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SUM RULE FUNCTIONS

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ERRATUM

p. (ii)	Line 15	'sum rules are obtained ....'
p. (iii)	Line 23	asterisk is superfluous
p. (iv)	Line 9	(Journal of Chemical Physics 48, No. 10, 4716-17)
p. 35	Line 24	'Then any A, E, L, or R transformation....'
p. 7		In the proof of theorem 7 it is necessary to assume that $\beta_0 > 0$. This can be done without loss of generality since $V(\varepsilon)$ can easily be transformed so that this assumption is met. [e.g. We could replace $V(\varepsilon)$ by $\varepsilon^{+\alpha} V(\varepsilon)$ where α is suitably chosen, & then $\beta \in [\beta_0, \infty)$ becomes $\beta \in [\beta_0 + \alpha, \infty)$].

SUM RULE FUNCTIONS I*

by

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INTRODUCTION

Many physical properties of an atom or molecule can be expressed in terms of the summations,[∓] known as <u>sum rules</u>,

$$S(k) = \sum_j{}' \varepsilon_{qj}^{-k} v_{qj}$$

where v_{qj} is an oscillator strength corresponding to a transition from state q to state j, ε_{qj} being the corresponding energy shift. If all the v_{qj}'s are positive for a particular q, for example q = o, then such a family of summations (as k ranges over all real values such that S(k) is convergent) is a particular example of a <u>sum rule function</u>. More generally, when the first N of the v_{qj}'s for a fixed q are negative, as would occur, for example, in the case of dipole oscillator strengths with q > o, then S(k) takes the form of a sum rule function plus an <u>N-sum rule function</u>. Thus, there is an immediate interest in the <u>nature</u> of sum rule functions and of N-sum rule functions. This is discussed in this paper.

For atoms the <u>dipole</u> oscillator strengths have been especially studied and it is usually possible to calculate or measure various of the corresponding S(k)'s directly*. For example, the Reiche-Thomas-Kuhn Sum Rule gives S(0) = number of electrons of the atom (using

*See "Advances in Quantum Chemistry" Vol. 1 Academic Press Inc. New York (1964) 'Recent Developments in Perturbation Theory' by Joseph O. Hirschfelder, W. Byers Brown and Saul T. Epstein.

∓ It is preferable to write $S(\beta) = \sum_j{}' \varepsilon_{qj}^{-\beta-1} v_{qj}$ since then S(0) has a value independent of the choice of energy scale.

atomic units.) This motivates the current interest in the problem of bounding sum rules in terms of other sum rules and in the problem of interpolation between sum rules. Dalgarno and Kingston (1970 Proc. Roy. Soc. A259, 424) have found that for the ground state (q = 0) the S(k)'s can be approximated by the expression

$$S(k) = n\left[\mathcal{E}_{10} + a(2{\cdot}5-k)^{-1} + b(2{\cdot}5-k)^{-2}\right]^{k}$$

providing the fqj's are dipole oscillator strengths. Here n is the number of electrons in the atom or molecule, "1" is the first excited state with nonvanishing oscillator strength, and the constants a and b are adjusted to make this equation correct for two selected values of k (usually k = -1 and k = -2). However, it must be stressed that this is only an approximate expression, with no bounding properties. In this paper we show how the problem of sum rule interpolation can be approached in such a way that the very best possible bounds to all (quantum mechanical) sum rules (based on any given set of sum rules). For a large class of given sets of sum rules we present an explicit construction for the appropriate interpolation functions. We also show the manner in which such constructions may be applied to other sets of given sum rules.

Let us digress briefly to give an example of precisely what is meant by "best possible". Suppose we are told that a certain function of a real variable is a sum rule function which we shall call $S(\beta)$. Suppose moreover that we are given the following information $\{S(\beta_0); S(\beta_1); \beta_0, \beta_1\}$ where β_0 and β_1 are finite real numbers. Then we can construct, given only this information, a function $S_1(\beta)$ which

(i) agrees with $S(\beta)$ at precisely $\beta = \beta_o$; $\beta = \beta_1$

(ii) gives lower bounds to $S(\beta)$ for $\beta \notin [\beta_o, \beta_1]$

(iii) gives upper bounds to $S(\beta)$ for $\beta \varepsilon (\beta_o, \beta_1)$

Moreover, these bounds are EXTENSIVE (i.e., every value of $S(\beta)$ is given a bound as β ranges through the real numbers); they are OPTIMAL (i.e., the lower bounds cannot possibly be improved on, on the basis of the information given); and finally, they are EXCLUSIVE (i.e., where $S_1(\beta)$ imposes a lower bound one cannot by any method which utilizes only the information which we are given, impose any upper bound except $+\infty$; and where $S_1(\beta)$ imposes an upper bound one cannot by any method which utilizes only the information which we are given impose any lower bound except zero). In the case of more than two given sum rules the best possible statement becomes slightly altered, but no less powerful. In general we shall be able to obtain both upper and lower bounds throughout various closed intervals, although in such cases we shall of course be forced to use more than two known sum rules.

The rigorous upper and lower bounds to sum rules that we can obtain may often be remarkable close; also they have applications. For example, Russell T. Pack (Chemical Physics Letters, Volume 5, Number 5, P. 257-259) has given a simple formula for an upper bound to the Van der Waals force constant in the interaction between any two atoms, in terms of the non-integer dipole sum rules $S(-1.5)$. Without concern for units his formula* is $Cab \leqslant 3/4\ Sa(-1.5)Sb(-1.5)$. Using rigorous upper bounds to the $S(-1.5)$'s we can obtain simple rigorous upper bounds to Cab. This formula was also derived independently by Howard L. Kramer

("Inequalities for Van der Waals Force Constants and Quantum Mechanical Sum Rules" which will be published in J. C. P.). Again, the Hylleraas variational principle has been applied by Davison (J. Phy. B (1968) Series 2, Vol. 1, 567-604) to yield lower bounds to the Van der Waal's force constants in terms of sum rules. Use of alternative trial functions to the ones used by Davison yields lower bounds in terms of various non-integer sum rules, and bounds on these yields bounds on the constants. Similar remarks apply to a variational principle given by Epstein (Journal of Chemical Physics 48). Finally, Barnsley has obtained excellent simple approximations to the Van der Waals force constants by using the interpolation functions directly. It is among the purposes of this paper to establish an initial reference to the theory of sum rule functions on which results concerning the above mentioned applications may be based.

More generally, sum rule functions arise whenever a series of Stieltjes occurs and hence the applications of their theory must ~~thus~~ be numerous. More precisely, if $F(z) = \int_0^\infty (1+uz)^{-1} dg(u) = \sum_{n=0}^\infty (-z)^n \int_0^\infty u^n dg(u)$ is a series of Stieltjes then the function $S(\beta) = \int_0^\infty u^\beta dg(u)$ is a sum rule function.

We remark that this paper can only serve as an introduction and that there is much work yet to be done. The proofs themselves are believed to be complete although a knowledge of elementary real analysis is often assumed, [3]. There is no doubt that the final formal theory will be far more elegant and the proofs simpler.

ABBREVIATIONS

The following abbreviations are used:

" $\Rightarrow$ " meaning "it follows that"

" $\exists$ " meaning "there exists"

" s.t. " meaning "such that"

" O.B.G.I." meaning "on the basis of the given information"

" cts. " meaning "continuous"

" cgs. " meaning "converges"

I. Unrestrained N-Sum Rule Functions and N-Sum Rule Functions

DEFINITION: If a function of a real variable β can be written in the form $\mathcal{S}_N(\beta) = \sum_{n=1}^{N} V_n / E_n^{\beta}$ where $V_n \neq 0$, V_n is real, and $0 < E_1 < \ldots\ldots\ldots < E_N$; then $\mathcal{S}_N(\beta)$ is an unrestrained N-sum rule function.

DEFINITION: If a function of a real variable β can be written in the form $S_N(\beta) = \sum_{n=1}^{N} V_n / E_n^{\beta}$ where $V_n > 0$, V_n is real, and $0 < E_1 < E_2 < \ldots < E_N$; then $S_N(\beta)$ is an N-sum rule function.

Unless otherwise stated, $\mathcal{S}_N(\beta)$ will denote an unrestrained N-sum rule function; $S_N(\beta)$ will denote an N-sum rule function.

THEOREM 1: $\mathcal{S}_N(\beta)$ has at most (N-1) zeros, the zeros at ∞ not being counted.

PROOF: We prove this by induction.

True for the case N = 1.

Suppose true N = 1,2,...,K.

Consider the zeros of $\mathcal{S}_{K+1}(\beta)$ where

$$\mathcal{S}_{K+1}(\beta) = \sum_{n=1}^{K+1} V_n/E_n^{\beta} = V_1/E_1^{\beta}\left[\sum_{n=2}^{K+1} \frac{(V_n/V_1)}{(E_n/E_1)^{\beta}} + 1\right]$$

which has the form:

$$\mathcal{S}_{K+1}(\beta) = V_1/E_1^{\beta}\left[\mathcal{S}_K(\beta) + 1\right]$$

Since $V_1/E_1^{\beta} \neq 0$ IT FOLLOWS THAT $S_{K+1}(\beta)$ has as many zeros as $f(\beta)$ where $f(\beta) = (S_K(\beta)+1)$. Now notice that $\partial S_n(\beta)/\partial\beta$ is an unrestrained m-sum rule function with m $\leq$ n. Hence $\partial f(\beta)/\partial\beta$ has at most (K-1) zeros, by the inductive hypothesis. Hence $f(\beta)$ has at most K zeros. Hence $S_{K+1}(\beta)$ has at most K zeros. This completes the induction.

THEOREM 2: Any $S_N(\beta)$ is uniquely defined by the values $S_N(\beta_i)$ $i=1,\ldots\ldots,2N$ where $-\infty < \beta_1 < \ldots\ldots < \beta_{2N} < \infty$.

PROOF: Suppose $\tilde{S}_N(\beta)$ is an unrestrained N-sum rule function which agrees with $S_N(\beta)$ for $\beta = \beta_i$, $i=1,\ldots\ldots,2N$. Then $S_M(\beta) = S_N(\beta) - \tilde{S}_N(\beta)$ is either an unrestrained M-sum rule function with $1 \leq M \leq 2N$ having $2N$ zeros or else $S_M(\beta) \equiv 0$. The first alternative is not possible by Theorem 1. Hence $S_N(\beta)$ is unique.

THEOREM 3: If $S_{N+1}(\beta)$ is an arbitrary (N+1)-sum rule function and $S_N(\beta)$ is an arbitrary N-sum rule function; then $(S_{N+1}(\beta) - S_N(\beta))$ has at most 2N zeros.

PROOF: $(S_{N+1}(\beta) - S_N(\beta)) = S_M(\beta)$ with $M \leq 2N+1$

Hence by Theorem 1, $(S_{N+1}(\beta) - S_N(\beta))$ has at most 2N zeros.

THEOREM 4: Given any $S_N(\beta)$, and any closed interval I = [a,b], then $\exists$ an $S_{N+1}(\beta)$ s.t. $|S_N(\beta) - S_{N+1}(\beta)| < \varepsilon_1$

for all $\beta \in I$; $|S_N(\beta) - S_{N+1}(\beta)| > M$ FOR ALL $\beta \in [b+\epsilon_2, \infty)$ where $1 > \epsilon_1 > 0$, $1 > \epsilon_2 > 0$ are arbitrarily small prescribed numbers; $M > 1$ is an arbitrarily large prescribed number.

PROOF: Take $V_{N+1} = (\epsilon_1/2)(\epsilon_1/4M)^{b/\epsilon_2}$; $E_{N+1} = (\epsilon_1/4M)^{1/\epsilon_2}$ and then let $S_{N+1}(\beta) = S_N(\beta) + V_{n+1}/E_{N+1}^{\beta}$.

THEOREM 5: Given any $S_N(\beta)$ and any closed interval $I = [a,b]$, then $\exists$ an $S_{N+2}(\beta)$ S.T. $|S_N(\beta) - S_{N+2}(\beta)| < \epsilon_1$ for all $\beta \in I$; $|S_N(\beta) - S_{N+2}(\beta)| > M_1$ FOR ALL $\beta \in [b+\epsilon_2, \infty)$ AND $|S_N(\beta) - S_{N+2}(\beta)| > M_2$ FOR ALL $\beta \in (-\infty, a-\epsilon_3]$ where $0 < \epsilon_1 < 1$, $0 < \epsilon_2 < 1$, AND $0 < \epsilon_3 < 1$, are arbitrarily small prescribed numbers; and $M_1 > 1$, $M_2 > 1$ are arbitrarily large prescribed numbers.

PROOF: Define $S_{N+1}(\beta)$ as in Theorem 4, replacing ϵ_1 by $\epsilon_1/2$. Take $V_{N+2} = (\epsilon_1/4)(8M_2/\epsilon_1)^{a/\epsilon_3}$; $E_{N+2} = (8M_2/\epsilon_1)^{1/\epsilon_3}$ and then let $S_{N+2} = S_{N+1}(\beta) + V_{N+2}/E_{N+2}^{\beta}$.

THEOREM 6: Given any $S_N(\beta)$ and any closed interval $I = [a,b]$; then for any integer $R \geq N+2$, $\exists$ AN $S_R(\beta)$ S.T. $|S_N(\beta) - S_R(\beta)| < \epsilon_1$ FOR ALL $\beta \in I$; $|S_N(\beta) - S_R(\beta)| > M_1$ FOR ALL $\beta \in [b+\epsilon_2, \infty)$; $|S_N(\beta) - S_R(\beta)| > M_2$ FOR ALL $\beta \in (-\infty, a-\epsilon_3]$; where $0<\epsilon_1<1$, $0<\epsilon_2<1$, AND $0<\epsilon_3<1$ are arbitrarily small prescribed numbers; AND $M_1, M_2 > 1$ are arbitrarily large prescribed numbers.

<u>PROOF</u>: Construct $S_{N+2}(\beta)$ as in theorem 4, replacing ϵ_1 by $(\epsilon_1/2)$. Choose a REAL POSITIVE NUMBER ϵ SUCH THAT $\left[\epsilon\left[1-\epsilon^{R-N-1}\right]/\left[1-\epsilon\right]\right] < (\epsilon_1/2)$. Then we can find an $S_{N+3}(\beta)$ S.T. $|S_{N+3}(\beta) - S_{N+2}(\beta)| < \epsilon$ FOR $\beta \in I$, ALSO AN $S_{N+4}(\beta)$ S.T. $|S_{N+4}(\beta) - S_{N+3}(\beta)| < \epsilon^2$ FOR $\beta \in I$, ALSO AN ...., AND FINALLY $S_R(\beta)$ S.T. $|S_R(\beta) - S_{R-1}(\beta)| < \epsilon^{R-N-2}$ FOR $\beta \in I$;

where each $S_{N+J}(\beta)$ is constructed from $S_{N+J-1}(\beta)$ as in theorem 4. Then $S_R(\beta)$ has the required properties.

Theorems 4, 5, and 6 are presented primarily to illustrate the nature of N-sum rule functions.

N-sum rule functions and unrestrained N-sum rule functions are the fundamental structures of sum rule function theory. It is their properties which dictate the nature of sum rule functions.

We stress the following points: an (unrestrained) N-sum rule function is a smooth infinitely differenciable function on the whole real line having at most N-1 zeros (which follows from the important detail that $0 < E_1 < \ldots\ldots < E_N$) so that no (unrestrained) N-sum rule function can ever vanish identically.

The nomenclature and notation for these functions (and for sum rule functions) stresses their connection with quantum mechanical sum rules.

Pictures of (unrestrained) N-sum rule functions

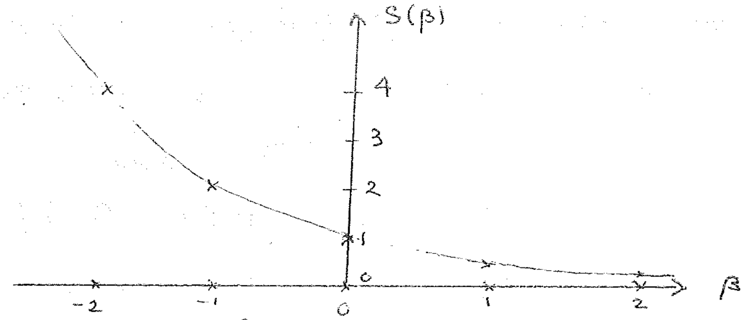

Fig. I $S_1(\beta) = 1/2^{\beta}$ (Monotone decreasing)

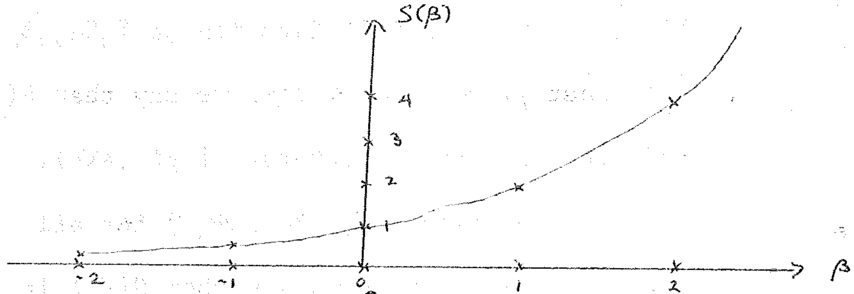

Fig. II $S_1(\beta) = 1/(1/2)^{\beta}$ (Monotone increasing)

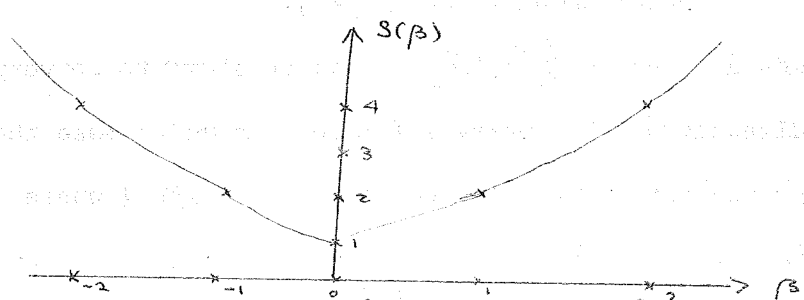

Fig. III $S_2(\beta) = (1/2)/2^{\beta} + (1/2)/(1/2)^{\beta}$

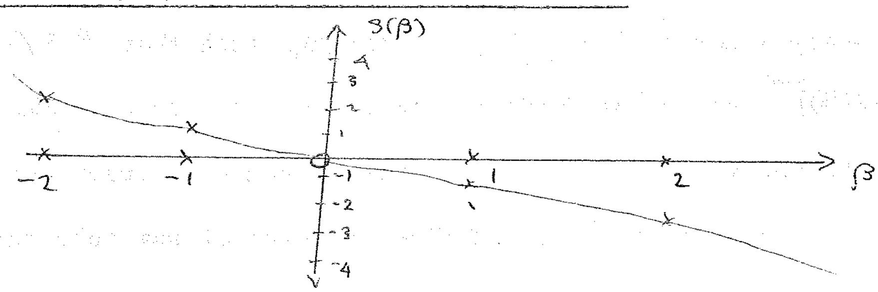

Fig. III $\mathcal{S}_2(\beta) = (1/2)/(1/2)^{\beta} - (1/2)/(2)^{\beta}$

II. SUM RULE FUNCTIONS

Definition: $S(\beta)$ is a sum rule function on the interval $[\beta_0, \beta_1]$, where $-\infty < \beta_0 < \beta_1 < +\infty$, if there exists a sequence of N-sum rule functions $\{S_N(\beta)\}_{N=1}^{\infty}$ such that

(i) $S(\beta)$ is finite for all $\beta \in [\beta_0, \beta_1]$

(ii) $S_N(\beta)$ tends uniformly to $S(\beta)$ for $\beta \in [\beta_0, \beta_1]$ as $N \longrightarrow \infty$.

If $S(\beta)$ is a sum rule function on $[\beta_0, \beta_1]$ for all β_1 such that $\beta_0 < \beta_1 < \infty$ then we say that $S(\beta)$ is a sum rule function on the interval $[\beta_0, \infty)$. If $S(\beta)$ is a sum rule function on $[\beta_0, \beta_1]$ for all β_0 such that $-\infty < \beta_0 < \beta_1$, then we say that $S(\beta)$ is a sum rule function on $(-\infty, \beta_1]$.

Sometimes a sequence $\{S_N(\beta)\}_{N=1}^{\infty}$ can be shown to converge uniformly to $S(\beta)$ directly on the interval $[\beta_0, \infty)$ in which case the same sequence converges uniformly to $S(\beta)$ on every $[\beta_0, \beta_1]$ where β_1 is such that $\beta_0 < \beta_1 < \infty$. However, the converse of this is not true. Namely, it is not true that if $\{S_N(\beta)\}_{N=1}^{\infty}$ converges uniformly to $S(\beta)$ on every interval $[\beta_0, \beta_1]$ with β_1 such that $\beta_0 < \beta_1 < \infty$ then $\{S_N(\beta)\}_{N=1}^{\infty}$ converges uniformly to $S(\beta)$ directly on $[\beta_0, \infty)$. This can be understood from the examples of sum rule functions (given in Theorem 7) which follow, and also in terms of sum rule scaling which we shall discuss later.

Our main interest is in sum rule function on intervals of the form $[\beta_0, \infty)$, and in particular, in those sum rule functions which are described in Theorem 7.

<u>Theorem 7</u> If $S(\beta)$ can be written in the form:

$S(\beta) = \int_{E_0}^{\infty} u^{-\beta}\, d\Phi(u)$; $E_0 > 0$; the integral being convergent for $\beta \in [\beta_0, \infty)$ and where $\Phi(u)$ is

(i) monotone non decreasing

(ii) and taking ∞ many values on $[E_0, \infty)$;

then $S(\beta)$ is a sum rule function on $[\beta_0, \infty)$

<u>Proof</u>: We will construct a requisite $\{S_N(\beta)\}_{N=1}^{\infty}$ sequence in a particular case and then indicate how this is generalized.

<u>Particular case</u>: Suppose $E_0 = 2$ and that the integral can be decomposed into $S(\beta) = \sum_{n=1}^{\infty} V_n E_n^{-\beta} + \int_{E}^{\infty} \frac{V(\varepsilon)}{\varepsilon^{\beta}}\, d\varepsilon$ for $\beta \in [\beta_0, \infty)$, where

(i) $V_n > 0$; $n = 1, 2, 3, \ldots$

(ii) $2 \leq E_1$; $E_n < E_{n+1}$; $\lim_{n \to \infty} E_n \leq E$

(iii) $V(\varepsilon) > 0$ and is a continuous function for $E \leq \varepsilon < \infty$

We will establish the existence of an $\{S_N(\beta)\}_{N=1}^{\infty}$ sequence as required by the definition of a sum rule function, with the uniform convergence taking place directly on the interval $[\beta_0, \infty)$.

Let $e > 0$ be prescribed.

Consider $\int_{E}^{\infty} V(\varepsilon)\varepsilon^{-\beta}\, d\varepsilon$. Since $\int_{E}^{\infty} V(\varepsilon)\varepsilon^{-\beta_0}\, d\varepsilon$ exists there must also exist an $F > E$ such that $\int_{F}^{\infty} \frac{V(\varepsilon)}{\varepsilon^{\beta}}\, d\varepsilon \leq \int_{F}^{\infty} \frac{V(\varepsilon)}{\varepsilon^{\beta_0}}\, d\varepsilon < \frac{e}{4}$ for all $\beta \in [\beta_0, \infty)$. (1)

Consider $\int_{E}^{F} \frac{V(\varepsilon)}{\varepsilon^{\beta}}\, d\varepsilon$. Define a sequence of equipartitions $\{\Delta_N\}_{N=1}^{\infty}$, of the interval [E,F], Δ_M being the set of (M + 1) equally spaced points $E = a_0^M < a_1^M < \ldots < a_M^M = F$.

Define two M-sum rule function on Δ_M

(i) $S^U_{\Delta M}(\beta) = \sum_{n=1}^{M} \overline{V}_n^M [a_n^M - a_{n-1}^M]/[a_{n-1}^M]^\beta$

(ii) $S^L_{\Delta M}(\beta) = \sum_{n=1}^{M} \nu_n^M [a_n^M - a_{n-1}^M]/[a_n^M]^\beta$

Where $\begin{cases} \overline{V}_n^M = Max\{V(\varepsilon) \mid \varepsilon \in [a_{n-1}^M, a_n^M]\} \\ \nu_n^M = Min\{V(\varepsilon) \mid \varepsilon \in [a_{n-1}^M, a_n^M]\} \end{cases}$

Then $S^U_{\Delta N}(\beta) > \int_E^F \frac{V(\varepsilon)}{\varepsilon^\beta} d\varepsilon > S^L_{\Delta N}(\beta)$ for all $\beta \in [\beta_0, \infty)$ (2)

Since $\int_E^F \frac{V(\varepsilon)}{\varepsilon^\beta} d\varepsilon \to 0$ as $\beta \to \infty$; $\Rightarrow \exists$ a $\beta_1 \in (\beta_0, \infty)$

s.t. $\int_E^F \frac{V(\varepsilon)}{\varepsilon^\beta} d\varepsilon < \frac{1}{4} e$ for all N if $\beta \in [\beta_1, \infty)$ (3)

Hence $0 < \int_E^F \frac{V(\varepsilon)}{\varepsilon^\beta} d\varepsilon - S^L_{\Delta N}(\beta) < \frac{1}{4} e$ for all N if $\beta \in [\beta_1, \infty)$

Now suppose $\beta \in [\beta_0, \beta_1]$.

$$S^U_{\Delta N}(\beta) - S^L_{\Delta N}(\beta) = \sum_{n=1}^{\infty} \left[\frac{(\overline{V}_n^N - \nu_n^N)}{[a_{n-1}^N]^\beta} + \nu_n^N \left\{ \frac{1}{[a_{n-1}^N]^\beta} - \frac{1}{[a_n^N]^\beta} \right\} \right] [a_n^N - a_{n-1}^N]$$

Since $V(\varepsilon)$ is continuous on the compact set [E, F], there exists an N_1

s.t. $N \geq N_1 \Rightarrow 0 \leq \frac{\overline{V}_n^N - \nu_n^N}{[a_{n-1}^N]^\beta} \leq \frac{\overline{V}_n^N - \nu_n^N}{E^{\beta_0}} < \frac{e}{8} \cdot \frac{1}{(F-E)}$; $n = 1, 2 \ldots N$

for all $\beta \in [\beta_0, \beta_1]$

Since $V(\varepsilon)$ is cts. on the compact set [E, F], there exists a $V > 0$

s.t. $0 < V(\varepsilon) \leq V$ for all $\varepsilon \in [E, F]$

Since $\varepsilon^{-\beta}$ is cts. on the compact set [E, F], there exists an N_2

s.t. $N \geq N_2 \Rightarrow 0 < \frac{1}{[a_{n-1}^N]^\beta} - \frac{1}{[a_n^N]^\beta} < \frac{e}{V[F-E]} \cdot \frac{1}{8}$ for all $\beta \in [\beta_0, \beta_1]$.

Hence for N $\geq$ max $\{N_1, N_2\}$ we have

$0 < S^U_{\Delta N}(\beta) - S^L_{\Delta N}(\beta) < e/4$ for all $\beta \in [\beta_0, \beta_1]$

Hence, by (2), for N $\geq$ max $\{N_1, N_2\}$ we have

$$0 < \int_E^F V(\varepsilon)/\varepsilon^\beta \, d\varepsilon - S_{\Delta N}^L(\beta) < \mathscr{E}/4 \quad \text{for all } \beta \in [\beta_0, \beta_1]$$

Combining the last statement with ① and ③ we see that, for N $\geqslant$ max$\{N_1, N_2\}$ we have:

$$0 < \int_E^\infty \frac{V(\varepsilon)}{\varepsilon^\beta} d\varepsilon - S_{\Delta N}^L(\beta) < \tfrac{1}{2}\mathscr{E} \quad \text{for all } \beta \in [\beta_0, \infty) \qquad ④$$

Since $\sum_{n=1}^\infty V_n E_n^{-\beta}$ is convergent, there exists an N_3 s.t. $N \geqslant N_3 \Rightarrow 0 < \sum_{n=1}^\infty V_n E_n^{-\beta} - \sum_{n=1}^N V_n E_n^{-\beta} < \tfrac{1}{2}\mathscr{E}$ for all $\beta \in [\beta_0, \infty)$ where we have also used the monotonicity of the sums as functions of β .

Hence, if $N \geqslant \max\{N_1, N_2, N_3\}$ then

$$0 < S(\beta) - \sum_{n=1}^N V_n E_n^{-\beta} - S_{\Delta N}^L(\beta) < \mathscr{E} \quad \text{for all } \beta \in [\beta_0, \infty)$$

Hence, for each $\mathscr{E} > 0$ there exists an N-sum rule function $S_N^*(\beta)$ such that $0 < S(\beta) - S_N^*(\beta) < \mathscr{E}$ for all $\beta \in [\beta_0, \infty)$

Hence we can find a sequence $N_1 < N_2 < \dots < N_n < \dots$ of integers and a sequence of N-sum rule functions, $S_{Np}^*(\beta)$, such that

$$0 < S(\beta) - S_{N_p}^*(\beta) < 1/p \quad ; \; p = 1, 2 \dots$$

for all $\beta \in [\beta_0, \infty)$.

It is easily seen from the theory of N-sum rule functions that we can now construct a sequence $\{S_N(\beta)\}_{N=1}^\infty$ which is uniformly convergent on $[\beta_0, \infty)$, such that

$$S_{N_p}(\beta) = S_{N_p}^*(\beta) \quad \text{for} \quad p = 1, 2, 3 \dots$$

The existence of $\{S_N(\beta)\}_{N=1}^\infty$, proves that $S(\beta)$ is a sum rule function. We notice that the particular sequence we have constructed satisfies $S_N(\beta) < S(\beta)$.

Extension of proof to the general case:

Most generally we can write:

$$S(\beta) = \sum_{n=1}^{N} V_n E_n^{-\beta} + \sum_{n=1}^{M} \int_{I_n} V_n(\epsilon)\,\epsilon^{-\beta}\,d\epsilon$$

where either or both of M,N may be infinite but if the second sum does not exist (i.e., M = 0) then $N = \infty$; and if N is finite then $M \geq 1$; and where

(i) $V_n > 0$; $n = 1,2,\ldots N$; $0 < E_1 < E_2 < \ldots$

(ii) $I_n = (a_n, b_n)$ with $E_0 \leq a_1 < b_1 \leq a_2 < b_2 \leq a_3 < \ldots$

(iii) $V_n(\epsilon) \geq 0$ is continuous on I_n, taking at least one non zero value in this interval.

It should be clear that corresponding to each integral, for example, the integral over the interval I_n, we can find a sequence of N-sum rule functions $\left\{ S_N^{I_n}(\beta) \right\}_{N=1}^{\infty}$ which converges uniformly to that integral at least on every interval $[\beta_0, \beta_1]$ for all β_1 such that $\beta_0 < \beta_1 < \infty$. In fact it will be necessary to establish the uniform convergence on such intervals $[\beta_0, \beta_1]$ only in those cases where $I_n \cap [1,0] \neq \Phi$. Hence we can find a sequence of N-sum rule functions tending uniformly to the overall sum on any interval $[\beta_0, \beta_1]$ where β_1 is such that $\beta_0 < \beta_1 < \infty$. This completes the proof.

Theorem 7 can be weakened slightly, for it is easily shown that if the integral $\int_{E_0}^{\infty} u^{-\beta}\,d\phi(u)$ is convergent for $\beta = \beta_0$ then it is convergent for all $\beta \in [\beta_0, \infty)$.

It is believed that the converse of Theorem 7 is also true.

Conjecture 1. If $S(\beta)$ is a sum rule function on $[\beta_0, \infty)$ then it can be written in the form $S(\beta) = \int_{E_0}^{\infty} u^{-\beta}\,d\phi(u)$ with $E_0 > 0$, the integral being convergent for $\beta = \beta_0$; and where $\phi(u)$ is

(i) monotone non-decreasing

(ii) and taking ∞ many values on $[E_0, \infty)$.

Noticing that if $S(\beta)$ is a sum rule function on $[\beta_0, \infty)$ then $S(-\beta)$, which we call the reflection of $S(\beta)$, is a sum rule function on $(-\infty, -\beta_0]$, we are now able to extend Theorem 7 to the following

Theorem 8. If $S(\beta)$ can be written in the form:

$$S(\beta) = \int_0^\infty u^{-\beta} \, d\phi(u) \quad \text{the integral existing for}$$

$\beta = \beta_0, \beta_1$, and where $\phi(u)$ is

(i) monotone non-decreasing

(ii) taking infinitely many values on $[0, \infty)$

then $S(\beta)$ is a sum rule function on $[\beta_0, \beta_1]$.

Proof: We first notice that if the integral exists for $\beta = \beta_0, \beta_1$ then it exists for all $\beta \in [\beta_0, \beta_1]$.

We can write
$$S(\beta) = \int_0^1 u^{-\beta} \, d\phi(u) + \int_{1+}^\infty u^{-\beta} \, d\phi(u)$$
$$= S_I(\beta) + S_{II}(\beta)$$

It is clear that $S_I(\beta)$ is a convergent integral for all $\beta \leq \beta_1$, and that $S_{II}(\beta)$ is a convergent integral for all $\beta \geq \beta_0$. In order to treat the most general case we will suppose that $\phi(u)$ in fact takes infinitely many values both in $(0, 1]$ and in $(1, \infty)$. The extension of the proof to all other possible cases should be clear from what now follows. Since $\phi(u)$ takes infinitely many values in $(1, \infty)$ it follows from Theorem 7 that $S_{II}(\beta)$ is a sum rule function on $[\beta_0, \infty)$.

Consider $\tilde{S}_I(\beta) = S_I(-\beta) = \int_0^1 u^{\beta}\, d\phi(u)$ for $\beta \in [-\beta_1, \infty)$

We can write this as:

$$\tilde{S}_I(\beta) = \int_{+\infty}^{1} u^{-\beta}\, d\phi(1/u) = \int_1^{\infty} u^{-\beta}\, d(-\phi(1/u))$$

But if ϕ (u) satisfies

(i) monotone non-decreasing

(ii) taking ∞ many values in (0, 1)

Then it is easily seen that $\hat{\phi}(u) = -\phi(1/u)$ satisfies

(i) monotone non-decreasing

(ii) taking ∞ many values in $[1, \infty)$.

Hence $\tilde{S}_I(\beta)$ is a sum rule function on $[-\beta_1, \infty)$ by Theorem 7.

Hence $S_I(\beta)$ is a sum rule function on $(-\infty, \beta_1]$

It is now easy to show, since $S_{II}(\beta)$ is a sum rule function on $[\beta_0, \infty)$, that $S(\beta) = S_I(\beta) + S_{II}(\beta)$ is a sum rule function on $[\beta_0, \beta_1]$. This completes the proof.

It is believed that the converse of this theorem (conjecture 2) is also true; and if this is the case then Theorem 8 together with its converse represents a complete characterization of sum rule functions.

<u>Conjecture 2</u>: If $S(\beta)$ is a sum rule function on $[\beta_0, \beta_1]$ then it can be written in the form $S(\beta) = \int_0^{\infty} u^{-\beta}\, d\phi(u)$ with the integral being convergent for $\beta \in [\beta_0, \beta_1]$, where ϕ (u) is

(i) monotone non-decreasing

(ii) taking infinitely many values in the interval $0 \leq u < \infty$

.

We will now restrict our attention to those sum rule functions which can be written in the form given in Theorem 8. It emerged naturally from the proof of Theorem 8 that all "Theorem 8" sum rule functions can be written in the form $S(\beta) = R(\beta) + T(-\beta)$ where one or other or both of $R(\beta)$ and $T(\beta)$ are sum rule functions, but which can be written in the special form $\int_1^\infty u^{-\beta}\, d\phi^R(u)$ and $\int_1^\infty u^{-\beta}\, d\phi^T(u)$ where $\phi^R(u)$, $\phi^T(u)$ satisfy the conditions of Theorem 7, with the rider that one or other but not both of $\phi^R(u)$, $\phi^T(u)$ MAY HAVE a finite spectrum, and where we take $E_0 = 1$. We call $R(\beta)$ a right hand convergent sum rule function and $T(-\beta)$ a left hand convergent sum rule function. $R(\beta)$ is in general a monotone decreasing function and $T(-\beta)$ is a monotone increasing function. Neither function need diverge to infinity (for example, if the spectrum of $\phi^R(u)$ is bounded above then convergence of the integral anywhere ensures its convergence everywhere). From the above decomposition we can see that a sum rule function can have at most one turning point and this is a minimum. There is much more we could say about sum rule functions, but for the moment we will content ourselves with a brief mention of two important transformations. We will discuss them in terms of "Theorem 7" sum rule functions.

Sum Rule Scaling.

Definition: If $S(\beta) = \int_{E_0}^\infty u^{-\beta}\, d\phi(u)$ is a sum rule function on $[\beta_0, \infty)$, then by the E-scaled sum rule functions $S^E(\beta)$ we shall mean:

$$S^E(\beta) = E^{-\beta}\int_{E_0}^\infty u^{-\beta}\, d\phi(u) \quad \text{where } E > 0$$

If $S(\beta)$ is a sum rule function on $[\beta_0, \infty)$ then so is $S^E(\beta)$ for we have: $E^{-\beta}\int_{E_0}^\infty u^{-\beta}\, d\phi(u) = \int_{E_0 E}^\infty u^{-\beta}\, d\phi(u/E)$ and it is seen that if $\phi(u)$

satisfies the conditions of Theorem 7, then so does $\phi(u/E)$ with $E_0 \to E_0 E$.

If we are given $S(\beta)$ on $[\beta_0, \infty)$ in the form of Theorem 7, then by choosing $E = 1/E_0$ we can ensure that $S^E(\beta)$ is a monotone decreasing function on $[\beta_0, \infty)$, i.e., we can ensure that $S^E(\beta)$ is of the form of $R(\beta)$ given above. Sum rule scaling may well be a useful device for establishing convergence properties. (see also Appendix IV)

POSITIVE LINEAR CHANGE OF VARIABLE

A positive linear transformation on the variable $\beta \in \mathbb{R}$ is $L\beta = \alpha\beta + \gamma$ where $\alpha > 0$ and α, γ are finite real numbers.

If $S(\beta)$ is a sum rule function on $[\beta_0, \infty)$ then $\tilde{S}(\beta) = S(L\beta)$ is a sum rule function on $[L^{-1}\beta_0, \infty)$.

It should be clear that there is one to one correspondence between the set of all sum rule functions defined on an interval $[a,b]$ and the set of all sum rule functions defined on any other interval $[c,d]$, the transformation which effects this correspondence being merely the positive linear transformation relating these intervals.

We will make repeated use of positive linear change of variable, and of reflection (i.e., the mapping $\beta \to -\beta$). (see also Appendix IV)

We have so far been concerned with trying to characterize sum rule functions from their definition. Why do we use this definition? The answer is simple. It contains the weakest possible conditions on $S(\beta)$ such that (i) it will at least be a reasonable function, namely, that it is continuous*, and (ii) sum rule interpolation theory may be

* This is ensured by the existence of a sequence of continuous functions which are uniformly convergent to $S(\beta)$ on the interval of definition.

developed on the basis of such a definition. Until our conjectures have been established it will remain difficult to decide quite <u>what</u> a sum rule function <u>is</u>. This question will be to some extent answered later when we deal with sum rule interpolations. The existence and bounding properties of the interpolation functions themselves will in fact tell us a great deal about sum rule functions.

We will now present what are probably the most important theorems concerning sum rule functions. They will allow us later, when we are dealing with interpolating sum rule functions using N-sum rule functions, to establish that our results are best possible.

<u>Theorem 9</u>: If $S_N(\beta)$ is any given N-sum rule function and I is any of the following intervals

(i) $I = [\beta_0', \beta_1']$ for any given β_0', β_1' such that $-\infty < \beta_0' < \beta_1' < \infty$

(ii) $I = [\beta_0', \infty)$ for any given β_0' such that $-\infty < \beta_0' < \infty$

(iii) $I = (-\infty, \beta_1']$ for any given β_1' such that $-\infty < \beta_1' < \infty$

then there exists a sum rule function $\tilde{S}(\beta)$ on the interval I such that $\tilde{S}(\beta)$ is arbitrarily close to $S_N(\beta)$ for all $\beta \in I$, and such that $S(\beta^*) - S_N(\beta^*)$ is arbitrarily large at any given point $\beta^* \notin I$; $\beta^* \neq \pm\infty$.

<u>Theorem 10:</u> If $S_N(\beta)$ is any given N- sum rule function and I is either of the following intervals

(i) $I = [\beta_0', \beta_1']$ for any given β_0', β_1' such that $-\infty < \beta_0' < \beta_1' < \infty$

(ii) $I = [\beta_0', \infty)$ for any given β_0' such that $-\infty < \beta_0' < \infty$

~~* This is ensured by the existence of a sequence of continuous functions which are uniformly convergent to S( ) on the interval of definition.~~

then there exists a sum rule function $\tilde{S}(\beta)$ on the interval I satisfying the conditions of Theorem 7 such that $\tilde{S}(\beta)$ is arbitrarily close to $S_N(\beta)$ for all $\beta \in I$ and such that $\tilde{S}(\beta^*) - S_N(\beta^*)$ is arbitrarily large at any given point $\beta^* \notin I$; $\beta^* \neq \pm\infty$. .

Theorem 11. If $S_N(\beta)$ is any given N-sum rule function and I is either of the following intervals

(i) $I = [\beta_0', \beta_1']$ for any given β_0', β_1' such that $-\infty < \beta_0' < \beta_1' < \infty$

(ii) $I = [\beta_0', \infty)$ for any given β_0' such that $-\infty < \beta_0' < +\infty$

then there exists a Theorem 7 sum rule function $\tilde{S}(\beta)$ of the special form $\tilde{S}(\beta) = \sum_{n=1}^{\infty} v_n E_n^{-\beta} + \int_{E}^{\infty} V(\varepsilon)\varepsilon^{-\beta} d\varepsilon$ where

(a) $v_n > 0$; $n = 1, 2, 3 \ldots$

(b) $0 < E_1 < E_2 \ldots$; $\lim_{n\to\infty} E_n \leq E$

(c) $V(\varepsilon)$ is continuous in $[E, \infty)$, non negative, and taking at least one non-zero value in $[E, \infty)$; such that $\tilde{S}(\beta)$ is arbitrarily close to $S_N(\beta)$ for all $\beta \in I$, and such that $S(\beta^*) - S_N(\beta^*)$ is arbitrarily large at any given point $\beta^* \notin I$, $\beta^* \neq \pm\infty$.

Proofs of Theorems 9, 10 and 11

The most important, or strongest, statement in these theorems is the one which conerns the interval (i) or Theorem 9. The proof of this is immediate from Theorem 6. Namely, if we take the limit of $S_R(\beta)$ (described in Theorem 6) as $R \to \infty$; i.e., take

$$\tilde{S}(\beta) = \lim_{R\to\infty} S_R(\beta)$$

we see that $\tilde{S}(\beta)$ is a sum rule function with the required properties, providing we take $\beta_0' = a$, $\beta_1' = b$. In fact, $\tilde{S}(\beta)$ thus constructed could look something like this:

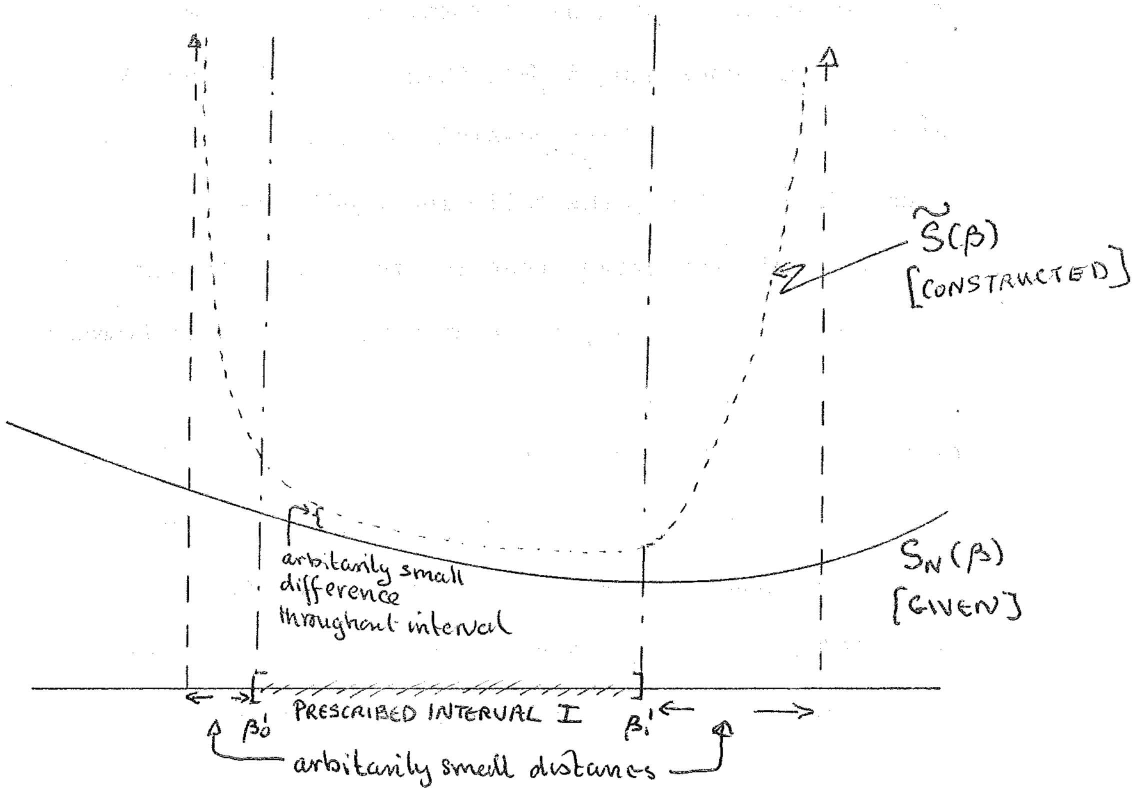

Diagram illustrating Theorem 9 with interval I = [β_0, β_1].

The proofs of all the other results are similar, constructions like those given in Theorems 4, 5 and 6 being used. We note that given any and any $\epsilon > 0$, we can find a positive continuous function $V(\varepsilon)$, $\varepsilon \in [E, \infty)$, such that $\int_E^\infty \varepsilon^{-\beta_0} V(\varepsilon)\, d\varepsilon < \epsilon$ and that in such a case the sum rule function thus defined satisfies $S(\beta) < \epsilon$ for all $\beta \in [\beta_0', \infty)$. We can make use of the reflection of such functions. At the end of Section IV we will be carrying out some of these constructions.

<u>Definition</u>: If $S(\beta)$ is a sum rule function on the interval I then the value of $S(\beta')$ for any $\beta' \in I$ is called a <u>sum rule</u>.

<u>Definition</u>: If $S(\beta)$ is known to be a sum rule function of a particular form* or of the most general form, and I is a set of further information concerning $S(\beta)$, then a set of bounds $B(\beta)$ on $S(\beta)$ is said to be <u>best possible</u> <u>O.B.G.I.</u> if and only if the bounds $B(\beta)$ satisfy the following conditions:

(i) $B(\beta)$ is <u>extensive</u>; that is, for $\beta \in \mathbb{R}$ the set $B(\beta)$ supplies at least either an upper or a lower bound to $S(\beta)$ O.B.G.I.;

(ii) $B(\beta)$ is <u>exclusive</u>; that is, O.B.G.I. no other non-trivial bounds can be imposed on $S(\beta)$, where zero and infinity are considered to be the trivial bounds;

(iii) $B(\beta)$ is <u>optimal</u>; that is, O.B.G.I. no improvement can be made on any bound contained in the set $B(\beta)$.

* For example, the different and more restricted types of sum rule function mentioned in Theorems 10 and 11 are particular forms of sum rule functions. The most general form is that given in the definition of a sum rule funtion. "O.B.G.I." stands for "on the basis of the given information".

III. Best Possible Upper and Lower Bounds To All Sum Rules Using Only Two Known Sum Rules.

THEOREM 12: (i) If $S_2(\beta)$ is an arbitrary 2-sum rule function, $\beta_0 < \beta_1$ are real numbers, then there is a unique ~~possibility to find~~ a 1-sum rule function such that

$$S_1(\beta_0) = S_2(\beta_0) \quad , \quad S_1(\beta_1) = S_2(\beta_1)$$

(ii) Moreover: $S_1(\beta) < S_2(\beta)$ if $\beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$

$S_1(\beta) > S_2(\beta)$ if $\beta \in (\beta_0, \beta_1)$

PROOF: We will prove the theorem for the case $\beta_0 = 0$, $\beta_1 = 1$. It is then easy to see that it is true for arbitrary $\beta_0 < \beta_1$ by making use of linear changes of variable.

Proof of (i):

Suppose $S_2(\beta) = V_1/E_1^{\beta} + V_2/E_2^{\beta}$. Then set $S_1(\beta) = V/\mathcal{E}^{\beta}$ where $V = S_2(0)$ and $\mathcal{E} = S_2(0)/S_2(1)$. The general interpolation formula is then $S_1(\beta) = S_2(\beta_0)\left[\dfrac{S_2(\beta_0)}{S_2(\beta_1)}\right]^{\frac{\beta_0-\beta}{\beta_1-\beta}}$.

This proves (i).

Proof of (ii):

Since $S_2(\beta)$ and $S_1(\beta)$, as constructed, are (N+1) & N-sum rule functions with N=1, it follows from theorem 3 with N=1 that $\left(S_2(\beta) - S_1(\beta)\right)$ can have at most two zeros. Hence, in this case,

$(S_2(\beta) - S_1(\beta))$ has exactly two zeros. Since $S_1(\beta)$ and $S_2(\beta)$ are continuous functions of β (being differenciable), it follows that the inequalities in (ii) are either true as they stand or else true with both the inequality signs reversed. Thus, it suffices as a completion of the proof to show that in the $\beta_0 = 0$; $\beta_1 = 1$ case, $S_2(2) > S_1(2)$.

i.e. wish to show that

$$V_1/E_1^2 + V_2/E_2^2 > \{V_1/E_1 + V_2/E_2\}^2 [V_1 + V_2]^{-1}$$

This is true $\Longleftrightarrow V_1 V_2 (1/E_1 - 1/E_2)^2 > 0$ which is true since $E_1 \neq E_2$. This proves (ii).

Finally, that $S_1(\beta)$ is unique follows from Theorem 2.

This completes the proof.

<u>THEOREM 13</u>: (i) If $S(\beta)$ is known to be a sum rule function; and $S(\beta_0), S(\beta_1)$; are known finite sum rules for some $\beta_0 < \beta_1$; then there is a unique 1-sum rule function such that:

$$S_1(\beta_0) = S(\beta_0) \quad , \quad S_1(\beta_1) = S(\beta_1)$$

(ii) Moreover:

$$S_1(\beta) \leq S(\beta) \quad \text{if} \quad \beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$$
$$S_1(\beta) \geq S(\beta) \quad \text{if} \quad \beta \in (\beta_0, \beta_1)$$

<u>PROOF</u>: Suppose $S_N(\beta)$ is any N-sum rule , with $V_1, \ldots, V_N; E_1, \ldots, E_N$ <u>known</u>. i.e. $S_N(\beta) = \sum_{n=1}^{N} \frac{V_n}{E_n^\beta}$

Let $\beta_0 < \beta_1$ be real numbers.

Since $V_{N-1}, V_N, E_{N-1}, E_N$ are <u>known</u>, it is possible to form the $S_1(\beta)$ approximation to $\frac{V_{N-1}}{E_{N-1}^\beta} + \frac{V_N}{E_N^\beta}$ which is exact at β_0, β_1 as in Theorem 12. Write this approximation as $\bar{V}_{N-1} / \mathcal{E}_{N-1}^{\beta}$.

Now let
$$\tilde{S}_{N-1}(\beta) = \sum_{n=1}^{N-2} \frac{V_n}{E_n{}^{\beta}} + \frac{V_{N-1}}{\mathcal{E}_{N-1}{}^{\beta}}$$

Then it is immediate that:

$$\tilde{S}_{N-1}(\beta) < S_N(\beta) \text{ if } \beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$$

$$\tilde{S}_{N-1}(\beta) > S_N(\beta) \text{ if } \beta \in (\beta_0, \beta_1)$$

with equality at β_0, β_1.

Now form $V_{N-2}/\mathcal{E}_{N-2}{}^{\beta}$ from $\frac{V_{N-2}}{E_{N-2}{}^{\beta}} + \frac{V_{N-1}}{\mathcal{E}_{N-1}{}^{\beta}}$ in the same way as before.

Let
$$\tilde{S}_{N-2}(\beta) = \sum_{n=1}^{N-3} \frac{V_n}{E_n{}^{\beta}} + \frac{V_{N-2}}{\mathcal{E}_{N-2}{}^{\beta}}.$$

Then
$$\tilde{S}_{N-2}(\beta) < \tilde{S}_{N-1}(\beta) < S_N(\beta)$$
$$\text{if } \beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$$
$$\tilde{S}_{N-2}(\beta) > \tilde{S}_{N-1}(\beta) > S_N(\beta)$$
$$\text{if } \beta \in (\beta_0, \beta_1)$$
with equality at β_0, β_1.

Proceed in this manner until $\tilde{S}_1(\beta) = V_1/\mathcal{E}_1{}^{\beta}$ is obtained.

Then

$$(1)\ \begin{cases} \tilde{S}_1(\beta) < \tilde{S}_2(\beta) < \cdots < \tilde{S}_{N-1}(\beta) < S_N(\beta) \\ \qquad \text{if } \beta \in (-\infty, \beta_0) \cup (\beta_1, \infty) \\ \tilde{S}_1(\beta) > \tilde{S}_2(\beta) > \cdots > S_{N-1}(\beta) > S_N(\beta) \text{ if } \beta \in (\beta_0, \beta_1) \end{cases}$$

with equality at β_0, β_1.

But $\tilde{S}_1(\beta)$ is uniquely defined by its values at β_0, β_1 i.e. it is completely defined by $S_N(\beta_0), S_N(\beta_1)$ with no knowledge of $V_1 \cdots V_N E_1 \cdots E_N$.

In fact $\tilde{S}_1(\beta) = S_N(\beta_0)\left\{S_N(\beta_0)/S_N(\beta_1)\right\}^{\frac{\beta_0-\beta}{\beta_1-\beta_0}}$

The point of going through the proceedure described above was to show that $\tilde{S}_1(\beta)$ has the bounding properties (1).

Now suppose that $S(\beta)$ is known to be a sum rule function & that $S(\beta_0)$, are known finite sum rules. Since $S(\beta)$ is a sum rule function, there exists a sequence $\left\{S_N(\beta)\right\}_{N=1}^{\infty}$ of N-sum rule functions such that $\lim_{N\to\infty} S_N(\beta) = S(\beta)$ for any fixed β on the interval of definition.

Let $S_1^{(N)}(\beta)$ be the 1-sum rule approximation to $S_N(\beta)$, exact at β_0, β_1.

(2) Let $S_1(\beta) = \lim_{N\to\infty} S_1^{(N)}(\beta) = S(\beta_0)\left\{\frac{S(\beta_0)}{S(\beta_1)}\right\}^{\frac{\beta_0-\beta}{\beta_1-\beta_0}}$

Then $S_1^{(N)}(\beta) < S_N(\beta)$ if $\beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$

and $S_1^{(N)}(\beta) > S_N(\beta)$ if $\beta \in (\beta_0, \beta_1)$

Taking limits as $N \to \infty$ we obtain

$$S_1(\beta) \leqslant S(\beta) \text{ if } \beta \in (-\infty, \beta_0) \cup (\beta_1, \infty)$$
$$S_1(\beta) \geqslant S(\beta) \text{ if } \beta \in (\beta_0, \beta_1)$$

(from 2) $S_1(\beta_0) = S(\beta_0)$; $S_1(\beta_1) = S(\beta_1)$

This completes the proof.

Theorem 13*: The set of bounds $B(\beta) = S_1(\beta)$ where $S_1(\beta)$ is the interpolation function to $S(\beta)$ constructed in Theorem 13 are best possible O.B.G.I. where the information we have concerning $S(\beta)$ is:

(i) $S(\beta)$ is a sum rule function either of the most general form or of the particular form given in Theorem 10 or of the particular form given in Theorem 11;

(ii) The finite sum rules $S(\beta_0)$, $S(\beta_1)$ and the respective points $-\infty < \beta_0 < \beta_1 < \infty$.

Proof: Let I be any closed interval that contains β_0 , and β_1 . Taking N = 1 in either Theorem 9 or Theorem 10 or Theorem 11, according respectively to the information that we are given in (i) above, and writing I in the form [β_0', β_1'], construct the $\tilde{S}(\beta)$ corresponding to a prescribed $\varepsilon > 0$ which has the properties ascribed to it by the respective Theorem. Then $0 \leqslant \tilde{S}(\beta_i) - S_1(\beta_i) = \varepsilon_i \leqslant \varepsilon$ for i = o,1 ; where the "o $\leqslant$ " follows from the manner in which it was suggested that the construction of $\tilde{S}(\beta)$ be carried out.

Now form the sum rule function

$$\tilde{\tilde{S}}(\beta) = \alpha E^{-\beta} \tilde{S}(\beta)$$

where $\alpha > o$ and E are chosen so that

$$\alpha E^{-\beta_0} \tilde{S}(\beta_0) = \tilde{S}(\beta_0) - e_0$$
$$\alpha E^{-\beta_1} \tilde{S}(\beta_1) = \tilde{S}(\beta_1) - e_1$$

Then $\tilde{\tilde{S}}(\beta)$ agrees with $S_1(\beta)$ at β_0 and β_1; is arbitrarily closed to $S_1(\beta)$ on the interval I and is arbitrarily divergent from it at any prescribed point outside. I. Alternatively $S_1(\beta)$ is the 1-sum rule interpolation function to $\tilde{\tilde{S}}(\beta)$, which is itself a sum rule function of respectively either the most general form of of one of the two particular forms given in Theorems 10 and 11, which has the usual bounding properties (Theorem 13). Hence, we can neither improve our lower bounds or our upper bounds O.B.G.I. (i.e. such bounds as $S_1(\beta)$ imposes are optimal). Moreover, since we neither can impose non-trivial upper bounds on $S(\beta)$ outside $[\beta_0, \beta_1]$; O.B.G.I.; nor, as can easily be demonstrated, can we impose non-trivial lower bounds inside $[\beta_0, \beta_1]$ O.B.G.I., it follows that the set of bounds is exclusive. It is clear that they are extensive. This completes the proof.

Theorem 13 has already been presented by H. L. Kramer [1], although the best possible statement was omitted. He shows that direct application to quantum mechanical sum rules leads to useful bounds on integer & non integer sum rules using any two known sum rules. My purposes in repeating the presentation are several. The statement and structure are here more formal & complete; the position of the theorem in a general theory of sum rule functions is expected to be correct; & the proof used in this paper should elucidate the nature & proofs of later theorems.

A particular case of theorem 13 has been given by ~~F.~~ Weinhold [2]. He shows that the matrix

$$G = \begin{vmatrix} S(2i) & S(i+j) & \cdots & S(i+k) \\ S(i+j) & S(2j) & \cdots & S(j+k) \\ \vdots & & & \\ S(i+k) & S(j+k) & \cdots & S(2k) \end{vmatrix}$$

must always be positive non-definite, where i,j,...k are any set of real numbers. This leads immediately to bounding relations on various sets of sum rules. Moreover the implied bounds must be optimal possible since G must be a metric matrix; & a both necessary and sufficient condition for this is that it be positive. Hence, wherever Weinhold's results are compatable with the results presented here, they must agree. Whereas Weinhold's bounds will always be optimal, our $S_2(\beta)$ bounds are best possible which, as already has been explained, is inclusive of optimal. For example, starting with only two sum rules known, G yields the optimal on exactly one other sum rule whereas theorem 13 yields the optimal bound on each of all other sum rules including of course the bound given by G. Similar remarks will later be seen to apply to any number of sum rules known.

Two Sum Rules Known

Weinhold: $$S(\beta_0)\,S(\beta_1) > \left[S\left(\frac{\beta_0+\beta_1}{2}\right)\right]^2$$

Theorem 13: $$S(\beta_0)\left[\frac{S(\beta_0)}{S(\beta_1)}\right]^{\frac{\beta_0-\beta}{\beta_1-\beta_0}} > S(\beta)$$

(Put $\beta = (\beta_0+\beta_1)/2$ to obtain Weinhold's Result.)

It is remarked that Weinhold's formalization may well have considerable relevance to a general theory of sum rule functions.

IV. Best Possible Upper & Lower Bounds To All Sum Rules Using Four Known Sum Rules.

THEOREM 14: (i) If $S_3(\beta)$ is an arbitrary 3-sum rule function & $\beta_0 < \beta_1 < \beta_2 < \beta_3$ are finite real numbers, then there is a unique 2-sum rule function such that $S_2(\beta_0) = S_3(\beta_0)$; $S_2(\beta_1) = S_3(\beta_1)$;

$S_2(\beta_2) = S_3(\beta_2)$; $S_2(\beta_3) = S_3(\beta_3)$

(ii) Moreover:

$S_2(\beta) < S_3(\beta)$ if $\beta \in (-\infty, \beta_0) \cup (\beta_1, \beta_2) \cup (\beta_3, \infty)$

$S_2(\beta) > S_3(\beta)$ if $\beta \in (\beta_0, \beta_1) \cup (\beta_2, \beta_3)$

PROOF: First we will prove the theorem in the case $\beta_0 = 0$; $\beta_1 = 1$, $\beta_2 = 2$, $\beta_3 = 3$. In this case the explicit construction is given. The extension to the case $\beta_n = \beta_0 + n\alpha$; $n = 0, 1, 2, 3$, β_0 and $\alpha \neq 0$ being real numbers, is then immediate using linear change of variable.

(I): The case $\beta_0 = 0$; $\beta_1 = 1$; $\beta_2 = 2$; $\beta_3 = 3$.

Suppose $S_3(0) = S_0$, $S_3(1) = S_1$, $S_3(2) = S_2$, $S_3(3) = S_3$.

Let $\varepsilon_1, \varepsilon_2$ be the roots of the quadratic equation:

$$(S_1 S_3 - S_2^2)\varepsilon^2 - (S_0 S_3 - S_1 S_2)\varepsilon + (S_0 S_2 - S_1^2) = 0$$

Let $x = (S_0 S_2 - S_1^2)\varepsilon_1^2 / (S_0 - 2S_1\varepsilon_1 + S_2\varepsilon_1^2)$; $y = S_0 - x$

Define $S_2(\beta) = x/\varepsilon_1^{\beta} + y/\varepsilon_2^{\beta}$.

Then it is a matter of substitution to verify that:

$S_2(0) = S_0$, $S_2(1) = S_1$, $S_2(2) = S_2$, $S_2(3) = S_3$.

To complete the proof of (i) we must verify that $S_2(\beta)$ thus defined is indeed a 2-sum rule function. That is, we must show that $x>0;\ y>0;\ \mathcal{E}_1>0;\ \mathcal{E}_2>0;\ \mathcal{E}_1 \neq \mathcal{E}_2$.

Suppose that $S_3(\beta) = V_1/E_1{}^\beta + V_2/E_2{}^\beta + V_3/E_3{}^\beta$

where $V_1>0;\ V_2>0;\ V_3>0;\ 0<E_1<E_2<E_3$.

Then:

$$(S_1S_3 - S_2^2) = \frac{V_1V_2}{E_1E_2}\left\{\frac{1}{E_1}-\frac{1}{E_2}\right\}^2 + \frac{V_2V_3}{E_2E_3}\left\{\frac{1}{E_2}-\frac{1}{E_3}\right\}^2 + \frac{V_3V_1}{E_3E_1}\left\{\frac{1}{E_3}-\frac{1}{E_1}\right\}^2 > 0$$

$$(S_0S_2 - S_1^2) = V_1V_2\left\{\frac{1}{E_1}-\frac{1}{E_2}\right\}^2 + V_2V_3\left\{\frac{1}{E_2}-\frac{1}{E_3}\right\}^2 + V_3V_1\left\{\frac{1}{E_3}-\frac{1}{E_1}\right\}^2 > 0$$

$$(S_0S_3 - S_1S_2) = V_1V_2\left\{\frac{1}{E_1}+\frac{1}{E_2}\right\}\left\{\frac{1}{E_1}-\frac{1}{E_2}\right\}^2 + V_2V_3\left\{\frac{1}{E_2}+\frac{1}{E_3}\right\}^2 + V_3V_1\left\{\frac{1}{E_3}+\frac{1}{E_1}\right\}\left\{\frac{1}{E_3}-\frac{1}{E_1}\right\}^2 > 0$$

Hence $a = (S_1S_3 - S_2^2) > 0;\quad -b = (S_0S_3 - S_1S_2) > 0;$
$c = (S_0S_2 - S_1^2) > 0$

Also
$$b^2 - 4ac = V_1^2V_2^2\left\{\frac{1}{E_1}-\frac{1}{E_2}\right\}^6 + V_2^2V_3^2\{-\}^6 + V_3^2V_1^2\{-\}^6$$
$$-2V_1V_2^2V_3\left\{\frac{1}{E_1}-\frac{1}{E_2}\right\}^3\left\{\frac{1}{E_2}-\frac{1}{E_3}\right\}^3 - 2(-)\{-\}^3\{-\} - 2(-)\{-\}\{-\}^3$$

Let $A = 1/E_1 - 1/E_2;\quad B = 1/E_2 - 1/E_3;$

so that $-(A+B) = 1/E_3 - 1/E_1$.

Then $A,\ B,\ (A+B) > 0$ and
$$b^2 - 4ac = \left[V_1V_2A^3 - V_2V_3B^3\right]^2 + 2\left[V_3V_1(A+B)^3\right]\left[V_2V_3B^3 + V_1V_2A^3\right] > 0$$

so $b^2 > b^2 - 4ac > 0$.

Hence the roots of the quadratic equation

$a\varepsilon^2 - b\varepsilon + c = 0$ are positive & non equal.

i.e. $\varepsilon_1 > 0$, $\varepsilon_2 > 0$; $\varepsilon_1 \neq \varepsilon_2$.

Finally, since $S_0 S_2 - S_1^2 > 0 \Rightarrow (S_0 - 2S_1\varepsilon_1^2 + S_2\varepsilon^2)$ is a positive definite fn. of ε. Hence $X > 0$. By symmetry $Y > 0$. Hence $S_2(\beta)$ is a sum rule function. That it is unique follows from Theorem 2.

We now prove (ii). By theorem 3, $S_3(\beta) - S_2(\beta)$ has at most four zeros. Hence in this case $S_3(\beta) - S_2(\beta)$ has exactly four zeros. Hence, since $S_2(\beta)$, $S_3(\beta)$ are cts. fns. of β the inequalities in (ii) are either true as they stand or else true with all the inequality signs reversed. Moreover, if they are true in any particular case (i.e. for some choice of $V_1^* > 0$; $V_2^* > 0$; $V_3^* > 0$; $0 < E_1^* < E_2^* < E_3^*$) then they are true in all cases. To see this we first notice that if $V_1 > 0$; $V_2 > 0$; $V_3 > 0$; $0 < E_1 < E_2 < E_3$ are given, then we can find a continuous transformation $\tilde{V}_1(\alpha), \tilde{V}_2(\alpha); \tilde{V}_3(\alpha); \tilde{E}_1(\alpha); \tilde{E}_2(\alpha); \tilde{E}_3(\alpha)$ defined on the interval $\alpha \in [0,1]$ s.t. $\tilde{V}_i(0) = V_i^*$; $\tilde{E}_i(0) = E_i^*$; $\tilde{V}_i(1) = V_i$; $\tilde{E}_i(1) = E_i$; $i = 1,2,3$, and such that $\tilde{V}_1(\alpha) > 0$; $\tilde{V}_2(\alpha) > 0$; $\tilde{V}_3(\alpha) > 0$; $0 < E_1(\alpha) < E_2(\alpha) < E_3(\alpha)$ for all $\alpha \in [0,1]$. If the inequality signs became reversed as α goes from 0 to 1, then for some $\alpha \in (0,1)$ the condition that $S_3(\beta) - S_2(\beta)$ has at most 4 zeros would be violated. So we need only verify the inequalities for one particular case & at one value of β_j; $\beta \neq$, $i = 0,1,2,3$.

[or else see P. 31].

A particular case: Define a 3-sum rule function by:

$$S_3(\beta) = 1/(\tfrac{1}{3})^\beta + 1/(\tfrac{1}{2})^\beta + 1/(1)^\beta$$

Find: $S_0 = 3$; $S_1 = 6$; $S_2 = 14$; $S_3 = 36$; $(S_0S_2 - S_1^2) = 6$; $(S_1S_3 - S_2^2) = 20$; $(S_0S_3 - S_1S_2) = 24$; $\varepsilon_1 = 0.844998975$; $\varepsilon_2 = 0.355051025$; $x = 1.4998713$; $y = 1.5001287$; $S_3(\tfrac{1}{2}) = 4.1463$; $S_2(\tfrac{1}{2}) = 4.1492$

Hence in this case $S_2(\beta)$ is an upper bound to $S_3(\beta)$ at $\beta = \frac{1}{2}$

This completes the proof of (ii) in the $\beta_0 = 0$; $\beta_1 = 1$; $\beta_2 = 2$; $\beta_3 = 3$ case. [Note: considering the increase in $S_3(\beta)$ as β goes from 0 to 1, the closeness of $S_3(\frac{1}{2})$ & $S_2(\frac{1}{2})$ is remarkable.

At $\beta = 3/4$ the results are indistinguishable within desk calculator accuracy].

II : We now extend the argument to the case of general interpolation points $\beta_0 < \beta_1 < \beta_2 < \beta_3$. We will concern ourselves with the existence of the interpolation function.

Given a 3-sum rule function $S_3(\beta)$ then there exists a 2-sum rule function $S_2^*(\beta)$ such that $S_2^*(\beta) = S_3(\beta)$ for $\beta = 0, 1, 2$, & such that $S_2^*(\beta) < S_3(\beta)$ for $\beta \in (2, \infty)$. This follows from the first part of the theorem. In fact we could take the $S_2^*(\beta)$ defined by $S_2^*(\beta) = S_3(\beta)$ for $\beta = -1, 0, 1, 2$, assuming we had known $S_3(-1)$. We are proving existence.

Now construct $S_2^{**}(\beta; \gamma)$ such that $S_2^{**}(\beta; \gamma) = S_2^*(\beta)$ for $\beta = 0, 1, 2$ & $S_2^{**}(3; \gamma) = [S_2^*(3) + \gamma]$ where $\gamma \in [0, \infty)$ (see appendix I).

Then $S_2^{**}(\beta; \gamma)$ is a continuous function of γ (see appendix).

Moreover $S_2^{**}(\beta, 0) < S_3(\beta)$ for $\beta \in (2, \infty)$ and $S_2^{**}(\beta, \gamma) \to \infty$ as $\gamma \to \infty$ for $\beta \in (2, \infty)$, (see appendix).

Let $\beta_3 \in (2, \infty)$ be given.

Then since $S_2^{**}(\beta_3, 0) < S_3(\beta_3)$, $S_2^{**}(\beta_3, \gamma) > S_3(\beta_3)$ for sufficiently large γ, & $S_2^{**}(\beta_3, \gamma)$ is a continuous function of γ, it follows that $\exists$ a $\gamma^* \in (0, \infty)$ s.t. $S_2^{**}(\beta_3; \gamma^*) = S_3(\beta_3)$.

We have constructed a 2-sum rule function, $S_2^{**}(\beta; \gamma^*)$ such that $S_2^{**}(\beta; \gamma^*) = S_3(\beta)$ for $\beta = 0, 1, 2, \beta_3 \in (2, \infty)$. Moreover it follows from continuity that $S_2^{**}(\beta, \gamma^*)$ has similar interlacing properties to the $S_2(\beta)$ which equals $S_3(\beta)$ at $\beta = 0, 1, 2, 3$. [This can be also seen in the following way: $S_2^{**}(\beta, \gamma^*)$ must be a lower bound when $\beta \notin [0, \beta_3]$ simply because, by theorem 9, it could not possibly be known to be always an upper bound & it must be always either an upper or a lower bound (see P.29).] Using the linear change of variable $\beta \to -\beta$, it follows now that given $S_3(\beta)$ it is possible to find an $S_2'(\beta)$ such that $S_2'(\beta) = S_3(\beta)$ for $\beta = \beta_0 \in (-\infty, 1)$; 1; 2; 3; with the usual bounding properties.

Hence, it is possible to find an $S_2^+(\beta)$ such that $S_2^+(\beta) = S_3(\beta)$ for $\beta = 1, 2, \beta_3, (2\beta_3 - 2)$ i.e. at $\beta = 1, 2, 2 + (\beta_3 - 2), 2 + 2(\beta_3 - 2)$; simply by again making use of linear change of variable on an $S_2'(\beta)$ type of interpolation.

Then $S_2^+(\beta)$ satisfies $S_2^+(\beta) = S_3(\beta)$ for $\beta = 1, 2, \beta_3$

& $S_2^+(\beta) < S_3(\beta)$ for $\beta \in (-\infty, 1)$.

Now construct $S_2^{++}(\beta; \gamma)$ such that $S_2^{++}(\beta; \gamma) = S_2^+(\beta)$ for $\beta = 1, 2, \beta_3$ & $S_2^{++}(0; \gamma) = (S_2^+(0) + \gamma)$ where $\gamma \in [0, \infty)$. (see appendix).

Then $S_2^{++}(0; \gamma)$ is a continuous function of γ (see appendix).

Moreover $S_2^{++}(\beta; 0) < S_3(\beta)$ for $\beta \in (-\infty, 1)$ and $S_2^{++}(\beta; \gamma) \longrightarrow \infty$ as $\gamma \longrightarrow \infty$ for $\beta \in (-\infty, 1)$ (see appendix)

Let $\beta_0 \in (-\infty, 1)$ be given.

Then since $S_2^{++}(\beta_0; 0) < S_3(\beta_0)$; $S_2^{++}(\beta_0, \gamma) > S_3(\beta_0)$ for sufficiently large γ, and $S_2^{++}(\beta_0; \gamma)$ is a continuous function of γ; it follows that $\exists\ \gamma^+$ such that $S_2^{++}(\beta_0; \gamma^+) = S_3(\beta_0)$.

We have constructed a 2-sum rule function s.t.

$$S_2^{++}(\beta; \gamma^+) = S_3(\beta) \text{ for } \beta = \beta_0, 1, 2, \beta_3$$

where $\beta_0 \in (-\infty, 1)$; $\beta_3 \in (2, \infty)$.

Clearly it has the expected bounding properties, from consideration of number of zeros.

Linear change of variable now completes the proof in its entirity.

THEOREM 15: If $S(\beta)$ is known to be a sum rule function, & if for some $\beta_0 < \beta_1 < \beta_2 < \beta_3$; $S(\beta_0)$, $S(\beta_1)$, $S(\beta_2)$, $S(\beta_3)$ are known finite sum rules, then there is a unique 2-sum rule function such that $S_2(\beta_i) = S(\beta_i)$ for $i = 0, 1, 2, 3$

Moreover: $S_2(\beta) \leq S(\beta)$ if $\beta \in (-\infty, \beta_0) \cup (\beta_1, \beta_2) \cup (\beta_3, \infty)$

$S_2(\beta) \geq S(\beta)$ if $\beta \in (\beta_0, \beta_1) \cup (\beta_2, \beta_3)$

PROOF: Follows exactly the same lines as Theorem 13. For completeness we will give the construction for $S_2(\beta)$ in the $\beta_0 = 0$; $\beta_1 = 1$; $\beta_2 = 2$; $\beta_3 = 3$ case, from which, by linear change of variable, the construction in the case $\beta_n = \Gamma + n\alpha$; $n = 0, 1, 2, 3$ is easily derived.

CONSTRUCTION: Let $S(0) = S_0$; $S(1) = S_1$; $S(2) = S_2$; $S(3) = S_3$

Let $\varepsilon_1, \varepsilon_2$ be the roots of the equation:

$$(S_1 S_3 - S_2^2)\varepsilon^2 - (S_0 S_3 - S_1 S_2)\varepsilon + (S_0 S_2 - S_1^2) = 0$$

Then form: $x = (S_0 S_2 - S_1^2)\varepsilon_1^2 / (S_0 - 2S_1\varepsilon_1 + S_2\varepsilon_1^2)$

$y = (S_0 - x)$

Then $S_2(\beta) = x/\varepsilon_1^\beta + y/\varepsilon_2^\beta$

has the desired properties. Other constructions are given in an appendix.

Theorem 15:* The set of bounds $B(\beta) = \{ S_2(\beta), S_1^i(\beta) : i = 1, 2, 3 \}$ where $S_2(\beta)$ is the interpolation function to $S(\beta)$ constructed in Theorem 15, and where the $S_1^i(\beta)$'s are 1-sum rule interpolation functions made exact at adjacent interpolation points,

β_{i-1} and β_i; are best possible O.B.G.I. where the information we have concerning $S(\beta)$ is:

(i) $S(\beta)$ is a sum rule function either of the most general form or of the form given in Theorem 10 or of the form given in Theorem 11;

(ii) The finite sum rules $S(\beta_i)$, $i = 0,1,2,3$; and the respective points $-\infty < \beta_0 < \beta_1 < \beta_2 < \beta_3 < \infty$

Before giving the basic result necessary for the proof of this theorem we refer the reader to the appendix on sum rule transformations. (Appendix IV)

PROOF OF THEOREM 15*: We will content ourselves with consideration of the case of interpolation points $\beta = 0,1,2,3$.

Let $S_2(\beta)$ be any given 2-sum rule function.

Our object will be to construct a sum rule function $S(\beta)$ which (i) agrees with $S_2(\beta)$ at $\beta = 0,1,2,3$;

(ii) is such that $|S_2(\beta) - S(\beta)| < \epsilon$ for all $\beta \in I$ where $\epsilon > 0$ has been prescribed and where $I = [a,b]$ is any closed real interval containing the points $\beta = 0,1,2,3$.

(iii) $S(\beta^*) - S_2(\beta^*)$ is arbitrarily large at any prescribed point $\beta^* \notin I$. Without loss of generality suppose $\beta^* > b$.

We first observe that there is a trivial proof in the case of the most general type of sum rule function. As follows: if $\{S^{(j)}(\beta)\}_{j=1}^{\infty}$ is a sequence of sum rule functions (not N-sum rule functions) that is uniformly convergent on an interval I then it converges to a sum rule function on that interval. This can be proven directly from the definition of a sum rule function. Thus, after the manner of Theorem 9, we could find a sum rule function which agrees with $S_2(\beta)$ on the interval I and is arbitrarily divergent from it at any other given point.

However, we will not rest our proof on this almost too remarkable construction. [What such a function looks like is simple; but its analytic nature is most puzzling!]

Instead, let us start with <u>any* monotone increasing sum rule</u> function which is convergent on $(-\infty, \infty)$; $\tilde{\tilde{S}}(\beta)$

Let $I = [a,b]$ be any closed interval which contains the points $\beta = 0,1,2,3$; and let $\beta^* > b$ be any such given point. Let $e^* > 0$ and $M > 0$ be arbitrarily small and arbitrarily large prescribed numbers respectively. Choose $a \in A$ and $\mathcal{E} \in E'$ s.t.

(i) $\tilde{S}(b) = a\,\mathcal{E}\,\tilde{\tilde{S}}(b) = e^*/2$

(ii) $\tilde{S}(\beta^*) = a\,\mathcal{E}\,\tilde{\tilde{S}}(\beta^*) = M$

Let $\tilde{S}(\beta) = a\,\mathcal{E}\,\tilde{\tilde{S}}(\beta)$. Now form the reflection of $\tilde{S}(\beta)$ through $\frac{1}{2}(a+b)$, $\tilde{S}(-\beta + \frac{1}{2}(a+b))$.

Let $S'(\beta) = \tilde{S}(\beta) + \tilde{S}(-\beta + \frac{1}{2}(a+b))$.

Then $S'(\beta)$ is a symmetric sum rule function, and must take its minimum value at $\frac{1}{2}(a+b)$.

Moreover $S'(a) = S'(b) < e^*$

$S'(\beta^*) = S'(-\beta^* + \frac{1}{2}(a+b)) > M$.

* This sum rule function may be chosen to be one of the <u>particular forms</u> which are mentioned in Theorems 10 and 11. Then any A, E, or R transformation will neither alter the <u>form</u> nor the interval of definition, $(-\infty, \infty)$.

Having constructed $S'(\beta)$ thus we will now forget about it for a while and consider another construction.

<u>Let $\tilde{S}_2(\beta)$ be any given 2-sum rule function</u>. Denote $\tilde{S}_2(i) = \tilde{S}_i$ for $i = 0,1,2,3$. As we saw in Theorem 15, an arbitrary 2-sum rule function $S_2(\beta)$ is itself a continuous function of the parameters $S_i = S_2(i)$, $i = 0,1,2,3$; which are themselves subject to the restraints

$$S_0 S_2 - S_1^2 > 0, \text{ etc.}$$

These left hand side of each of these restraints is also a continuous function of S_0, S_1, S_2, S_3. Hence there exists a spherical neighbourhood of radius α , where α is suitably small, centered on $(\tilde{S}_0, \tilde{S}_1, \tilde{S}_2, \tilde{S}_3)$ such that if

$(S_0, S_1, S_2, S_3) \in C_\alpha\{S_0, S_1, S_2, S_3\}$ then the above restraints are still satisfied, and $S_\alpha(\beta)$ exists.

Now Let $I = [a,b]$ be any closed interval which contains the points $\beta = 0,1,2,3$; and let

$$G(S_0, S_1, S_2, S_3) = \text{Max}\left\{ \left|\tilde{S}_2(\beta) - S_2(\beta)\right| : \beta \in I \right\}$$

be defined on $C_\alpha\{S_0, S_1, S_2, S_3\}$. Then $G(S_0, S_1, S_2, S_3)$ is itself a continuous function and takes the value zero uniquely at $(\tilde{S}_0, \tilde{S}_1, \tilde{S}_2, \tilde{S}_3)$. Hence there exists a new spherical neighbourhood $C_\gamma\{S_0, S_1, S_2, S_3\}$ such that

$$(S_0, S_1, S_2, S_3) \in C_\gamma\{S_0, S_1, S_2, S_3\}$$

implies (i) that $S_2(\beta)$ exists

(ii) $\left|\tilde{S}_2(\beta) - S_2(\beta)\right| < e$ for all $\beta \in I$ where $e > 0$ has been prescribed.

We are now ready to construct $S(\beta)$. Let $e > 0$ be prescribed. Find $C_\gamma\{S_0, S_1, S_2, S_3\}$ as above. Choose $e^* = \min\{e, \gamma\}$.

Construct $S'(\beta)$. Construct $S_2(\beta)$ defined by

$S_i = S_i - S'(i)$, $i = 0,1,2,3$.

Finally let $S(\beta) = S_2(\beta) + S'(\beta)$.

Then $S(\beta)$ has the required properties.

We will check this briefly.

(i) $S(i) = \tilde{S}_i$, where $i = 0,1,2,3$.

(ii) $S'(\beta) < e$ throughout I and $|S_2(\beta) - S_2(\beta)| < e$ thoughout I, so that $|\tilde{S}_2(\beta) - S_2(\beta)| < 2e$ throughout I

(iii) $S'(\beta^*)$ is arbitrarily large so that $S(\beta^*)$ is also arbitrarily large.

The theorem can now be established, using arguments similar to those used in Theorem 13^*.

V: Best Possible Upper And Lower Bounds To All Sum Rules Using Any Number of Known Sum Rules.

One sum rule known: $S(\beta_0)$. It is impossible to say anything about any other sum rules, apart from the trivial statement that they are positive.

Two sum rules known: $S(\beta_0)$, $S(\beta_1)$. Then we can use an $S_1(\beta)$ function to obtain upper bounds for $\beta \in (\beta_0, \beta_1)$ & lower bounds elsewhere. These bounds are best possible. (See remarks following theorem 8).

Three sum rules known: $S(\beta_0)$, $S(\beta_1)$, $S(\beta_2)$. We know that there exist numerous $S_2(\beta)$ functions through the points, but we can say nothing about their bounding properties with no more information. Since there exists an $S(\beta)$ arbitrarily close to each of these $S_2(\beta)$'s on any closed interval it follows that the best possible bounds that we can put on an arbitrary $S(\beta)$ through these three points are identical with the best possible bounds that we can put on an arbitrary $S_2(\beta)$ function through these points (see Theorem 5 & appendix) & these are easily seen to be given by $S_1(\beta)$ functions; one made exact at $\beta = \beta_0, \beta_1$, & one made exact at $\beta = \beta_1, \beta_2$. These will give best upper and lower bounds to $S(\beta)$

for $\beta \in (\beta_0, \beta_3)$; & best lower bounds elsewhere.

Four sum rules known: $S(\beta_0)$, $S(\beta_1)$, $S(\beta_2)$, $S(\beta_3)$.

The $S_2(\beta)$ made exact at $\beta = \beta_0, \beta_1, \beta_2, \beta_3$ gives best possible lower bounds for

$\beta \in (-\infty, \beta_0) \cup (\beta_1, \beta_2) \cup (\beta_3, \infty)$

& best possible upper bounds for $\beta \in (\beta_0, \beta_1) \cup (\beta_2, \beta_3)$. By similar reasoning to that used in the case of "three sum rules known" we see that best possible upper bounds for $\beta \in (\beta_1, \beta_2)$ are obtained from an $S_1(\beta)$ function made exact at β_1, β_2; & similarily for the remaining lower bounds.

Five sum rules known: $S(\beta_0), \ldots, S(\beta_4)$. By similar reasoning to the case of 'three sum rules known' we see that best possible bounds are given by $S_2(\beta)$ functions.

Any even number of sum rules known: $S(\beta_0) \ldots S(\beta_{2N-1})$.

Certainly if an $S_N(\beta)$ can be found, exact at $\beta_0, \ldots, \beta_{2N-1}$, then it will have best bounding properties. It is believed that it is in fact always possible to find such a function.

Any odd number of sum rules known: $S(\beta_0), \ldots\ldots, S(\beta_{2N})$.

It would certainly be true that the best possible bounds would be obtained using $S_N(\beta)$ functions, providing such interpolations exist.

F. Wienhold presents best possible bounds using particular sets of known sum rules. His results give bounds on a few other sum rules when various sum rules are known. Certainly the results he obtains in the cases of 2,3,4 & 5 sum rules known must be particular cases of the results given here since our results also are best possible.

Appendix I

THEOREM: If $S_2(\beta)$ is an arbitrary 2-sum rule function, with $S_2(n) = S_n$ for $n = 0, 1, 2, 3$; then $S_3 > S_2^2/S_1$, $S_0 > S_1^2/S_2$. Moreover, for any $\gamma > 0$ there exists a 2-sum rule function $S_2^*(0) = S_0$; $S_2^*(1) = S_1$, $S_2^*(2) = S_2$, $S_2^*(3) = (S_2^2/S_1) + \gamma$ with $\gamma \in (0, \infty)$. Similarily, there exists a 2-sum rule function $S_2^{**}(\beta)$ such that $S_2^{**}(0) = (S_1^2/S_2) + \gamma$ $S_2^{**}(1) = S_1$; $S_2^{**}(2) = S_2$; $S_2^{**}(3) = S_3$.

Moreover; $\begin{cases} S_2^*(\beta) \to \infty \text{ as } \gamma \to \infty, \text{ for } \beta \in (2, \infty) \\ S_2^{**}(\beta) \to \infty \text{ as } \gamma \to \infty, \text{ for } \beta \in (-\infty, 1) \end{cases}$

In particular, $\exists$ an $S_2^{***}(\beta)$ s.t., for $\gamma_1 \in [0, \infty)$, and $\gamma_2 \in [0, \infty)$; $S_2^{***}(0) = S_0 + \gamma_1$, $S_2^{***}(1) = S_1$, $S_2^{***}(2) = S_2$; $S_2^{***}(3) = S_3 + \gamma_2$, and

$$S_2^{***}(\beta) \to \infty \text{ as } \gamma_1 \to \infty \text{ for } \beta \in (-\infty, 1)$$
$$S_2^{***}(\beta) \to \infty \text{ as } \gamma_2 \to \infty \text{ for } \beta \in (2, \infty)$$

Moreover, the various 2-sum rule functions thus obtained are continuous functions of the γ's.

PROOF: That $S_3 > (S_2^2/S_1)$ and $S_0 > (S_1^2/S_2)$ is an immediate consequence of theorem 12.

If we parametrically solve the set of equations

$$x + y = S_0;\ x/\varepsilon_1 + y/\varepsilon_2 = S_1;\ x/\varepsilon_1^2 + y/\varepsilon_2^2 = S_2$$
$$x/\varepsilon_1^3 + y/\varepsilon_2^3 = S_3$$

then we obtain the relations

$$\mathcal{E}_1 = \frac{(S_1\mathcal{E}_2 - S_0)}{(S_2\mathcal{E}_2 - S_1)} \qquad \mathcal{E}_2 = \frac{(S_1\mathcal{E}_1 - S_0)}{(S_2\mathcal{E}_1 - S_1)}$$

$$x = \frac{\mathcal{E}_1(S_1\mathcal{E}_2 - S_0)}{(\mathcal{E}_2 - \mathcal{E}_1)} \qquad y = \frac{\mathcal{E}_2(S_1\mathcal{E}_1 - S_0)}{(\mathcal{E}_1 - \mathcal{E}_2)}$$

In particular;

$$S_3 = \frac{S_2^2\mathcal{E}_1^2 - S_1S_2\mathcal{E}_1 + (S_1^2 - S_0S_2)}{\mathcal{E}_1(S_1\mathcal{E}_1 - S_0)}$$

So that S_3 can be shown to be motone decreasing as a function of $\mathcal{E}_1$ in the domain $\left(\frac{S_0}{S_1}, \infty\right)$; going from $+\infty$ to S_2^2/S_1 . Moreover if

$\mathcal{E}_1 \in (S_0/S_1, \infty)$ then

$\mathcal{E}_2 > 0, \ x > 0, \ y > 0.$

Hence we can find a 2-sum rule function $S_2^*(\beta)$ s.t. for any $\gamma > 0$ we have $S_2^*(0) = S_0$; $S_2^*(1) = S_1$; $S_2^*(2) = S_2$; $S_2^*(3) = S_2^2/S_1 + \gamma$.

It is clear that $S_2^*(\beta)$ will be a continuous function of γ .

We will show that $S_2^*(\beta) \to \infty$ as $\gamma \to \infty$ for $\beta \in (2, \infty)$.

Let $\ell > 0$ be prescribed.

Take $\mathcal{E}_1 = S_0/S_1 + \ell_1$ where $\ell_1 > 0$ will be chosen later on.

Then $\varepsilon_2 = \dfrac{S_1^2 \ell_1}{(S_0 S_2 - S_1^2) + S_1 S_2 \ell_1}$.

Notice $(S_0 S_2 - S_1^2) > 0$.

Moreover; $y = \dfrac{\varepsilon_2 (S_1 \varepsilon_1 - S_0)}{(\varepsilon_1 - \varepsilon_2)}$.

Hence if we take $S_2^*(\beta) = \dfrac{x}{\varepsilon_1^\beta} + \dfrac{y}{\varepsilon_2^\beta}$

we see that $S_2^*(2+\ell) > \dfrac{y}{\varepsilon_2^{2+\ell}}$

But $$y/\varepsilon_2^{2+\ell} = \frac{(S_1 \varepsilon_1 - S_0)}{\varepsilon_2 (\varepsilon_1 - \varepsilon_2) \varepsilon_2^{\ell}}$$

$$= \frac{S_1 e_1 \left[(S_0 S_2 - S_1^2) + S_1 S_2 \ell_1\right]}{S_1^2 \ell_1 (\varepsilon_1 - \varepsilon_2) \varepsilon_2^{\ell}} > \frac{(S_0 S_2 - S_1^2)}{S_1 \varepsilon_1 \varepsilon_2^{\ell}}.$$

$\therefore$ Whatever the choice of $\ell > 0$ was, we can ensure by taking $\ell_1 > 0$ sufficiently small, that $S_2^*(2+\ell)$ is arbitrarily large.

Hence $S_2^*(\beta) \to \infty$ as $\beta \to \infty$ for $\beta \in (2, \infty)$.

Similarily $S_2^{**}(\beta)$ can be shown to exist. [For example, we could make use of a linear change of variable on a suitably chosen $S_2^*(\beta)$ type of function].

The results concerning $S_2^{***}(\beta)$ follow at once.

This completes the proof.

Appendix II

General proceedure for finding the S_2 interpolation function through various sets of integer interpolation points.

We will suppose that the values of four sum rules are given for integer points. By means of a linear change of variable we can transform the interpolation points to be $\beta = 0\,;\ 1\,;\ n_1\,;\ n_2$.
Practical proceedures in different cases vary, but the method described by examples below is the basic format which such proceedures must follow.

Example: Interpolation points $\beta = 0, 1, 2, 4$.

In the usual notation, $S_2(\beta) = \dfrac{X}{\varepsilon_1{}^\beta} + \dfrac{Y}{\varepsilon_2{}^\beta}$

Let S_0, S_1, S_2, S_4 be the given sum rules.

Using the parametric representations

$$\varepsilon_1 = \frac{(S_1\varepsilon_2 - S_0)}{(S_2\varepsilon_2 - S_1)}\ ; \quad \varepsilon_2 = \frac{(S_1\varepsilon_1 - S_0)}{(S_2\varepsilon_1 - S_1)}\ ; \quad X = \frac{\varepsilon_1(S_1\varepsilon_2 - S_0)}{(\varepsilon_2 - \varepsilon_1)}$$

etc.; express $S_2(4)$ in terms of $S_0\ S_1\ S_2\ \varepsilon_1\ \varepsilon_2$.

Obtain:

$$S_2(4) = S_4 = S_1\left[\frac{1}{\varepsilon_1{}^3} + \frac{1}{\varepsilon_1{}^2\varepsilon_2} + \frac{1}{\varepsilon_1\varepsilon_2{}^2} + \frac{1}{\varepsilon_2{}^3}\right] - \frac{S_0}{\varepsilon_1\varepsilon_2}\left[\frac{1}{\varepsilon_1{}^2} + \frac{1}{\varepsilon_1\varepsilon_2} + \frac{1}{\varepsilon_2{}^2}\right] \quad (1)$$

We ask: What is the value of $S_2(3)$ if $S_2(4) = S_4$?

If $S_2(\beta)$ passes through $S_0, S_1, S_2, S_2(3)$ then $\varepsilon_1, \varepsilon_2$

are the roots of

$$(S_1S_2(3)-S_2^{2})\varepsilon^{2}-(S_0S_2(3)-S_1S_2)\varepsilon+(S_0S_2-S_1^{2})=0 \quad (2)$$

Using "sum of roots", "product of roots" from (2) in (1) we obtain the following condition on $S_2(3)$:

$$S_0\{S_2(3)\}^{2}-2S_1S_2\{S_2(3)\}+\left[S_2^{3}-(S_0S_2-S_1^{2})S_4\right]=0$$

Whence

$$S_2(3)=\frac{S_1S_2}{S_0}+\frac{(S_0S_4-S_2^{2})^{1/2}(S_0S_2-S_1^{2})^{1/2}}{S_0}$$

The value of $S_2(3)$ together with S_0, S_1, S_2, are now used in the standard 0 1 2 3 interpolation formulae to yield the required $S_2(\beta)$ function.

<u>Example:</u> <u>Interpolation points $\beta = 1, 2, 4, 6$</u>.

Use a linear change of variable so the interpolation points become $\frac{1}{2}, 1, 2, 3$; know sum rules $S_{\frac{1}{2}}, S_1, S_2, S_3$. Suppose that $S_2(0) = S_1^{2}/S_2 + \alpha$ with $\alpha > 0$. Find 0, 1, 2, 3 interpolation function & look at $S_2(\frac{1}{2}, \alpha)$. Increase α until $S_2(\frac{1}{2};\alpha) = S_{\frac{1}{2}}$. Then $S_2(\beta;\alpha)$ is the required function.

In general it will be found necessary to solve

$$S_0 = x + y$$

$$S_1 = x/\varepsilon_1 + y/\varepsilon_2$$

$$S_{n_1} = x/\varepsilon_1^{\,n_1} + y/\varepsilon_2^{\,n_1}$$

$$S_{n_2} = x/\varepsilon_1^{\,n_2} + y/\varepsilon_2^{\,n_2}$$

and the form:

$$S_2(\beta) = \frac{X}{\varepsilon_1^{\beta}} + \frac{Y}{\varepsilon_2^{\beta}}$$

That they are solveable was proven (see appendix I).

Appendix III

Upper & Lower Bounds for Some Hydrogenic Sum Rules.

β	Lower Bound to $S^H(\beta)$	Upper Bound to $S^H(\beta)$
0.1	0.972	0.992
0.5	0.974	0.981
0.7	0.9813	0.9846
1.1	1.00764	1.00822
1.5	1.04955	1.05071
1.7	1.07681	1.07763
1.9	1.10799	1.10828
2.1	1.14265	1.14292
2.3	1.18073	1.18147
2.5	1.22256	1.22354
2.7	1.26816	1.26907
2.9	1.31758	1.31801
3.2	1.3978	1.3990
3.5	1.4852	1.4895
3.9	1.614	1.625

Here we take $S^H(\beta) = \sum' f_\ell^H / (\varepsilon_\ell^H)^\beta$ where ε_ℓ^H is the energy & f_ℓ^H is the dipole oscillator strength for the excitation of a neutral hydrogen atom from its ground state to a state ℓ.

Energies are expressed Rydberg & all other quantities in Atomic units. [4].

We present upper and lower bounds for $S^H(\beta)$ at various points, $\beta \in [0,4]$. To obtain these, the exact values, [4], of $S^H(0)$, $S^H(1)$ $S^H(2)$, $S^H(3)$, $S^H(4)$ were used to give $S_2(\beta)$ interpolation functions, exact at four points. The point is not to give a complete listing, but rather to demonstrate the closeness of the bounds.

Appendix IV. Sum Rule Transformations

We will discuss in more detail those invertable transformations which take sum rule functions into sum rule functions.

Let $\mathcal{S}$ denote the set of all sum rule functions.

(i) Scalar Transformations: The mapping $\alpha : \mathcal{S} \longrightarrow \mathcal{S}$ defined by $(\alpha)S(\beta) = \alpha S(\beta)$ for any $\alpha > 0$ and any $S(\beta) \in \mathcal{S}$ is called a scalar transformation. If A denotes the set of all scalar transformations then it is easily seen that if $\alpha \in A$ then $\alpha^{-1} \in A$. A scalar transformation also maps (unrestrained) N-sum rule functions invertably into (unrestrained) N-sum rule functions. The most important properties of a scalar transformation are that it is invertable, and that bounding relationships between [(unrestrained) N-] sum rule functions are invariant to it. For example, if $S(\beta) > S_N(\beta)$ for some $\beta \in \mathbb{R}$, then for that β, $\alpha S(\beta) > \alpha S_N(\beta)$.

(ii) Sum rule scaling transformations: we have already mentioned these. We denote by the operator $\mathcal{E}$ the mapping $\mathcal{E} : \mathcal{S} \longrightarrow \mathcal{S}$ which takes $S(\beta) \in \mathcal{S}$ into $\mathcal{E}S(\beta) = S^{(E)}(\beta) = E^{-\beta}S(\beta)$ where $E > 0$. If E_1 denotes the set of all sum rule scaling transformations then it is easily seen that if $\mathcal{E} \in E_1$ then $\mathcal{E}^{-1} \in E_1$. In fact $\mathcal{E}^{-1}S(\beta) = S^{(-E)}(\beta) = E^{\beta}S(\beta)$ for any $S(\beta) \in \mathcal{S}$. A sum rule scaling transformation also maps (unrestrained) N-sum rule functions invertably into (unrestrained) N-sum rule functions. The most important properties of any $S(\beta) \in \mathcal{S}$ are that it is invertable, and that bounding relationships between [(unrestrained) N-] sum rule functions are invariant to it.

We notice that A and E commute. Moreover, neither A nor E involves a change in the variable β, rather, they map a sum rule function on an interval I into a new sum rule function on I and preserve all bounding relationships on that interval. The following two types of transformation map sum rule functions into new sum rule functions on new intervals.

(iii) Positive Linear Change of Variable: we have already mentioned the transformations which are effected in this manner. Briefly, if $L \in \mathcal{L}$ then $LS(\beta) = S(L\beta)$ where $S(\beta) \in \mathcal{S}$ is defined on the interval I and $LS(\beta)$ is defined on the interval $L^{-1}I$. If $L \in \mathcal{L}$ then $L^{-1} \in \mathcal{L}$. L also maps any (unrestrained) N-sum rule function into an (unrestrained) N-sum rule function. The most important property of any $L \in \mathcal{L}$ is that it is invertable and that any bounding relationship between [(unrestrained) N-] sum rule functions on the interval I also hold on the transform of that interval between the transforms of the [(unrestrained) N-] sum rule functions.

(iv) Reflection: If $S(\beta) \in \mathcal{S}$ then $RS(\beta) = S(-\beta)$ is also a sum rule function on the reflection of the interval of definition of $S(\beta)$. Notice that R is its own inverse and that bounding relationships are preserved in the obvious sense.

We notice the following two properties of (N-) sum rule functions. If $S(\beta)$, $t(\beta)$ are (N-) sum rule functions defined on intervals I_s, I_t respectively, then so are $(S(\beta) + t(\beta))$ and $S(\beta)t(\beta)$ on $\{I_s \cap I_t\}$

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