The Smoothness of Physical Observables

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[A different point of view of the Garvey and Kelson Relations for Nuclear Masses]

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Outlook

- Garvey and Kelson Relations (GKR)
  - Assumptions
  - Algebraic expressions

- State-of-the-art
  - Systematic study of the whole nuclear chart
  - Quantum Chaos
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- GKRs: A different point of view
  - Example: Semi-empirical Mass Formula of Nuclei
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  - **Nuclear Physics:** Charge radii prediction for $^{195}$Pb.
  - **Particle Physics:** re-derivation of the Coleman-Glashow Mass Relation (octet $J^\pi = \frac{1}{2}^+$).
  - **Particle Physics:** Extension of the Coleman-Glashow Mass Relation (decuplet $J^\pi = \frac{3}{2}^+$).
  - **Particle Physics:** Extended 3D-GKRs. Gell-Mann Okubo Mass Relation (octet $J^\pi = \frac{1}{2}^+$).
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Garvey & Kelson Relations (GKR)
Motivation: “A mass formula will be in general too approximate to make predictions to a sufficient degree of accuracy.”

Proposal: “It is possible to develop certain simple relations between nuclidic masses”

Main assumption: “No assumptions are made about the quantitative aspects of the description except that the position of the single-particle levels, and the residual interactions between nucleons in them, vary slowly with atomic number”

FIG. 1. Diagram of the single-particle levels entering into Eq. (1) for the case $N=Z=2n$. From the figure it is evident that it expresses a set of identitities, as the same configurations appear for each single-particle level on both sides of the equation. As the configurations are encountered in different nuclei, it is necessary to assume a slow variation of the Hartree-Fock field with atomic number.
“New Nuclidic Mass Relationship” [PRL 16 (1966) 197]

\[
M(N+2, Z-2) - M(N, Z) = M(N+1, Z-2) - M(N, Z-1) + M(N+2, Z-1) - M(N+1, Z).
\] (1)

Generalization:

\[
M(N+\Delta T, Z-\Delta T) - M(N, Z) = \sum_{i=1}^{\Delta T} \left[ M(N+i, Z-\Delta T-i+1) - M(N-1+i, Z-\Delta T+i) \right].\] (2)

Some tests:

\[
\begin{align*}
10^{15}C_6^{15} - 8^{16}O_8^{16} &= 9^{15}C_6^{15} + 8^{17}N_7^{15} + 10^{17}N_7^{17} - 9^{17}O_8^{17} \quad (0.01 \text{ MeV}), \\
22^{36}S_{16}^{38} - 15^{38}K_{19}^{38} &= 20^{36}S_{16}^{36} - 19^{38}C_{17}^{38} + 21^{38}C_{17}^{38} - 20^{38}A_{18}^{38} \\
&\quad + 22^{40}A_{18}^{40} - 21^{40}K_{19}^{40} \quad (0.30 \pm 0.15 \text{ MeV}), \\
129^{211}Pb_{82}^{211} - 125^{211}Fr_{87}^{211} &= 125^{207}Pb_{82}^{207} - 123^{207}Bi_{83}^{207} + 126^{209}P_{83}^{209} - 123^{209}Po_{84}^{209} \\
&\quad + 127^{211}Po_{84}^{211} - 123^{211}At_{85}^{211} + 128^{213}At_{85}^{213} - 127^{213}Rh_{86}^{213} \\
&\quad + 128^{215}Rh_{86}^{215} - 123^{215}Fr_{87}^{215} \quad (0.55 \pm 0.35 \text{ MeV}),
\end{align*}
\]
State–of–the–art: Two examples
“We discuss the Garvey and Kelson mass relations in an extended formalism and show how they can be used to test and improve the consistency of the most commonly used mass formulas to achieve more accurate predictions.”

\[
\begin{align*}
M(N - 2, Z + 2) + M(N - 2, Z - 2) + M(N + 2, Z + 2) + M(N + 2, Z - 2) \\
- 2M(N + 2, Z - 1) - 2M(N + 2, Z + 1) \\
- 2M(N - 2, Z - 1) - 2M(N - 2, Z + 1) \\
- 2M(N - 1, Z - 2) - 2M(N + 1, Z - 2) \\
- 2M(N - 1, Z + 2) - 2M(N + 1, Z + 2) \\
+ 2M(N + 2, Z) + 2M(N - 2, Z) \\
+ 2M(N, Z - 2) + 2M(N, Z + 2) \\
+ 4M(N + 1, Z) + 4M(N - 1, Z) \\
+ 4M(N, Z - 1) + 4M(N, Z + 1) \\
- 12M(N, Z) = 0.
\end{align*}
\] (4)

**TABLE 1.** The rms deviations for masses (in keV) calculated with the GK relations for different \( n \).

|      | \( n \geq 1 \) | \( n \geq 4 \) | \( n \geq 7 \) | \( n = 12 \) |
|------|----------------|----------------|----------------|-----------|
| \( A \geq 16 \) | 182            | 152            | 123            | 87        |
| \( A \geq 60 \)   | 115            | 98             | 86             | 76        |
It has been suggested that chaotic motion inside the nucleus may significantly limit the accuracy with which nuclear masses can be calculated. Using a power spectrum analysis we show that the inclusion of additional physical contributions in mass calculations, through many-body interactions or local information, removes the chaotic signal in the discrepancies between calculated and measured masses. Furthermore, a systematic application of global mass formulas and of a set of relationships among neighboring nuclei to more than 2000 nuclear masses allows one to set an unambiguous upper bound for the average errors in calculated masses, which turn out to be almost an order of magnitude smaller than estimated chaotic components.
“Nuclear Masses Set Bounds on Quantum Chaos” [PRL94 (2005) 102501]

In summary, a careful use of several global mass formulas and a systematic application of the Garvey-Kelson relations imply that there is no evidence that nuclear masses cannot be calculated with an average accuracy of better than 100 keV. While mass errors in mean-field calculations like the FRDM behave like quantum chaos, with a slope in their power spectrum close to $-1$, microscopic models' results correspond to smaller slopes. Finally, for the local GK relations the remaining mass deviations behave very much like white noise. These re-

FIG. 1 (color online). Differences, in MeV, between the measured masses [24] and those obtained in LDM, FRDM, DZ, and GK, plotted against the order number $f$.

FIG. 2 (color online). Squared amplitudes of the Fourier transforms of the mass differences obtained in LDM, FRDM, DZ, and GK, plotted against the frequency $\omega = k/N$. 
GKRs: A different point of view
GKR: A different point of view I

Assumption: smoothness of the underlying physical observable \( O \).

- Within this assumption, if the observable \( O \) depends on \( n \) independent variables \( O(x_1, x_2, \ldots, x_n) \) one can always expand the unknown function in a Taylor series.

Choosing the particular case of \( n = 2 \) for comparison with GKR's and expanding around \( x \to x_0 \) and \( y \to y_0 \),

\[
O(x, y) = \sum_{\ell=0}^{\infty} \sum_{\kappa=0}^\ell \frac{\Delta x^{\ell-\kappa} \Delta y^\kappa}{\kappa!(\ell-\kappa)!} \frac{\partial^\ell O(x, y)}{\partial x^{\ell-\kappa} \partial y^\kappa}
\]

where \( \Delta x \equiv x - x_0 \) and \( \Delta y \equiv y - y_0 \). Applying the GKR (a),

\[
O(x + 2, y - 2) - O(x, y) + O(x, y - 1) - O(x + 1, y - 2) + O(x + 1, y) - O(x + 2, y - 1) = \frac{\partial^3 O(x, y)}{\partial x \partial y^2} - \frac{\partial^3 O(x, y)}{\partial x^2 \partial y} + O[\partial^4 O]
\]

A smooth function in \( x \) and \( y \to \) smallest contribution as higher are the derivatives.
GKR: A different point of view II

Within this procedure one can easily find 3 relations more proportional to the third derivatives which are linearly independent:

\[ O(x + 2, y) - O(x, y - 2) + O(x + 1, y - 2) - O(x + 2, y - 1) + \]

\[ O(x, y - 1) - O(x + 1, y) = \frac{\partial^3 O(x, y)}{\partial x \partial y^2} + \frac{\partial^3 O(x, y)}{\partial x^2 \partial y} + O[\partial^4 O] \]

\[ O(x + 2, y) - 3O(x + 1, y) + 3O(x, y) - O(x - 1, y) = \frac{\partial^3 O(x, y)}{\partial x^3} + O[\partial^4 O] \]

\[ O(x, y + 2) - 3O(x, y + 1) + 3O(x, y) - O(x, y - 1) = \frac{\partial^3 O(x, y)}{\partial y^3} + O[\partial^4 O] \]

Thus, it is a helpful tool for the study of smooth observables described within a good established theory or not.
GKR: A different point of view III

The accurate description of the experiment shown for the relation involving 21 neighbor nuclei (c) proposed by Barea et al. in reference Phys. Rev. C77 (2008) 041304(R) has, within our point of view, an easy explanation:

\[
\Delta M_{21 \text{ Masses}} = 2 \frac{\partial^6 O(x, y)}{\partial x^4 \partial y^2} + 2 \frac{\partial^6 O(x, y)}{\partial x^2 \partial y^4} + \mathcal{O}[\partial^4 O]
\]

And within the generalization (b) proposed by GK,

\[
M(N + \Delta T, Z - \Delta T) - M(N, Z) - \sum_{\ell=1}^{\Delta T} [M(N + \ell, Z - \Delta T - 1 + \ell) - M(N - 1 + \ell, Z - \Delta T + \ell)] = \frac{1}{6} (\Delta T + 1) \Delta T (\Delta T - 1) \left( \frac{\partial^3 M(N, Z)}{\partial N \partial Z^2} - \frac{\partial^3 M(N, Z)}{\partial N^2 \partial Z} \right)
\]

one gets –for smooth observables as the nuclear masses– worst results with increasing values of \(\Delta T\) (i.e. more masses).
Thus, GKR are more general and more powerful than originally assumed. Have been shown:

- the mathematical reasons why the GKR works for any smooth observables.
- that are model independent (insensitive to the underlying dynamics provided the slowly-varying assumption of the observable).
- different relations can improve the accuracy of the original GKR by progressively removing third and higher order derivatives.
Example: Semi-empirical Mass Formula of Nuclei I

If $M(A, Z)$ is represented by the smooth liquid drop formula:

$$M(A, Z) \equiv m_p Z + m_n (A - Z) - B(A, Z)$$

$$B(A, Z) \equiv a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(A - 2Z)^2}{A}$$

And applying the GKR (a) and (c),

$$\Delta M_{6 \text{ Masses}} = -2 \frac{36 A a_a + 3 A (5/3) a_c + 72 a_a Z + 4 A (2/3) a_c Z}{9 A^3}$$

$$\Delta M_{21 \text{ Masses}} = 32 \frac{972 a_a + 35 A^{2/3} a_c}{81 A^5}$$
Examples beyond nuclear masses
Nuclear Physics: $R_{\text{ch}}$ prediction for $^{195}\text{Pb}$ within $\Delta R_6$

To illustrate the generality and the flexibility of the approach we extend, in this example, the application of the GKR to nuclear charge radius.

| Nucleus | $R_{\text{ch}}$(fm) | Nucleus | $R_{\text{ch}}$(fm) |
|---------|---------------------|---------|---------------------|
| $^{197}_{82}\text{Pb}$ | 5.4420 | $^{195}_{80}\text{Hg}$ | 5.4347 |
| $^{193}_{80}\text{Hg}$ | 5.4239 | $^{195}_{82}\text{Pb}$ | —— |
| $^{194}_{80}\text{Hg}$ | 5.4311 | $^{194}_{81}\text{Tl}$ | 5.4233 |
| $^{194}_{81}\text{Tl}$ | 5.4304 | $^{196}_{80}\text{Hg}$ | 5.4311 |
| $^{196}_{82}\text{Pb}$ | 5.4420 | $^{196}_{82}\text{Pb}$ | 5.4420 |
| $^{196}_{81}\text{Tl}$ | 5.4304 |

| $|\Delta R_6^{(2)}|$ | 0.0001 | $|\Delta R_6^{(1)}|$ | 5.4385 |

In this particular case, exist 4 of 12 possible estimates for $^{195}\text{Pb}$ involving different neighbors leading to an average value of $R_{\text{ch}}(^{195}\text{Pb}) = 5.437(5)$ fm.
Particle Physics: re-derivation of the Coleman-Glashow Mass Relation (octet \(J^\pi = \frac{1}{2}^+\))

\[
\begin{align*}
\Sigma^- & \quad \Sigma^0 & \quad \Lambda & \quad \Sigma^+ \\
\Xi^- & \quad \Xi^0 & \quad q = +1 \\
q = -1 & \quad q = 0
\end{align*}
\]

\[
\Delta_{CG} = (p - n) - (\Sigma^+ - \Sigma^-) + (\Xi^0 - \Xi^-)
\]

\[
= \frac{\partial^3 m_8(S, Q)}{\partial S \partial Q^2} + \frac{\partial^3 m_8(S, Q)}{\partial S^2 \partial Q} + O[\partial^4 m_8(S, Q)]
\]

where \(m_8(S, Q)\) is the underlying ground-state baryon octet mass function. The equation \(\Delta_{CG} = 0\) is the celebrated Coleman-Glashow (CG) mass relation, derived originally using unbroken flavor \(SU(3)\) and later by methods as the \(1/N_c\) expansion.
Particle Physics: extension of the Coleman-Glashow Mass Relation (decuplet $J^\pi = \frac{3}{2}^+$)

\[ \Delta^*_\text{CG} = (\Delta^+ - \Delta^0) - (\Sigma^{*+} - \Sigma^{*-}) + (\Xi^0 - \Xi^{*-}) \approx 1.2\, \text{MeV} ! \]
Particle Physics: extended 3D-GKRs. Gell-Mann Okubo
Mass Relation (octet $J^{\pi} = \frac{1}{2}^+$)

\[ \begin{align*}
\Sigma^- & \quad \Sigma^0 & \quad \Lambda & \quad \Sigma^+ \\
\Xi^- & \quad \Xi^0 & \quad \Lambda & \quad \Xi^+ \\
q = -1 & \quad q = 0 & \quad q = +1
\end{align*} \]

3D-Relation (Check in MeV)

\[
\begin{array}{c}
\Xi^0 + n - \Lambda - \Sigma^0 \approx 95 \\
\Sigma^+ + n + \Xi^- - \Lambda - 2\Sigma^0 \approx 91 \\
\Sigma^- + \Lambda - n - \Xi^- \approx 93 \\
p + \Xi^- - \Lambda - \Sigma^0 \approx -89 \\
\end{array}
\]

\[\Delta m_8\]

\[
\begin{align*}
(\partial^2_{q^2} - \partial^2_{q,s} - \frac{1}{2} \partial^2_{q,l} - \frac{1}{4} \partial^2_{l^2})m_8 \\
(\partial^2_{q^2} - \frac{1}{2} \partial^2_{q,s} - \frac{1}{4} \partial^2_{l^2})m_8 \\
(\partial^2_{q^2} - \frac{1}{4} \partial^2_{l^2})m_8
\end{align*}
\]

Gell-Mann Okubo

\[
\begin{align*}
3\Lambda + \Sigma^0 - 2\Xi^0 - 2n & \approx 154 \\
(-2\partial^2_{q^2} - \partial^2_{q,q} - \partial^2_{q,l})m_8
\end{align*}
\]
Conclusions
Conclusions of our study

The validity of the GK relations hinges exclusively on the smoothness of the underlying function and on nothing else. So,

1. any slowly-varying physical observable satisfies the GK relations.
2. the GK relations are model independent.
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Moreover,

▸ we hope that the present study may already inspire to consider applications in other fields and perhaps even to areas outside of physics.
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Thank you!
Additional information
link: http://pdg.lbl.gov/2008/mcdata/mass_width_2008.csv

| MASS(MeV)    | I   | J   | P  | Name       | Quarks |
|-------------|-----|-----|----|------------|--------|
| 938.2720    | 1/2 | 1/2 | +  | p(P11)     | uud    |
| 939.5654    | 1/2 | 1/2 | +  | n(P11)     | udd    |
| 1189.3700   | 1   | 1/2 | +  | Σ(P11)     | uus    |
| 1192.6420   | 1   | 1/2 | +  | Σ(P11)     | uds    |
| 1197.4490   | 1   | 1/2 | +  | Σ(P11)     | dds    |
| 1314.8600   | 1/2 | 1/2 | +  | Ξ(P11)     | uss    |
| 1321.7100   | 1/2 | 1/2 | +  | Ξ(P11)     | dss    |
| 1115.6830   | 0   | 1/2 | +  | Λ(P01)     | uds    |
### Particle Data Base (2008)

**link:** http://pdg.lbl.gov/2008/mcdata/mass_width_2008.csv

| MASS (MeV) | I   | J   | P   | Name               | Charge | Quarks |
|------------|-----|-----|-----|--------------------|--------|--------|
| 1.23200E+03 | 3/2 | 3/2 | +   | ∆(1232)(P33)       | ++     | uuu    |
| 1.23200E+03 | 3/2 | 3/2 | +   | ∆(1232)(P33)       | +      | uud    |
| 1.23200E+03 | 3/2 | 3/2 | +   | ∆(1232)(P33)       | 0      | udd    |
| 1.23200E+03 | 3/2 | 3/2 | +   | ∆(1232)(P33)       | -      | ddd    |
| 1.3828E+03  | 1   | 3/2 | +   | Σ(1385)(P13)       | +      | uus    |
| 1.38370E+03 | 1   | 3/2 | +   | Σ(1385)(P13)       | 0      | uds    |
| 1.3872E+03  | 1   | 3/2 | +   | Σ(1385)(P13)       | -      | dds    |
| 1.53180E+03 | 1/2 | 3/2 | +   | Ξ(1530)(P13)       | 0      | uss    |
| 1.5350E+03  | 1/2 | 3/2 | +   | Ξ(1530)(P13)       | -      | dss    |
| 1.67245E+03 | 0   | 3/2 | +   | Ω                   | -      | sss    |
Essential to the derivation of the GK relations is the structure of the octet, decuplet,... but not the particular case of the ground state baryons. Thus, replacing strange quarks by charm quarks in the decuplet \( J = \frac{3}{2}^+ \) one can find:

\[
\Delta_{q=2} = \Delta^{++} - 3\Sigma_c^{++} + 3\Xi_{cc}^{++} - \Omega_{ccc}^{++} \approx 0 \\
3\Xi_{cc}^{++} - \Omega_{ccc}^{++} \approx 3\Sigma^{++} - \Delta^{++} \approx 6328\text{MeV}
\]

Note that a recent theoretical study based on the Bethe-Salpeter equation yields a value of 6396 MeV for this combination, (see Eur. Phys. J. A28, 41 (2006)) or a 1% discrepancy