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COMMENT

Bounds to the extreme eigenvalues of the Lanczos Hamiltonian of a quantum system

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Abstract. The Lanczos method is an iterative scheme which when applied to the Hamiltonian H of a quantum system and starting from an initial vector (which is, in principle, an arbitrary vector of the associated Hilbert space) produces very good approximations to the eigenvalues at the extreme ends of the spectrum after a few iterations. In this comment we derive analytically a lower bound to the smallest eigenvalue and an upper bound to the largest eigenvalue of the Lanczos Hamiltonian of the system in terms of the expectation values of H evaluated at the initial vector.

The calculation of the lower bounds to the eigenvalues of the time-independent Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle, \tag{1}$$

where H is the Hamiltonian of the physical system under consideration, is not as easy as calculating the upper bounds. The latter can be readily and accurately obtained by means of the Rayleigh-Ritz variational method. However, several methods of obtaining the lower bounds have been derived (Bazley and Fox 1961, Hill 1980, Löwdin 1965).

Here we present a new, entirely different method which allows us to calculate the lower bounds to the smallest eigenvalue and the upper bounds to the largest eigenvalue of the Hamiltonian H projected onto a subspace of the Hilbert space of the system. The bounds are given by means of the expectation values of the Hamiltonian evaluated at an, in principle, arbitrary vector $|1\rangle$ of the Hilbert space. Therefore, the bounds are state dependent, thus the better the choice of the vector $|1\rangle$ the more accurate are the resulting bounds.

This problem, apart from its intrinsic interest, appears in applying the well known Lanczos method (Bullet *et al* 1980, Haydock 1976, Lanczos 1950, Mattis 1981, Schaeffer 1977, Whitehead *et al* 1977) to solve the eigenvalue problem (1). Up to now, only numerical algorithms to estimate the largest eigenvalue have been developed (Parlett *et al* 1982).

The Lanczos (1950) method defines a computational algorithm to diagonalise the Hamiltonian H of a quantum mechanical system very efficiently, especially if one is interested in the first few lowest-lying or the last few highest-lying eigenvalues and the corresponding eigenvectors. This method, widely applied in numerous branches of physics (Bullet *et al* 1980, Haydock 1976, Mattis 1981, Schaeffer 1977†, Whitehead *et*

† See especially the contribution of Roos, Haussman, Bender and Seigbahn.

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al 1977), starts from an initial vector $|1\rangle$ which is an arbitrary vector of the Hilbert space of the system, generates the sequence of vectors $\{|n\rangle;\ n=1,2,3,\ldots,N\}$ which is the so-called Lanczos' basis and converts the eigenvalue problem (1) into one of finding the eigensolutions of the so-called Lanczos Hamiltonian matrix H'.

The only non-vanishing entries of this N-dimensional real symmetric tridiagonal matrix are denoted by $H'_{n,n}=a_n$; $H'_{n,n+1}=b_n$. The matrix H' has the following property: the characteristic polynomials $\{P_n(E);\ n=0,1,\ldots,N\}$ of the principal submatrices satisfy the recursion relation

$$P_n(E)=(E-a_n)P_{n-1}(E)-b_{n-1}^2P_{n-2}(E)$$
$$P_{-1}(E)=0, \qquad P_0(E)=1, \qquad n=1,2,\ldots,N.$$

This recurrence implies that the polynomials $\{P_n(E)\}$ form (Dehesa 1978, 1981) an orthogonal set whose weight function is the spectral density $w_1(E)$ of the vector $|1\rangle$ with respect to the Hamiltonian of the system. This function $w_1(E)$ gives the distribution of the vector $|1\rangle$ among the eigenstates of the system; it is usually called the 'local density of states' in solid state theory (Bullet *et al* 1980, Haydock 1976) and the 'strength function' in nuclear physics (Whitehead *et al* 1977, 1980). For example, if $|1\rangle$ represents a single-particle state of a nucleus, then $w_1(E)$ gives in the nuclear shell model the spreading of the single-particle state among the exact shell model eigenstates. Often the quantity $w_1(E)$ can be experimentally measured and calculated by different analytical models.

Therefore the problem of calculating the eigenvalues of H' reduces to finding the zeros of the polynomials $P_n(E)$. As a trivial consequence the smallest and the largest eigenvalue of H' are the smallest and the largest zero of the polynomial $P_N(E)$. Then we are faced with the problem of determining a lower bound to the smallest zero and an upper bound to the largest zero of an orthogonal polynomial in terms of its weight function. Questions of this nature have received a lot of attention (Szegö 1975) for some particular systems of orthogonal polynomials (e.g. Jacobi, Hermite, Laguerre) but only recently have they been attacked for a general set of orthogonal polynomial (Costabile and Gautschi 1980)

Let the weight function $w_1(E)$ of the polynomials $\{P_n(E)\}$ have a finite or half-finite support $[a,b]$, $a<b\leqslant 0$, and such that all its moments around the origin are finite, i.e.

$$m_k=\int_a^b E^k w_1(E)\,\mathrm{d}E=\langle 1|H^k|1\rangle<\infty$$

for $k=0,1,2,\ldots$. Also, we assume that

$$E_1^{(n)}<E_2^{(n)}<\ldots<E_n^{(n)}<0$$

are the zeros of $P_n(E)$, where $E_i^{(n)}$, $i=1,2,\ldots,n$ denote the energies of the bound states of the physical system.

Following the lines of Costabile and Gautschi (1980) one readily finds that the zero $E_1^{(n)}$, which corresponds to the smallest eigenvalue of the Lanczos Hamiltonian of the system, is bounded from above by

$$E_1^{(n)}\leqslant \tau_{2n-1}-h_n/m_{2n-1}\leqslant \tau_{2n-2}, \qquad n>1 \tag{2}$$

where

$$\tau_k=m_{k+1}/m_k, \qquad k=0,1,2,\ldots$$

and

$$h_n = \int_a^b P_n^2(E) w_1(E)\, \mathrm{d}E. \tag{3}$$

It has been shown (Dehesa 1978) that h_n is equal to the norm of the member $|n+1\rangle$ of the Lanczos basis. Further (Dehesa 1978),

$$h_n = \langle n+1|n+1\rangle = D_n / D_{n-1}$$

where D_k denotes the determinant

$$D_k = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_k & \mu_{k+1} & \cdots & \mu_{2k} \end{vmatrix}.$$

Here the μ symbols denote the moments of $w_1(E)$ around the centroid $m_1 = \langle 1|H|1\rangle \equiv \langle H\rangle$, and are related to the moments around the origin by

$$\mu_r = \langle 1|(H - \langle H\rangle)^r|1\rangle = \sum_{j=0}^{r} \binom{r}{j} m_{r-j}(-m_1)^j.$$

On the other hand one can make a straightforward use of Costabile and Gautschi (1980) to obtain a lower bound to the largest eigenvalue $E_n^{(n)}$. For simplicity let us assume that the support of $w_1(E)$ is $[-a, 0]$, $a > 0$. Then it turns out that $E_n^{(n)}$ is bounded from below as follows

$$E_n^{(n)} > \tau'_{2n-1} - h'_n / m'_{2n-1} - a > \tau'_{2n-2} - a, \qquad n > 1 \tag{4}$$

where

$$m'_k = \int_0^a (x+a)^k w_1(x)\, \mathrm{d}x = \sum_{j=0}^{k} \binom{k}{j} a^{k-j} \int_{-a}^{0} x^j w_1(x)\, \mathrm{d}x$$

and

$$\tau'_k = m'_{k+1} / m'_k, \qquad k = 0, 1, 2, \ldots.$$

The h' quantities are defined as in (3) but with the integration interval $[-a, 0]$.

Usually the terms h_n / m_{2n-1} in (2) and h'_n / m'_{2n-1} in (4) are very small with respect to τ_{2n-1} and τ'_{2n-1} respectively. This allows us to avoid the calculation of the numerically badly behaved D objects. Therefore we suggest using the values τ_{2n-2} and $\tau'_{2n-2} - a$ as the upper bound to the energy $E_1^{(n)}$ of the deepest bound level and the lower bound to the energy $E_n^{(n)}$ of the least bounded level of the system (in the subspace under consideration) respectively.

Summarising, we have bounded the two most extreme bound energy levels of a quantum system which lie in the subspace expanded by the Lanczos basis generated from a vector $|1\rangle$ of the Hilbert space. The bounds are given in a simple way by means of the expectation values of the Hamiltonian operator evaluated at the vector $|1\rangle$.

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