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# Many-Body Orthogonal Polynomial Systems

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**Abstract**

The fundamental methods employed in the Moment Problem, involving Orthogonal Polynomial Systems, the Lanczos Algorithm, Continued Fraction analysis, and Padé Approximants has been combined with a cumulant approach and applied to the extensive Many-Body problem in physics. This has yielded many new exact results for Many-Body systems in the thermodynamic limit - for the ground state energy, for excited state gaps, for arbitrary ground state averages - and are of a nonperturbative nature. These results flow from a confluence property of the three-term recurrence coefficients arising and define a general class of Many-Body Orthogonal Polynomials. These Theorems constitute an analytical solution to the Lanczos Algorithm in that they are expressed in terms of the three-term recurrence coefficients $\alpha$ and $\beta$. These results can also be applied approximately for non-solvable Models in the form of an expansion, in a descending series of the system size. The zeroth order of this expansion is just the manifestation of the Central Limit Theorem in which a Gaussian measure and Hermite polynomials arise. The first order represents the first non-trivial order, in which classical distribution functions like the binomial distributions arise and the associated class of Orthogonal Polynomials are Meixner Polynomials. Amongst examples of Systems which have infinite order in the expansion are $q$-Orthogonal Polynomials where $q$ depends on the system size in a particular way.

## 1 Physical Questions

Our motivation is to employ the Moment Formalism to the static, homogeneous properties of extensive Many-body Systems at zero temperature such as the many examples of strongly coupled systems with essentially an infinite number of degrees of freedom arising in condensed matter physics or quantum field theories. In such problems what is of interest are the spectral properties, such as ground state energies, excited state or mass gaps, and other averages such as order parameters and correlation functions. We will give definite answers to these questions, but the additional questions concerning the precise forms of the orthogonal polynomials, etc that arise is of less importance in this context. In fact such additional detail is usually unattainable and often unneccesary in the physical context. In the second Section we review the solution to the Moment Problem and establish connections with apparently diverse areas of analysis and the physical formalism, and set out our notations and conventions. The third Section contains our essential contribution, in the Extensivity Conjecture, and gives all the recently proved Theorems following from this and some new results which complete the picture. In the fourth Section we examine the approximate employment of these Theorems in the form of an expansion, a large size expansion or the "Plaquette" Expansion. Here we make interpretations of the zeroth and first order approximations in the Expansion, and the relationship with physical Models, statistical distributions and Orthogonal Polynomial Systems.

## 2 Formal Moment Problem

We give the Hamiltonian formulation of the Many-Body quantum mechanical problem, which is the one most closely connected with the Moment Problem. In the Hermitian Lanczos Algorithm[1, 2] the Subspace $|\psi_0\rangle, |\psi_1\rangle, \dots$ is generated by the recurrence

$$|\psi_{n+1}\rangle = \frac{1}{\beta_{n+1}}[(H-\alpha_n)|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle] \tag{1}$$

with Lanczos coefficients $\alpha_n = \langle\psi_n|H|\psi_n\rangle$ and $\beta_n = \langle\psi_{n-1}|H|\psi_n\rangle$. The norm is defined as $\langle\cdot\rangle \equiv \langle\psi_0|\cdot|\psi_0\rangle$ with respect to the trial state $|\psi_0\rangle$ which is completely arbitrary other than having a non-zero overlap with the true ground state and being translationally invariant. The Hamiltonian in this basis is tri-diagonal and the eigenvalue problem reduces to

$$T_n = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & & \beta_n \\ & & & \beta_n & \alpha_n \end{pmatrix} . \tag{2}$$

The Lanczos process is entirely equivalent to the three term recurrence for an Orthogonal Polynomial System[3, 4]

$$Q_{n+1}(E) = (E-\alpha_n)Q_n(E) - \beta_n^2 Q_{n-1}(E) \tag{3}$$

or through a positive definite linear functional being defined by the measure on the real line

$$\mathcal{L}[\cdot] \equiv \int_{-\infty}^{+\infty} d\rho(E) . \tag{4}$$

The direct connections are given by the determinant $Q_{n+1}(E) = (-)^{n+1}|T_n - EI_{n+1}|$ so that the zeros of the Orthogonal Polynomial are eigenvalues of Hamiltonian.

A key ingredient in the classical solution to the Moment Problem, the Resolvent is simply the analytic continuation of the Laplace transform of the cumulant generating function (see Eq. (13))

$$R(E) = \int_0^\infty dt\, e^{-Et}\langle e^{tH}\rangle = \langle\frac{1}{E-H}\rangle \qquad \Re(E) > E_0 . \tag{5}$$

Its formal Laurent series establishes a direct link with Hamiltonian moments

$$R(E) = \sum_{i=0}^{\infty} \frac{\mu_i}{E^{i+1}} \tag{6}$$

where the Hamiltonian moments are defined $\mu_n = \langle H^n\rangle$, $\mu_0 = 1$. The Resolvent has a real Jacobi-fraction continued fraction form[5, 6]

$$R(E) = -\mathbf{K}_{n=0}^{\infty} - \left(\frac{\beta_n^2}{E-\alpha_n}\right) . \tag{7}$$

The density of states is given by the discontinuity of the Resolvent across the branch cut delinateing the spectrum

$$n(E) = -\frac{1}{\pi}\Im\, R(E+i0^+) . \tag{8}$$

The $n$-th continuant of the Resolvent is then the [n-1/n] Padé Approximant formed from the numerator and denominator Orthogonal Polynomials

$$R_n(E) = \frac{P_n(E)}{Q_n(E)} \tag{9}$$

with the initial terms

$$\begin{aligned} P_0(E) &= 0 \qquad P_1(E) = 1 \\ Q_{-1}(E) &= 0 \qquad Q_0(E) = 1 \ . \end{aligned} \tag{10}$$

The solutions for the Lanczos or recurrence coefficients $\alpha_n$ and $\beta_n^2$, in terms of the moments, are given explicitly in terms of the Hankel determinants or Selberg Integrals[5, 7],

$$\begin{aligned} \Delta_n &= |\mu_{i+j-2}|_{i,j=1}^{n+1} = \int_{-\infty}^{+\infty} d\rho(x_1)\ldots d\rho(x_{n+1}) \prod_{i<j} |x_i - x_j|^2 \\ \Delta'_n &= |\mu_{i+j-1}|_{i,j=1}^{n+1} = \int_{-\infty}^{+\infty} d\rho(x_1)\ldots d\rho(x_{n+1}) x_1 \ldots x_{n+1} \prod_{i<j} |x_i - x_j|^2 \end{aligned} \tag{11}$$

for $n \geq 0$, in the following closed form expressions,

$$\alpha_n = \frac{\Delta'_{n-2}}{\Delta'_{n-1}} \frac{\Delta_n}{\Delta_{n-1}} + \frac{\Delta'_n}{\Delta'_{n-1}} \frac{\Delta_{n-1}}{\Delta_n} \ , \qquad \beta_n^2 = \frac{\Delta_n \Delta_{n-2}}{\Delta_{n-1}^2} \qquad n \geq 2 \ . \tag{12}$$

As is well known, this Hamburger Moment Problem has a solution if and only if all $\beta_n^2 > 0$ and the $\alpha_n$ are real. For a finite sized Many-Body System however, the Lanczos Process must terminate when the Hilbert Space has been exhausted, whereupon a particular $\beta_n^2$ will vanish. Generally this will occur after a very large number (usually exponentially large with respect to the number of sites) of iterations and we are of course intending to take the system size to infinity.

# 3 Extensivity Properties

The $n$-th cumulant, or connected moment, is denoted by $\nu_n \equiv \langle H^n \rangle_c$ and defined in terms of its generating function[8]

$$\langle e^{tH} \rangle = \sum_{n=0}^{\infty} \mu_n \frac{t^n}{n!} = \exp\left( \sum_{n=1}^{\infty} \nu_n \frac{t^n}{n!} \right) \ . \tag{13}$$

The interrelationship between moments and cumulants can be made explicit and so one can go from the first $n$ moments to the first $n$ cumulants or vice versa. Cumulants scale directly with the size of the system[8] so that for the Extensive Many-Body Problem we have $\nu_n = c_n N$ in the ground state sector, or $\nu_n = c_n N + m_n$ in any other sector[9]. In arriving at this we have ignored all boundary effects and conditions as we want to take the limit $N \to \infty$, after termination of the Lanczos process. In all that follows we consider only Hamiltonian and energy densities, $\epsilon \equiv E/N$, consequently the Lanczos coefficients are divided by the system size and we use the same symbol to denote these.

We have found a confluence property of the Lanczos coefficients,

Conjecture 1 (Extensivity Conjecture[10]) *The exact Lanczos density coefficients of any extensive Many-Body system have the following confluence properties as $n, N \to \infty$*

$$\begin{aligned} \alpha_n(N) &= \alpha(n/N) + \mathrm{O}(1/N) \\ \beta_n^2(N) &= \beta^2(n/N) + \mathrm{O}(1/N) \end{aligned} \tag{14}$$

*in terms of the scaled Lanczos iteration number $s = n/N$.*

Great simplification will arise from this observation. We consider this to be true of homogeneous systems with local interactions of a reasonably short-ranged nature. We do not know if this is the weakest formulation of the true confluence behaviour but it is certainly sufficient to make a number of strong statements, that are to follow. This limiting behaviour defines a class of Orthogonal Polynomials which we call Many-Body Orthogonal Polynomials, where an additional parameter appears, $N$, with the above limiting value. Actually to be strictly correct this system is not an Orthogonal Polynomial System because it always terminates for finite $N$ and in the limit $n, N \to \infty$ the Orthogonal Polynomials become orthogonal functions. But because so much of the classical formalism is the basis of all the results for this system, its parentage could never be in doubt. We define the spectral envelope functions

$$e_n(N) = 1/2\left\{\alpha_n + \alpha_{n-1} - [(\alpha_n - \alpha_{n-1})^2 + 16\beta_n^2]^{1/2}\right\} \xrightarrow[n,N\to\infty]{} e(s) = \alpha(s) - 2\beta(s) \ , \tag{15}$$

and the following exact results can be found.

**Theorem 1** (Exact Ground State Energy[10]) *The exact ground state energy of the extensive Many-Body system in the thermodynamic limit is given by*

$$\epsilon_0 = \inf_s[e(s)] \ . \tag{16}$$

This result follows from the bounds and equalities on the extreme zeros of orthogonal polynomials found in Leopold[11] and van Doorn[12] where in the last work the lowest zero of the n-th order orthogonal polynomial is

$$x_{n1} = \max_{\mathbf{h}}\left\{\min_{1\le i<n}\frac{1}{2}\left(\alpha_i + \alpha_{i-1} - \left[(\alpha_i - \alpha_{i-1})^2 + \frac{4\beta_i^2}{a_i}\right]^{1/2}\right)\right\} \tag{17}$$

where $\{a_i\}_1^n$ is a chain sequence with a parameter sequence $\{h_i\}$ given by $a_i = (1-h_i)h_{i+1}$ and $h_1 = 0, h_n = 1$ and $0 < h_i < 1$. Further use is made of the maximal constant chain sequence[13] $a_i \to a = 1/4\cos^2(\pi/(n+2))$. If the infimum occurs at a finite point, we denote this by $s_0$.

**Theorem 2** (Ground State Averages[14]) *The exact ground state average of an operator $O$ of an extensive Many-Body system in the thermodynamic limit is*

$$\langle O\rangle = \left[\delta^O\alpha(s) - \frac{\delta^O\beta^2(s)}{\beta(s)}\right]_{s_0} \tag{18}$$

*where the shifted Lanczos coefficients $\delta^O\alpha, \delta^O\beta^2$ are constructed from the shifted cumulants*

$$\delta^O\nu_{n+1} = \sum_{k=0}^{n}\langle H^{n-k}OH^k\rangle_c \ . \tag{19}$$

This follows directly from the ground state energy theorem, by just appending the operator $O$ to the Hamiltonian in a "piggy-back" fashion and carrying the analysis through, and then appealing to the Hellmann-Feynman theorem.

**Theorem 3** (Exact Excited State Gaps - different sector[9]) *The exact gap between the first excited state and the ground state, where the excited state belongs to a different sector than the ground state, of the extensive Many-Body system in the thermodynamic limit is*

$$\Delta\epsilon = N\left[\delta^G\alpha(s) - \frac{\delta^G\beta^2(s)}{\beta(s)}\right]_{s_0} \tag{20}$$

*where the shifted Lanczos coefficients $\delta^G\alpha, \delta^G\beta^2$ are constructed from the shifted cumulants*

$$\nu_n^P = c_n N + \delta^G c_n \ . \tag{21}$$

This gap is simply the difference in the ground state energies of two distinct sectors of the Hilbert space, and leads to the above result.

**Conjecture 2** (Exact Excited State Gaps - same sector[15]) *The exact gap between the first excited state and the ground state, where the both states belong to the same sector, of the extensive Many-Body system in the thermodynamic limit is*

$$\Delta\epsilon = 2\lim_{n,N\to\infty} N\left[e(s) - e_n(N)\right]_{s_0} \ . \tag{22}$$

This result suggests that the gap is the consequence of a "peeling operation" on the finite-size spectral envelope function.

## 4 Large Size Expansion

If one uses cumulants in place of moments in the solution for the Lanczos coefficients Eqs. (11,12) and expands the result with respect to the size of the system then a very simple result emerges[16, 17]. The descending series of these coefficients with respect to $N$ has the leading terms

$$\alpha_n = c_1 + \frac{n}{N}\left[\frac{c_3}{c_2}\right] + \frac{n(n-1)}{2N^2}\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{2c_2^4}\right] + \dots \tag{23}$$

for $n \geq 0$, and

$$\beta_n^2 = c_2\frac{n}{N} + \frac{n(n-1)}{2N^2}\left[\frac{c_2c_4 - c_3^2}{c_2^2}\right] + \frac{n(n-1)(n-2)}{6N^3}\left[\frac{-12c_3^4 + 21c_2c_3^2c_4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{2c_2^5}\right] + \dots \tag{24}$$

for $n \geq 1$ and arises from the following general form of a constant term for the Hankel determinants[18], one example being

$$\Delta_n = \frac{1}{(n+1)!}\prod_{1\leq i<j\leq n+1}\left(\frac{\partial}{\partial t_i} - \frac{\partial}{\partial t_j}\right)^2 \exp\left\{N\sum_{l=1}^{\infty}\frac{c_l}{l!}p_l(t)\right\}\Bigg|_{t=0} \tag{25}$$

where the power sums are defined $p_l(t) = \sum_{i=1}^{n+1} t_i^l$. This expansion clearly satisfies the Extensivity Conjecture and is in fact the principal motivation for it.

The lowest level approximation, referred to as the zeroth level, that is to say just retaining $c_1$ and $c_2$ with all others zero has

$$\alpha_n = c_1 \ , \qquad \beta_n^2 = c_2\frac{n}{N} \ . \tag{26}$$

The recurrence relation for the denominator orthogonal polynomials, namely Eq. (3), is just that for the Hermite polynomials and the Gaussian weight function on the unbounded interval $(-\infty, +\infty)$. The results at this order are the manifestation of the Central Limit Theorem in our scheme, but it cannot represent any physical model because the spectrum is not bounded below.

The Lanczos coefficients at the next order in the size expansion are

$$\alpha_n = c_1 + c_3/c_2\frac{n}{N} \ , \qquad \beta_n^2 = c_2\frac{n}{N} + \frac{n(n-1)}{2N^2}\left[\frac{c_2c_4 - c_3^2}{c_2^2}\right] \ . \tag{27}$$

The classical distributions appearing in Statistics, which are exactly represented at this order, include the Binomial distribution[19], where $\alpha_n = p + (1-2p)n/N$ and $\beta_n^2 = pqn/N - pqn(n-1)/N^2$. A physical Model which is treated exactly at this order is that of $N$ bosons interacting harmonically and confined in a common harmonic well[20], in one dimension

$$H = \frac{1}{2}\left[\sum_{i=1}^{N}\left(-\frac{d^2}{dx_i^2} + \omega^2 x_i^2\right) + g^2\sum_{i<j}(x_i - x_j)^2\right] \ . \tag{28}$$

There are two primary cases of Orthogonal Polynomials Systems which arise at this order, depending on the parameters

$$I \equiv 3c_3^2 - 2c_2c_4 \ , \qquad D \equiv \frac{c_2c_4 - c_3^2}{2c_2^2} \ . \tag{29}$$

1. $I > 0$ - there exists a real minima of $e(s)$ at a finite $s$-value and the corresponding ground state energy and spectral gap are[21] with $N \to \infty$

$$\epsilon_0 = c_1 + \frac{\sqrt{I} - c_3}{2D} \ , \qquad \Delta\epsilon = \frac{\sqrt{I}}{c_2} \ . \tag{30}$$

For finite $N$ the Orthogonal Polynomials appropriate to this case are the Meixner Polynomials of the first kind,

$$\left(\frac{\sqrt{I}-c_3}{2c_2N}\right)^n m_n\left(\frac{c_2N}{\sqrt{I}}[\epsilon-\epsilon_0];\frac{c_2N}{D},\frac{c_3-\sqrt{I}}{c_3+\sqrt{I}}\right) \tag{31}$$

in terms of the standard notation of Chihara[4]. The Resolvent is given by[21]

$$\frac{1}{R(\epsilon)}=[\epsilon-c_1](1-r)+\frac{[\epsilon-\epsilon_0]r(1-a)^{-c_2N/D}}{{}_2F_1\left(\frac{r}{1-r^2D}N[\epsilon-\epsilon_0],-\frac{c_2}{D}N;\frac{r}{1-r^2D}N[\epsilon-\epsilon_0]+1;a\right)} \tag{32}$$

where the auxiliary parameters are $r=[-c_3\pm\sqrt{I}]/2c_2D$ and $a=r^2D$ such that $|r^2D|<1$. Within this case there are two further distinct sub-cases -

1(a) - Bounded spectrum $D<0$:
This leads to the following unnormalised density of states in the $N\to\infty$ regime

$$n(x)=n_0[x(1-x)]^{-1/2}[(1+a)^{-1}a^x x^{-x}(1-x)^{-(1-x)}]^{-c_2N/D} \tag{33}$$

for the scaled and shifted energy on the interval $x\equiv(\epsilon-\epsilon_0)|D|/\sqrt{I}\in(0,1)$.

1(b) - Unbounded spectrum $D>0$:
In this case the unnormalised density of states in the same limit is

$$n(x)=n_0[x(1+x)]^{-1/2}[(1-a)a^x x^{-x}(1+x)^{(1+x)}]^{c_2N/D} \tag{34}$$

on the interval $x\in(0,\infty)$.

2. $I<0$ - In the remaining case one can show that the envelope function $e(s)$ is monotonically decreasing and not bounded below. Consequently there is no ground state energy, nor any physical system representing this case. The Orthogonal Polynomials arising in this case are the Meixner Polynomials of the second kind whose spectrum is $(-\infty,+\infty)$,

$$\left(\frac{\sqrt{-I}}{c_2N}\right)^n M_n\left(\frac{2c_2N}{\sqrt{-I}}[\epsilon-c_1+\frac{c_3}{2D}];\frac{c_3}{\sqrt{-I}},\frac{c_2N}{D}\right) \tag{35}$$

Examples of Many-body OPS at higher orders (infinite order) in the size expansion include $q$-orthogonal polynomials with $q=1-1/N$. One of the simplest cases is the Al-Salam Carlitz Polynomials with $a<0$[4].

$$\alpha_n=(1+a)q^n\ ,\qquad \beta_n^2=-aq^{n-1}(1-q^n)\ . \tag{36}$$

The zeros of these OPS are located at $aq^n$ and $q^n$ for $n\geq 0$ and thus on the interval $[a,1)$. The bottom of the spectrum is $\epsilon_0=a$ and the first excited state gap is

$$\epsilon_1-\epsilon_0=\frac{-a}{N}\ . \tag{37}$$

The envelope function is then simply

$$e(s)=(1+a)e^{-s}-2\sqrt{-a}[e^{-s}(1-e^{-s})]^{1/2}\ , \tag{38}$$

and one can easily verify all the above theorems.

# 5 Conclusions

We have carried out the application of the Lanczos Process, or equivalently the solution of the Moment Problem, to the extensive Many-Body Problem in Quantum Mechanics and been able to analytically and exactly diagonalise this eigenproblem. Thus we have rendered all questions concerning the ground state spectrum and other averages in terms of the Lanczos coefficients, or matrix elements, which can be found directly from the connected moments of certain operators. In formulating our results we defined a very general class of orthogonal polynomial, the Many-Body orthogonal polynomials, from a certain confluence property of the three-term recurrence coefficients. We have also found that two types of hypergeometric Orthogonal Polynomial Systems, Hermite and Meixner, arise from the first two orders, in association with classical distribution functions. No other examples within the Askey scheme of hypergeometric orthogonal polynomials appear relevant for Many-Body orthogonal polynomials. However higher orders in this expansion certainly include $q$-orthogonal Polynomials as examples but these basic hypergeometric orthogonal polynomials would not represent the most general type, nor necessarily any realistic physical model.

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# References


[1] C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255 (1950).

[2] Y. Saad, *Numerical Methods for Large Eigenvalue Problems*, Lecture Notes, 1991.

[3] G. Szegö, *Orthogonal Polynomials*, Colloquium Publications **23**, American Mathematical Society, Providence, Rhode Island, fourth edition, 1975.

[4] T. Chihara, *An Introduction to Orthogonal Polynomials*, Gordon and Breach, New York, 1978.

[5] W. Jones and W. Thron, *Continued Fractions - Analytic Theory and Applications*, Addison-Wesley Publishing Company, Reading, Massachusetts, 1980.

[6] L. Lorentzen and H. Waadeland, *Continued Fractions with Applications*, North-Holland, Amsterdam, 1992.

[7] J. Shohat and J. Tamarkin, *The Problem of Moments*, American Mathematical Society, Providence, Rhode Island, 1943.

[8] R. Kubo, J. Phys. Soc. Japan **17**, 1100 (1962).

[9] L. Hollenberg, M. Wilson, and N. Witte, Phys. Lett. B **361**, 81 (1995).

[10] L. Hollenberg and N. Witte, Phys. Rev. B (1997).

[11] E. Leopold, J. Approx. Th. **43**, 15 (1985).

[12] E. van Doorn, J. Approx. Th. **51**, 254 (1987).

[13] M. Ismail and X. Li, Proc. Am. Math. Soc. **115**, 131 (1992).

[14] N. Witte, L. Hollenberg, and Z. Weihong, Phys. Rev. B (1997).

[15] N. Witte and L. Hollenberg, Excited state gaps in an analytic lanczos expansion, 1997.

[16] L. Hollenberg, Phys. Rev. D **47**, 1640 (1993).

[17] N. Witte and L. Hollenberg, Z. Phys. B **95**, 531 (1994).

[18] N. Witte, Selberg integrals in the application of the moment formalism to the many-body problem, 1997.

[19] L. Hollenberg, private communication, 1995.

[20] J. Cioslowski, Int. J. Quantum Chem.: Quant. Chem. Symp. **21**, 563 (1987).

[21] N. Witte and L. Hollenberg, Z. Phys. B **99**, 101 (1995).