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Nuclear cohesion, Weizsacker's mass formula and statistical equilibrium in atomic nuclei

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Abstract

The nuclear cohesion is put in terms of the virial theorem, Weizsacker's mass formula is derived from free nucleons moving in a mean-field potential well, and the one-particle nuclear ground-state and energy spectrum are shown to not be able to sustain an excited nucleus.

The generic nucleus. The nucleon in the atomic nuclei has a radius $a = 1.5 \times 10^{-15} m \, (= 1.5 fm)$ and an average binding energy $\varepsilon \simeq 8 MeV$ (denoted also by u, or u_b for "bulk", or $-q$). On the other hand, it has a rest energy $E_b = Mc^2 \simeq 1 GeV$. It follows that the nucleon extends over the Compton wavelength $\lambda = \hbar c / E_b \sim 10^{-16} m = 0.1 fm$, and, consequently, it may move over distance a with energy of the order $\varepsilon \simeq 8 MeV$. It has a momentum $p \sim \hbar / a$ and a velocity $v \sim \varepsilon / p = \varepsilon a / \hbar \simeq 2 \times 10^7 m/s$, such that $v^2 / c^2 \sim 10^{-3}$, which indicates that the nucleon moves non-relativistically (as expected from the ratio of the two characteristic energies ε and E_b).

The virial theorem. Let $\dot{q} \partial T / \partial \dot{q} = 2T$ be Euler's identity for the kinetic energy T of a generic motion of coordinates q. T is a homogeneous function of degree two of velocities $\dot{q}$. Integrating by parts over motion time t we get

$$2T = (qp)_t / t - q\dot{p} = (qp)_t / t + q \partial U / \partial q \tag{1}$$

for time averages, where U is the potential energy and p denotes the momenta. For a bound motion the momenta are finite at time $t \to \infty$, so we are left with $2T = q \partial U / \partial q$.

This is the well-known theorem of the virial. For matter cohesion it may have a particular significance. First, we note that $q \partial U / \partial q$ is an oscillatory function of time, due to the oscillatory behaviour of the coordinates in a bound motion. Therefore, the time average of $q \partial U / \partial q$ retains only the uniform component of this function, which corresponds to certain initial values of the coordinates. These values correspond to the integrals of the motion, like energy, number of particles, etc. Next, the cohesion of the matter exhibits the phenomenon of saturation, *i.e.* energy, volume and number of particles are proportional to each other. It follows that coordinates q correponding to a certain energy define the volume of the body corresponding to that energy. This implies independent particles moving in a mean-field and purely attractive short-range forces. Then, matter cohesion is a statistical average over all the mechanical energies, as all the corresponding motions are possible. It is different from short-range forces with minima of potential energy. It follows that we have to average over q in equation (1) over the motion volume enclosed by a surface S and get the corresponding average with respect to number of particles, or energy. The result is the energy asociated with cohesion.

Doing so, and integrating by parts in equation (1) we obtain

$$2T + U = (qU)_S/q \ , \tag{2}$$

for space averages, where q denotes the range of the spatial average. This is the virial theorem for matter cohesion. The averages in equation (2) corresponds to the energy of matter aggregation via attractive short-range interaction. In addition, the derivation given above presupposes the quasi-classical description of matter aggregation.

Mechanical energies $E = un$, where u is a constant and n number of particles, are distributed in cohesion with equal weights dn/N, so that the mean energy is $\bar{E} = uN/2$ and the mean square energy is $\bar{E^2} = u^2N^2/3$. The dispersion is therefore $1/\sqrt{3}$, independent of the size N. Macroscopic matter is statistical, so that the sum of dispersion is governed by the $1/\sqrt{N}$-law: $(\sum \delta f_i)^2 = \sum (\delta f_i)^2 \sim N$, and dispersion goes like $1/\sqrt{N}$, where N is now the number of sub-ensembles.

All this applies to attractive short-range forces. The situation is different for cohesion by long-range Coulomb forces. In this case, the relevant coordinates are collective ones, related to the electron density. This change the dependence of the kinetic and potential energy, so the virial theorem has different coefficients (though numerically, of course, the energies are the same). In addition, the long-range Coulomb cohesion results in effective short-range binding with minima of the potential energy, and the corresponding collective, global dynamics removes the statistical character of the cohesion, so that the resulting mechanical energy is the cohesion energy.[1]

If the surface is a virtual one in the bulk, the term $(qU)_S/q$ is negative. We denote it by $-E_s$ and have the binding energy for the bulk

$$E_b = T + U = -T - E_s < 0 \ . \tag{3}$$

For a real surface the term $(qU)_S/q$ vanishes in equation (2) and we get the binding energy

$$E = T + U = -T = E_b + E_s < 0 \ , \tag{4}$$

on account of the same value of the kinetic energy in both cases. One can see that the binding energy of a body is higher than the binding energy of the bulk by the surface term E_s. Indeed, in order to break down a body we have to supply the fracture with its surface energy.

It is easy to see from (2) that the surface energy goes like number $N^{2/3}$ of surface particles, since $(qU)_S/q$ involves a summation over those particles only (which is the integration over the surface), while the bulk energy goes like N. Therefore, we can write $E_s = u_s N^{2/3}$ and $E_b = -u_b N$, and notice that the coefficients u_s and u_b are close in value to each other. For large N we can see that the surface energy can be neglected in comparison with bulk energy. For instance, averaging over large N we get $\langle E_s \rangle \, / \, \langle E_b \rangle = 6/5N^{1/3} \sim 0.2$ for $N = 200$.

We apply these results to the cohesion of the atomic nuclei, which indeed exhibit the saturation phenomenon. There, N is of course the mass number A.

Weizsacker's mass formula. It is customary to view the nucleons as free fermions, embedded in a square potential well $U = -N\varepsilon_0$, and write down $N = gVp_F^3/6\pi^2\hbar^3$, or $p_F = (6\pi^2/g)^{1/3}\hbar/a$, where V denotes the volume of a sphere of radius $R = aN^{1/3}$, p_F is the Fermi momentum and g is a statistical weight (for instance, $g = 4$, spin and isotopic spin included). Then we get the Fermi energy $\varepsilon_F = p_F^2/2M$ and the kinetic energy $T = 3N\varepsilon_F/5$. It is worth noting that in employing such

[1] See L. C. Cune and M. Apostol, ***Metallic Binding***, **apoma**, MB (2000).

formulae, the thermodynamic limit $N \to \infty$ is assumed, so that the surface energy is vanishing. According to (4) we get the binding energy of the bulk $E = -N\varepsilon_0 + 3N\varepsilon_F/5 = -3N\varepsilon_F/5$. We are interested in estimating the change q in energy for a change $\delta N = 1$ in number of particles at constant concentration. It is easy to see that it is given by $q = -3\varepsilon_F/5$. We emphasize that q differs from the chemical potential $\mu = \varepsilon_F$. Using $a = 1.5 \cdot 10^{-15}m$ we get $\varepsilon_F = \mu = 46MeV$ (for $g = 4$), the potential depth parameter $-\varepsilon_0 = -6\varepsilon_F/5 = 55.2MeV$ and $q = -3\varepsilon_F/5 = 27.6MeV$. (The fermions have also a pressure $p = 2\varepsilon_F/5a^3$, compensated by the pressure produced by the potential well ε_0).

In order to compare these results with the empirical mass formula we average over number of nucleons, in compliance with the requirement of the virial theorem (2) for matter cohesion. This average with respect to N amounts to taking half of the figures given above ($\int NdN/N = N/2$). We get therefore the (average) Fermi energy $\langle\varepsilon_F\rangle = 23MeV$, the depth parameter of the potential well $-\langle\varepsilon_0\rangle = 27.6MeV$ and $u_b \simeq -u_s = -q = 3\langle\varepsilon_F\rangle/5 = 13.8MeV$, a figure which compares well with the experimental fits. It is worth noting that $q = -13.8MeV$ differs from the empirical binding energy per particle $q = E/N \simeq -8MeV$ on account of additional energy contributions, like surface energy and the Coulomb repulsion, not included herein.

Weizsacker's mass formula reads therefore untill now

$$E = -u_b N + u_s N^{2/3} + ... \ , \tag{5}$$

where $u_b = u_s \simeq 13.8MeV$.

The Coulomb interaction for atomic nuclei can be written as $E_c \sim Z(Z-1)e^2/2R = Z(Z-1)N^{-1/3}e^2/2a$, where e is the electron charge (the factor 2 has been introduced in the denominator in order to account for the distribution over the volume R^3). Writing $E_c = u_c Z(Z-1)N^{-1/3}$ we get the coefficient $u_c = e^2/2a = 0.48MeV$, which agrees with the empirical value. Weizsacker's mass formula (5) becomes

$$E = -u_b N + u_s N^{2/3} + u_c Z(Z-1)N^{-1/3} + ... \ , \tag{6}$$

where $u_c = 0.48MeV$.

The last contribution to the mass formula comes from the symmetry effect, which is a consequence of the exclusion principle. It should increase the energy from a $g = 4$-degenerate energy level under a transform which replaces a proton by a neutron, or conversely, a neutron by a proton. This energy contribution, denoted E_r, should read $E_r = u_r(Z-N)^2/A$, where Z denotes the number of protons, N denotes now the number of neutrons and $A = Z + N$ is the mass number. In the limit $A \to \infty$ this term should compensate the bulk contribution, so that we get a value $u_{r1} \simeq -u_b = 13.8MeV$. Actually, this value should be somewhat larger, because E_r can also be written as $E_r = u_r(A-2Z)^2/A = u_r A x^2 < u_r A$, where $x = 1 - 2Z/A$. We average x^2 around $x = 1$, over the range described by the tangent to x^2 at $x = 1$. We get $\langle x^2\rangle = 7/12$ and the second value $u_{r2} \simeq 23MeV$. Finally, we get the mean value $u_r = (u_{r1} + u_{r2})/2 = 18.4MeV$, which agrees well with the empirical value. Weizsacker's mass formula becomes finally[2]

$$E = -u_b A + u_s A^{2/3} + u_c Z(Z-1)A^{-1/3} + u_r(Z-N)^2/A \ , \tag{7}$$

with $u_r \simeq 18.4MeV$.

Statistical equilibrium. For a consistent description of the statistical equilibrium of an ensemble of particles a series of inequalities of the type

$$\varepsilon_{eq} > T > \delta\varepsilon_f > \delta\varepsilon_{ex} \gg \delta\varepsilon_q > \delta\varepsilon_{obs} \tag{8}$$

[2] C. F. von Weizsacker, Z. Phys. **96** 431 (1935).

must be satisfied, where ε_{eq} is a mean (scale) energy, T is the temperature, $\delta\varepsilon_f = T(\partial\varepsilon/\partial T)^{1/2}$ is the thermal fluctuation energy, $\delta\varepsilon_{ex}$ is the uncertainty in the energy of the elementary excitations, $\delta\varepsilon_q$ is the spacing between the quantal energy levels and, finally, $\delta\varepsilon_{obs}$ is the uncertainty in the observed (measured) energy, all per particle. For a large number of particles such inequalities are fulfilled, in general, but for small numbers of particles they may not be satisfied, which means that the ensemble is not in equilibrium, since, for instance, ε_{eq} may be comparable with $\delta\varepsilon_q$ in this case. The meaning of such inequalities resides in the succession of time intervals

$$\tau_{eq} < \tau_{th} < \tau_f < \tau_{life} \ll \tau_q < \tau_{obs} \tag{9}$$

required for measuring consistent mean values of various quantities, according to the generic uncertainty relationship $\tau \sim \hbar/\delta\varepsilon$. In (9) $\tau_{th} = \hbar/\varepsilon_{th}$ is the time needed to establish the thermal equilibrium, and τ_{life} is the lifetime of the elementary excitations.

For fermions at zero temperature ε_{eq} is of the order of the mean energy per particle, or Fermi energy ε_F, the next two terms in (8) do not appear, while the rest of inequalities in (8) keep their meaning. It is interesting to note that even in the absence of the thermal equilibrium we may still have a statistical equilibrium. Indeed, the mean energy is $\varepsilon_{eq} = 3\varepsilon_F/5$, while its mean square is $\bar{\varepsilon^2} = 3\varepsilon_F^2/7$, which is comparable with ε_{eq}^2. It shows how effective the establishing of the statistical equilbrium can be in this case, by exchanging energy during collisions. The fact that the statistical equilbrium may be independent of temperature originates in describing ensembles by probabilities, which is unavoidable when talking about such ensembles of particles in terms of particles. For a degenerate gas of fermions the discussion is similar, and for high temepratures the gas behaves classically. In both cases the meaning of (8) is defined.

For bosons at low temperature the scale energy ε_{eq} is the temperature $T_0 \sim \hbar^2/mr^2$ of the Bose-Einstein condensation, where r is the mean inter-particle distance and m is the particle mass. Above the condensation temperature the role of the ε_{eq} is played by the chemical potential (its absolute value), which for high temperatures becomes again that of a classical gas. A similar discussion holds also for other ensembles of particles (of an academic interest in this context might be the Bose-Einstein condensation of relativistic particles, more exactly relativistic corrections to the Bose-Einstein condensation), the black-body radiation included.

According to the discussion given above, the nucleons may be brought into statistical equilibrium in time $\tau_{eq} = \hbar/\varepsilon$, providing energy ε is shared among a large number of energy levels. This is not the case for the atomic nucleus with mean-field nucleons, the "shell-model" included. Indeed, the momentum of free fermions is given by $p = \hbar n/R$, where $R = aN^{1/3}$ is the radius of the nucleus, and the Fermi momentum is $p_F \sim \hbar n_F/R = \hbar n_F/aN^{1/3}$, hence the Fermi number $n_F \sim N^{1/3} \sim 6$ for $N \sim 200$. The energy levels are given by $\varepsilon_n = (\hbar^2/MR^2)n^2 = (\hbar^2/Ma^2)n^2/N^{2/3}$, and for $n = n_F$ we get the Fermi energy $\varepsilon_F \sim \hbar^2/Ma^2$ ($\sim 15MeV$).[3] We see that only a few energy levels are occupied ($n_F \sim 6$), as a consequence of the spatial degeneracy. The energy separation is $\delta\varepsilon \sim (\hbar^2/MR^2)n$, and $\delta\varepsilon_F \sim (\hbar^2/Ma^2)/N^{1/3} \sim \varepsilon_F/6$, which is comparable to the Fermi energy. Consequently, we cannot have a statistical equilibrium. The free nucleons in a square potential well are purely a quantal ensemble, unable to sustain thermalization.

A self-consistent potential well of a mean field does not change the situation. The nucleons may accommodate to each other through mutually correlated motions over the entire volume of the nucleus, such as to produce a mean field acting as an external potential. It is usually a central-force field, like an oscillator potential, and it explains satisfactorily the nuclear shells and magic numbers. The energy separation is then reduced to somewhat extent ($1 - 2MeV$), but the degeneracy is

[3] Actually, this value of the Fermi energy is changed to somewhat extent by specific numerical factors, see the previous section.

still present, as indicated by the ~ 7 nuclear shells. The equilibrium is still unattainable. Even if, ideally, we distribute all the nucleons uniformly over an energy of the order ε_F, and get an energy separation $\delta\varepsilon \sim \varepsilon_F/N$, this separation is still insufficient for a consistent statistical equilibrium, in the sense that we would have then large fluctuations ($\sim 7\%$ for $N \sim 200$).

The atomic nucleus is too small to have a statistics of quasi-independent particles. It is cold, and there is no nuclear temperature, as long as such a gas-like ground-state and energy spectrum are maintained. In order to get a thermodynamics, and the nucleus to be able to get excited, the atomic nucleus must change its ground-state and enery spectrum.[4]

[4]The mean field may still work for special excitations, like the radiative capture of slow neutrons, where the neutron is gently accommodated. On the other hand, as it is well-known, one-particle nuclear models describe satisfactorily the nuclear shells, magic numbers, and even the mass formula.