Analytic Solution for the Ground State Energy of the Extensive Many-Body Problem

Lloyd C.L. Hollenberg and N.S. Witte

Research Centre for High Energy Physics,
School of Physics, University of Melbourne,
Parkville, Victoria 3052, AUSTRALIA.

Abstract

A closed form expression for the ground state energy density of the general extensive many-body problem is given in terms of the Lanczos tri–diagonal form of the Hamiltonian. Given the general expressions of the diagonal and off-diagonal elements of the Hamiltonian Lanczos matrix, $\alpha_n(N)$ and $\beta_n(N)$, asymptotic forms $\alpha(z)$ and $\beta(z)$ can be defined in terms of a new parameter $z \equiv n/N$ ($n$ is the Lanczos iteration and $N$ is the size of the system). By application of theorems on the zeros of orthogonal polynomials we find the ground-state energy density in the bulk limit to be given in general by $\mathcal{E}_0 = \inf [\alpha(z) - 2 \beta(z)]$. 
I. INTRODUCTION

Finding analytic means of calculating details of the energy spectrum of strongly interacting many-body systems has long been a goal of theoretical physics, with applications from low energy scales in condensed matter physics to high energy particle physics. In particular, accurate calculations of the ground state energy are important to settle issues relating to the character of the ground state, or vacuum state, itself. While there has arisen a range of theoretical tools to tackle problems that cannot be treated by perturbation theory, many suffer from the effects of uncontrolled approximation to the extent that each, alone cannot be trusted to give a reliable answer. It is only when several independent methods point in the same direction, that one can confidently state something about the character of a system. Examples include mean field theories neglecting correlations in fluctuations thereby reinforcing a tendency to order; exact diagonalisation and Monte-Carlo studies, at zero temperature, on relatively small clusters and the extrapolation to the bulk limit; finite temperature Monte-Carlo simulation of somewhat larger systems, but at temperatures above the interesting low energy scales.

In this paper a simple fundamental relationship is found between the tri-diagonal form of the Hamiltonian and the ground state energy density. A general theorem is proved for the ground state energy density in terms of the coefficients generated by the Lanczos method, evaluated in a limiting process incorporating convergence of the Lanczos iterates and the thermodynamic limit. The Lanczos method is based on the following recursion: starting from an appropriate trial state, one recursively generates new basis states with repeated application of the Hamiltonian

\[ |v_n\rangle = \frac{1}{\beta_{n-1}} \left[ (H - \alpha_{n-1}) |v_{n-1}\rangle - \beta_{n-2} |v_{n-2}\rangle \right], \tag{1} \]

where \( \alpha_n = \langle v_n | H | v_n \rangle \) and \( \beta_n = \langle v_{n+1} | H | v_n \rangle \). At the \( n \)th iteration of this recursion the Hamiltonian matrix in the new basis of states is given by the tri-diagonal, \( T_n \), i.e.
The power of the Lanczos phenomenon is that the dimension of the tri-diagonal basis, required to describe the low-lying states of the system, determined by the recursion level is significantly smaller than the original basis. The outermost eigenvalues of $T_n$ rapidly converge to those of the Hamiltonian. In computing the Lanczos coefficients, $\alpha_n$ and $\beta_n$, exactly one is usually restricted to an early termination of the recursion in the analytic case treating large systems, or to small systems in a numerical calculation taken to complete convergence. To date all methods, however the Lanczos basis has been generated, require the numerical diagonalisation of the tri-diagonal $T_n$ matrices for the ground state energy. In this paper we will demonstrate how the diagonalisation can be carried out analytically for extensive systems, thereby providing a solution for the ground state energy density in terms of the tri-diagonal form. By introducing a new parameter, $z = n/N$, where $N$ is the size of the system, the asymptotic forms $\alpha(z)$ and $\beta(z)$ are related to the ground state energy by

$$E_0 = \inf [\alpha(z) - 2 \beta(z)].$$

(3)

II. THERMODYNAMIC LIMIT OF THE TRI-DIAGONAL FORM

Using the initial state, $|v_1\rangle$, one forms Hamiltonian moments, and from these the connected moments,

$$\langle H^n \rangle_c \equiv \langle v_1 | H^n | v_1 \rangle_c.$$  (4)

The connected moments encapsulate the essential physics of the system because they scale with the size of the system, $N$, as
\[ \langle H^n \rangle_c \equiv c_n N. \] (5)

Here \( N \) is a quantitative measure of the size of the system whether it be the number of sites in a lattice of localised spins, or the volume in a continuum model with itinerant particles. Although this form is restricted to the ground state or vacuum sector of the model, generalisations can be easily made to excited states.

A \( 1/N \) expansion of the Lanczos matrix elements, \( \alpha_n(N) \) and \( \beta_n(N) \), reveals a surprising analytic property – a simple polynomial \( n \) dependence. In terms of the connected coefficients \( c_n \), this cluster expansion for the Hamiltonian density are [1,2]

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

\[
\beta_n^2(N) = \frac{n}{N}c_2 + n(n-1) \frac{1}{N^2} \left[ \frac{c_2c_4 - c_3^2}{2c_2^2} \right]
\]

\[
+ n(n-1)(n-2) \frac{1}{N^3} \left[ \frac{21c_2c_3^2c_4 - 12c_3^4 - 4c_2c_3c_4^2 - 6c_2^2c_3c_5 + c_3^3c_6}{12c_2^3} \right] + O \left( \frac{1}{N^4} \right). \] (6)

We first define a parameter \( z \equiv n/N \) which remains finite as the Lanczos recursion proceeds in the bulk limit, \( n \to \infty \) and \( N \to \infty \). In this limit the expansions become a series in \( z \), i.e.

\[
\alpha(z) \equiv \lim_{n,N \to \infty} \alpha_n(N) = c_1 + z \left[ \frac{c_3}{c_2} \right] + z^2 \left[ \frac{3c_3^2 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^2} \right] + O(z^3),
\]

\[
\beta^2(z) \equiv \lim_{n,N \to \infty} \beta_n^2(N) = z c_2 + z^2 \left[ \frac{c_2c_4 - c_3^2}{2c_2^2} \right]
\]

\[
+ z^3 \left[ \frac{21c_2c_3^2c_4 - 12c_3^4 - 4c_2c_3c_4^2 - 6c_2^2c_3c_5 + c_3^3c_6}{12c_2^3} \right] + O(z^4). \] (8)

The cluster expansion guides us to the observation that, more generally, we have for the exact problem the asymptotic forms in the \( n \to \infty \) and \( N \to \infty \) regime

\[
\alpha_n(N) = \alpha(z) + O(1/N),
\]

\[
\beta_n^2(N) = \beta^2(z) + O(1/N). \] (10)
We observe here a confluence of the two limiting regimes: that of convergence of the Lanczos iterates and of the thermodynamic limit into a single scaled Lanczos iteration number $z$.

III. ORTHOGONAL POLYNOMIALS AND VAN DOORN’S THEOREM

The connection between the Lanczos tri-diagonal form of the Hamiltonian and the associated system of orthogonal polynomials is simple. The characteristic polynomial $D_n(x) = \det(T_n - xI_n)$ of the Lanczos tri-diagonal matrix representation satisfies the following recursion relation:

$$D_n(x) = (\alpha_n - x)D_{n-1}(x) - \beta_{n-1}^2 D_{n-2}(x),$$

which in turn defines $P_n(x) \equiv (-1)^n D_n(x)$ as an orthogonal polynomial, the zeros of which are the eigenvalues of the $T_n$ matrices. The analytic forms for the $\alpha_n(N)$ and $\beta_n(N)$ define a special class of orthogonal polynomials relevant to the many-body problem which are distinguished by a certain dependence on the size parameter $N$.

For the orthogonal polynomials $P_n(x)$ satisfying the recursion relation

$$P_n(x) = (x - \alpha_n)P_{n-1}(x) - \beta_{n-1}^2 P_{n-2}(x)$$

there exits a powerful theorem by Van Doorn [3] on the lower bound on the lowest zero which has been generalised by Ismail and Li [4] to include an upper bound to the largest zero. Simply stated Ismail and Li’s result is the following: if $x_k^{(1)}$ and $x_k^{(k)}$ are the smallest and largest zeros respectively of $P_k(x)$ with $k > 1$ then they are bounded by the interval $(A, B)$ where

$$A = \min\{f_n^- : 1 \leq n < k\}$$

$$B = \max\{f_n^+ : 1 \leq n < k\}$$

and the bound sequence is given by

$$f_n^\pm = \frac{1}{2} \left[ (\alpha_n + \alpha_{n+1}) \pm \sqrt{(\alpha_n - \alpha_{n+1})^2 + \frac{4}{a_n} \beta_n^2} \right].$$
In the above expression for \( f_n^\pm \), \( \{a_n\}_1^{k-1} \) is a chain sequence. That is, there exists a parameter sequence \( \{g_n\}_1^k \) for which we have the factorisation of \( a_n \)

\[
a_n = g_{n+1}(1-g_n), \quad 1 \leq n < k
\]  

(15)

where \( 0 \leq g_1 < 1 \) and \( 0 < g_n < 1 \) for \( 1 < n \leq k \). Van Doorn’s theorem is for strict equality, whereby maximising the lower bound with respect to the parameter sequence gives the lowest eigenvalue exactly:

\[
x_k^{(1)} = \max_{\{g\}} \left[ \min_n \{f_n^- : 1 \leq n < k\} \right]
\]  

(16)

for \( k > 1 \). Only a technical difference occurs with this theorem in that \( g_1 = 0 \) and \( g_k = 1 \).

For finite \( N \) the termination of the Lanczos recursion occurs at some \( n_{\text{max}} \) when the sector of Hilbert space, determined by the trial state, has been exhausted. In general the basis of states grows faster than any linear enumeration with \( N \). Taking the minimum of \( f_n^- \) to occur at some \( \bar{n} = \bar{z}N \) (\( \bar{n} < n_{\text{max}} \)), the asymptotic forms for \( \alpha_n(N) \) and \( \beta_n(N) \) give the leading order behaviour of the lowest energy level as

\[
x_n^{(1)} = \max_{\{g\}} \left[ \alpha(\bar{z}) - \frac{1}{\sqrt{a_n}} \beta(\bar{z}) + O(1/N) \right].
\]  

(17)

Since \( \beta_n(N) > 0 \), to maximise the RHS of the above expression with respect to the chain sequence we may choose the maximal constant chain sequence

\[
a = \frac{1}{4 \cos^2 \left( \frac{\pi}{n_{\text{max}}+2} \right)}.
\]  

(18)

We can now obtain the ground state energy density, \( \mathcal{E}_0 \), in the bulk limit:

\[
\mathcal{E}_0 = \lim_{N \to \infty} x_n^{(1)}.
\]  

(19)

In the \( N \to \infty \) limit, we also have \( n_{\text{max}} \to \infty \) giving \( a \to 1/4 \), and it is straightforward to establish that in general \( \bar{z} \) is obtained by finding the greatest lower bound with respect to \( z \). The ground state energy density of the general extensive many-body problem in the bulk limit is therefore

\[
\mathcal{E}_0 = \inf_{z>0} [\alpha(z) - 2 \beta(z)].
\]  

(20)
IV. EXAMPLES

As a first illustration of this exact analytic diagonalisation of extensive systems we consider the purely mathematical model defined by the tri-diagonal form

\[
\alpha_n(N) = \left(1 + \frac{a n}{N^2}\right)^N, \\
\beta_n(N) = \left(1 + \frac{b n}{N^2}\right)^N - 1.
\] (21)

The lowest eigenvalue in the \(N \to \infty\) limit is

\[
E_0 = \inf \left[ e^{az} - 2e^{bz} + 2 \right] = \left(\frac{r}{2}\right)^{r/(1-r)} (1 - r) + 2,
\]

where \(r = a/b\). The minimum occurs at \(z_{\text{min}} = \ln(2/r)/b(r - 1)\). It is a straightforward matter to numerically diagonalise this system for increasing \(N\) to demonstrate the convergence of the numerical results to the analytic expression. The results of this exercise are shown in Figure 1 (for a typical case \(a = 3\) and \(b = 2\)) where we plot the error, defined as the difference from the exact value, of numerical diagonalisations for increasing \(N\). The approach to the analytic solution is clear as \(N \to \infty\).

Secondly we compare the analytic diagonalisation with numerical results using the truncated Lanczos coefficients given by the plaquette expansion. We do this here for the case of the anti-ferromagnetic Heisenberg chain, for which the expansions have been derived to high order using the classical Néel state as the trial state. This state is an poor choice for the isotropic Heisenberg model but is sufficiently simple to allow the computation of moments up to \(< H^{28} >_c\). Employing the traditional analysis of the plaquette expansion the \(T_n\) matrices are diagonalised numerically for increasing chain size \(N\) \(\ll 1\). In Figures 2 and 3 we demonstrate the approach of the numerical diagonalisation for the ground state to the analytic expression as the \(N \to \infty\) limit is approached. We show the two typical cases which can occur due to the truncation of the expansions for \(\alpha(z)\) and \(\beta(z)\). Figure 2 corresponds to an order of the plaquette expansion for which \(\alpha(z) - 2\beta(z)\) has no minimum – a point of inflection develops, reflecting the fact that the expansion naturally breaks down
at some large enough value of $z$. Figure 3 shows a case where a minimum develops – the numerical values for the lowest eigenvalue in the large volume limit match onto the value of at the minimum.

We must emphasis that the plaquette expansion is a series expansion of the exact Lanczos coefficients about $z = 0$ and truncated, and is therefore only reliable for small $z$. The error involved grows rapidly with $z$ which can occur with either sign, and thus the large $z$ behaviour of the truncated approximations bear no relation to the exact behaviour. Because of this we don’t expect that at every order at which the truncation is made, that a minima would arise.

**V. CONCLUSIONS**

We have found an expression for the ground state energy density for the extensive many-body problem which is completely general and, since the Hamiltonian was diagonalised exactly, is non-perturbative. Given the Hamiltonian in tri-diagonal form the expression can be used immediately. So far, the exact analytic transformation of a system to tri-diagonal form has not been achieved for any examples of solvable systems. This state of affairs may change as the theorem proved here gives impetus to efforts in this direction. However, an immediate approximate tri-diagonalisation of the general problem does exist in the plaquette expansion and studies of the usefulness of this method with better trial states also merits further work. The analytic nature of this expansion uncovered the existence of the scaled Lanczos iteration parameter $z = n/N$ and the asymptotic forms $\alpha(z)$ and $\beta(z)$ for the exact problem.

An interesting extension of this work is to consider a similar analysis on excited states. An indication that the solution for the mass-gap of the general extensive many-body system may in fact be possible is the fact that the mass-gap of the first order plaquette expansion has already been solved analytically \[\text{[6,7].}\] Such a generalisation is presently under active investigation.
FIGURES

FIG. 1. Comparison of the analytic solution with numerical diagonalisation for the simple case, \( \alpha_n(N) = (1 + an/N^2)^N \) and \( \beta_n(N) = (1 + bn/N^2)^N - 1 \), with \( a = 3 \) and \( b = 2 \).

FIG. 2. Plaquette expansion of the 1D AFH model at an order \((1/N^{11})\) where a point of inflection develops due to the breakdown of the expansion. The numerical diagonalisation for increasing \( N \) converges to the function \( \alpha(z) - 2\beta(z) \).

FIG. 3. Plaquette expansion of the 1D AFH model at an order \((1/N^7)\) where a minimum develops in \( \alpha(z) - 2\beta(z) \). The numerical diagonalisation data at \( N = 5 \times 10^4 \) clearly display the convergence to the value of \( \min[\alpha(z) - 2\beta(z)] \).
REFERENCES

[1] L.C.L. Hollenberg, *Phys. Rev.* D47 (1993) 1640.

[2] N.S. Witte and L.C.L. Hollenberg, *Z. Phys.* B95 (1994) 531.

[3] E.A. Van Doorn, *J. Approx. Th.* 51 (1987) 254.

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

[5] L.C.L. Hollenberg, Phys. Lett. A182 (1993), 238.

[6] N.S. Witte and L.C.L. Hollenberg, *Z. Phys.* 99 (1995) 101.

[7] L.C.L. Hollenberg, M.P. Wilson and N.S. Witte, *Phys. Lett.* B in press.

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$z = \frac{n}{N}$

$\varepsilon_0$

$\alpha(z) - 2 \beta(z)$

$N = 10^2$, $N = 10^5$, $N = 10^3$
\[ z = \frac{n}{N} \]

\[ \varepsilon_0 = \min[\alpha(z) - 2\beta(z)] \]

\[ N = 10^2 \]

\[ N = 5 \times 10^4 \]