation energies

Level density data available in the IAEA RIPL-3 database

Alternatively, you can get theoretical level-density estimates from the BRUSLIB database or the TALYS code (accessible from NNDC page)



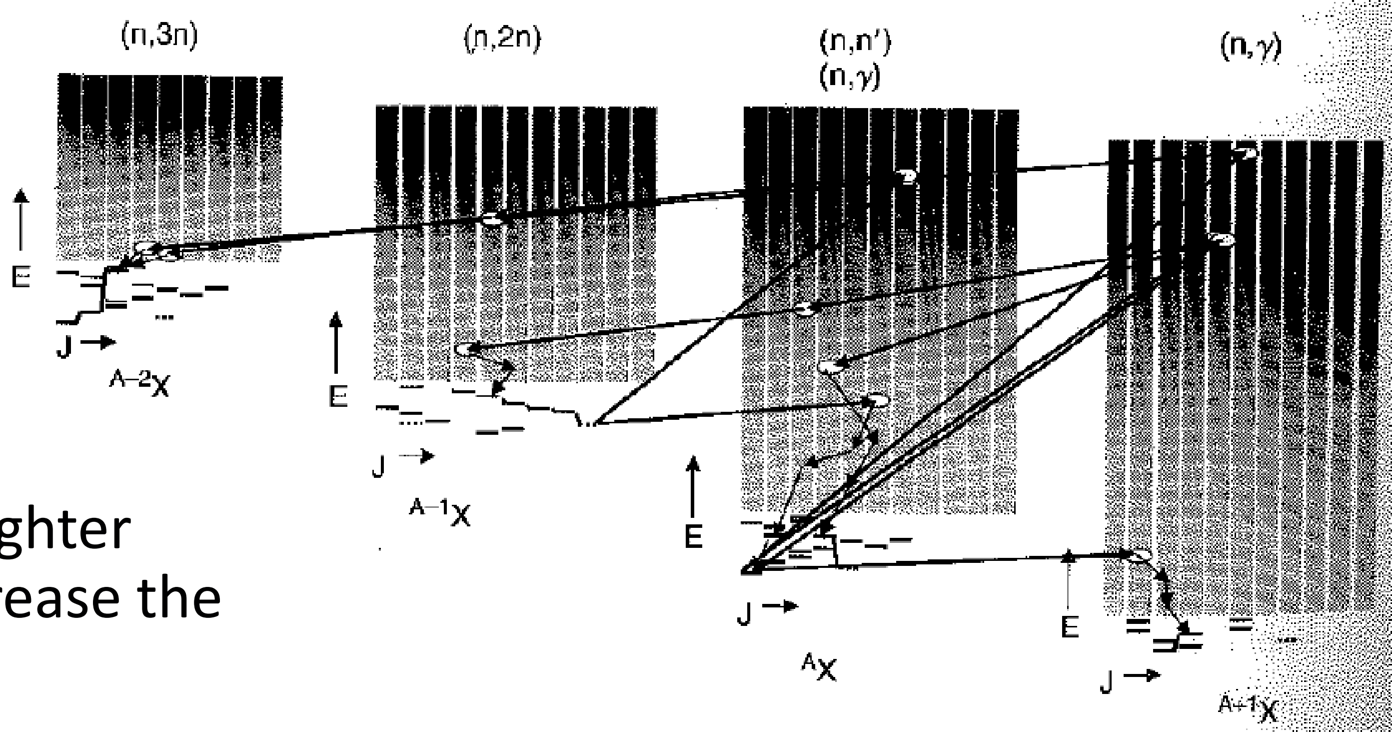
Arguably the best single text to consult on statistical nuclear physics

H're art the leveleth density paramet'rs, 'mongst oth'r things

Implications of level density for excited state decay

- When a nucleus is formed via a nuclear reaction, it may be energetically possible for the newly formed compound nucleus to break up into different sets of components (a.k.a. decay through different channels)
- The probability to decay via one channel or another is going to be directly proportional to the number of accessible final levels for that channel, since we assume the likelihood of populating any given level is equal (essentially the ergodic hypothesis)
- Therefore, a higher level-density in the daughter nucleus formed by a decay channel will increase the likelihood of forming that daughter nucleus (a.k.a. the cross section)

Decay modes for ^{A}X+n



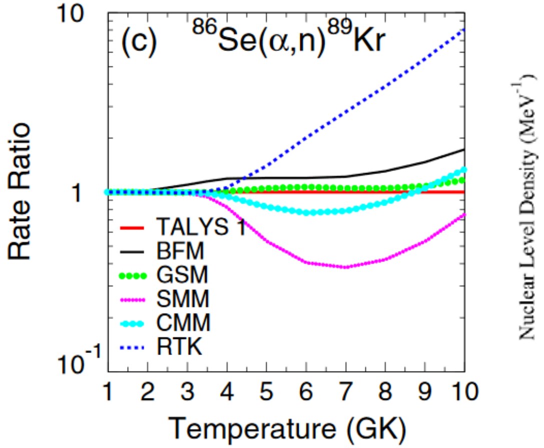
Thompson & Nunes, Nuclear Reactions for Astrophysics (2009)

- Later, when we discuss the Hauser-Feshbach theory for nuclear reaction rates, we will see that the level density gets multiplied by so-called Transmission coefficients to make the cross section

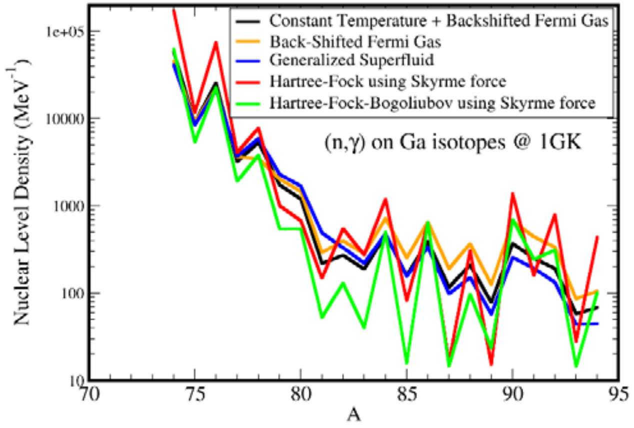
Level Density Impact (Selected examples)

Astrophysical Reaction Rates

Pereira & Montes, Phys.Rev.C (2016)

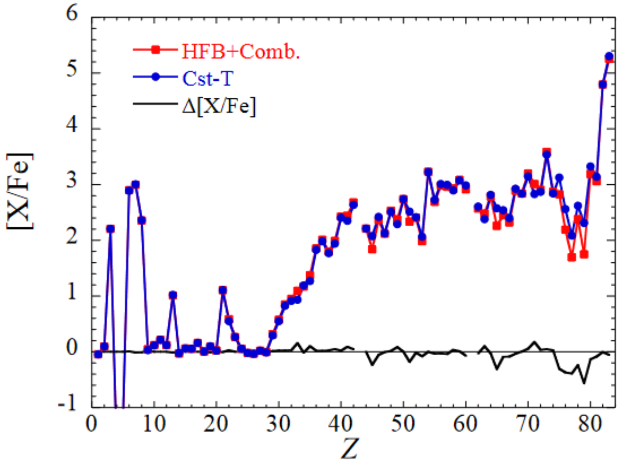


S. Nikas et al., arXiv:2010.01698 (2020)

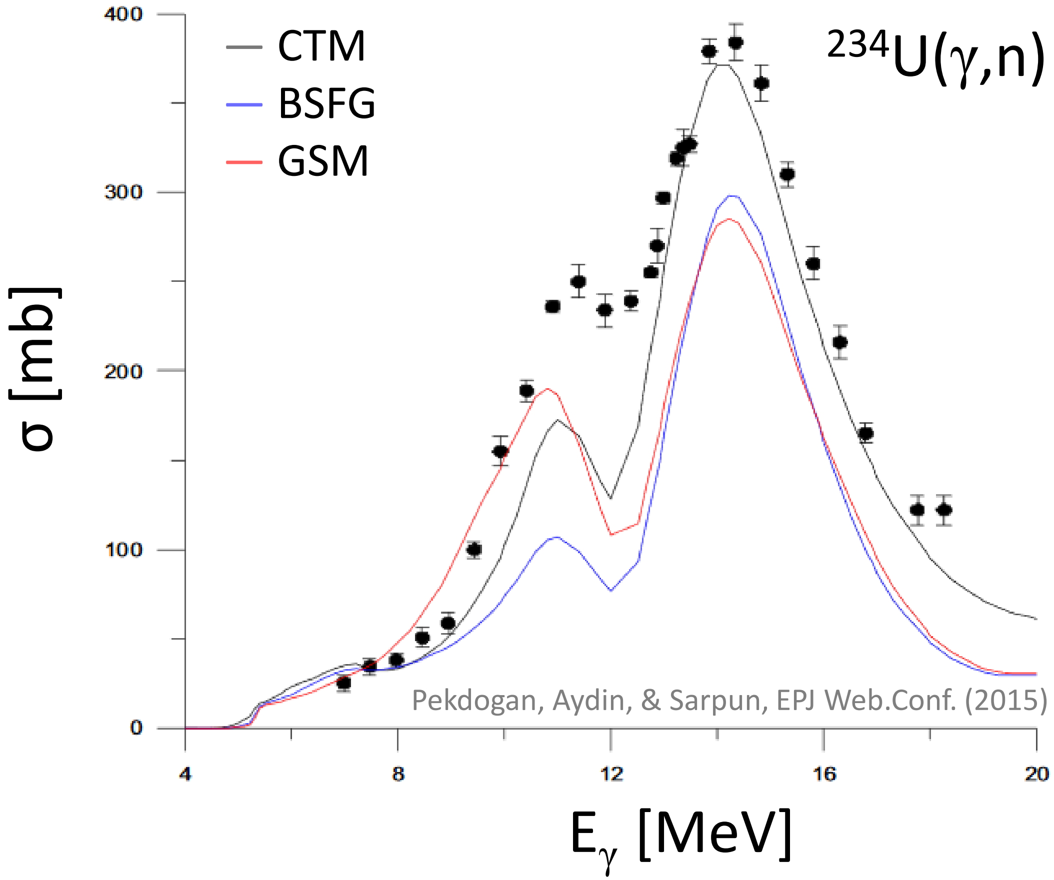


and associated nucleosynthesis

Goriely, Siess, & Choplin, A&A (2021)



Special Nuclear Material Detection



Further Reading

- Chapter 6: Modern Nuclear Chemistry (Loveland, Morrissey, Seaborg)
- Chapter 7: Nuclear & Particle Physics (B.R. Martin)
- Chapter 5, Section F: Introduction to Nuclear Physics & Chemistry (B. Harvey)
- Chapter 2: Statistical Models for Nuclear Decay (A.L. Cole)
- Chapter 2, Section 1i: Nuclear Structure Volume 1 (A. Bohr & B. Mottelson)
- Chapter 8 (Fermi Systems): Lecture Notes on Condensed Matter Physics (H. Glyde)
- Chapter 6: IAEA RIPL2 Handbook
- Chapter 4, Section 7: Talys User Manual
- Chapter 11: Nuclear Reactions for Astrophysics (I. Thompson & F. Nunes)