Truncated space calculations of "exact" bound-state energies

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A method is developed for correcting truncated harmonic oscillator basis calculations of one-body bound-state energies for the omitted matrix elements of the kinetic energy operator. The method is only applicable when the potential energy operator is accurately represented in the truncated space. As an example of the method, the Hartree-Fock potential for the oxygen nucleus is considered with the Tabakin nucleon-nucleon potential. In a very large space this potential has only one bound s state, though solving the Schrödinger equation in coordinate space yields two. The method gives this second bound state's energy quite accurately.

[NUCLEAR STRUCTURE Approximate eigenvalues, infinite matrix, truncated basis.]

In many types of calculations it is convenient to use a representation of discrete basis states and instead of solving integral equations, diagonalize finite dimensional matrices. Naturally one only obtains, in this way, an approximation to the exact solutions. It will be shown here that, under certain conditions, it is possible to obtain an extremely accurate estimate of the difference between the approximate and exact solutions without resorting to the diagonalization of larger matrices.

The integrodifferential equations to be solved are typically of the form

$$-\frac{\hbar^2}{2m}\nabla^2\psi_\lambda(\vec{r})+\int d^3r' U(\vec{r},\vec{r}')\psi_\lambda(\vec{r}')=\epsilon_\lambda\psi_\lambda(\vec{r}), \tag{1}$$

Here U is the one-body potential, possibly nonlocal, which may be derived from some two-body interaction, as in Hartree-Fock calculations, or simply postulated.

The unknown wave function $\psi_\lambda(\vec{r})$ can be expanded in the set of harmonic oscillator states $\phi_\alpha(\vec{r})$,

$$\psi_\lambda(\vec{r})=\sum_\alpha C_\lambda^\alpha\phi_\alpha(\vec{r}). \tag{2}$$

Here α represents the quantum numbers $nljm$ and τ_z. It will be assumed that $\psi_\lambda(\vec{r})$ is a state of sharp ljm and τ_z, as could be the case for a spherically symmetric nucleus in a Hartree-Fock calculation, although this is not essential. Still, in principle, the sum should contain an infinite number of terms but in practice some truncated space of N states of each ljm and τ_z is considered.

The Schrödinger equation then becomes a set of N by N matrix equations, for each relevant ljm and τ_z, in the usual way:

$$\sum_{\alpha=1}^{N}\{\langle\beta|h|\alpha\rangle\}C_\lambda^\alpha=\epsilon_\lambda C_\lambda^\beta \quad (\beta=1,N), \tag{3}$$

where

$$\langle\alpha|h|\beta\rangle=\langle\alpha|t+U|\beta\rangle$$
$$=\int d^3r\phi_\beta^*(\vec{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\phi_\alpha(\vec{r})$$
$$+\int d^3r\int d^3r'\phi_\beta^*(\vec{r})U(\vec{r},\vec{r}')\phi_\alpha(\vec{r}').$$

Diagonalization of these matrices will yield sets of N eigenvalues and eigenfunctions, some of which will be bound (negative ϵ) and some unbound. The solutions of the full integrodifferential equation will also be divided into two classes, some finite (usually) number of bound states and a continuum of positive energy states. The problem considered here is that of finding the "exact" energies of these bound state solutions without leaving the N-dimensional spaces. In this way one may readily test whether or not a large enough space has been utilized, by calculating the difference between the bound state energies and the corresponding eigenvalues in the truncated space. Of particular importance in scattering calculations is a knowledge of just the *number* of bound states in a potential, for this determines the value of the phase shift at zero energy, assuming it is zero at infinite energy. This may not coincide with the number of negative ϵ states in an N-dimensional calculation, and an example where there is disagreement will be given.

The complete set of harmonic oscillator wave functions can be used to define two projection operators P and Q.[1] The first projects onto components in the N-dimensional space used in the matrix problem, while Q projects onto all other components:

$$P=\sum_{\alpha=1}^{N}|\alpha\rangle\langle\alpha|, \quad Q=\sum_{\alpha=N+1}^{\infty}|\alpha\rangle\langle\alpha|, \tag{4}$$
$$P+Q=1, \quad PP=P, \quad QQ=Q.$$

(There are, actually, P and Q operators for each space of states given by the same ljm and τ_z. Since the matrices do not connect these spaces, only one will be considered in order to simplify the notation.)

The full Schrödinger equation which should be solved instead of Eq. (3) is

$$\sum_{\alpha=1}^{\infty}\langle\beta|h|\alpha\rangle C_\lambda^\alpha=\epsilon_\lambda C_\lambda^\beta \quad (\beta=1,\infty), \tag{5}$$

whereas Eq. (3) can be rewritten as

$$\sum_{\alpha=1}^{N}\langle\beta|PhP|\alpha\rangle \tilde{C}_\lambda^\alpha=\tilde{\epsilon}_\lambda \tilde{C}_\lambda^\beta \quad (\beta=1,N). \tag{6}$$

Multiplying these equations by $|\beta\rangle$ and summing over all β gives

$$(h-\epsilon_\lambda)|\lambda\rangle=0 \tag{7}$$

as the exact equation and

$$(php-\tilde{\epsilon}_\lambda)|\tilde{\lambda}\rangle=0 \tag{8}$$

as the equation solved in the truncated spaces.

In many situations the matrix elements of the potential part of h decrease very rapidly with increasing n, the principle quantum number of the harmonic oscillator state. For a short range potential, for example, the matrix elements would be (approximately) proportional to $1/n!$ For a typical Hartree-Fock[2] potential, as is shown in Table I, the diagonal matrix elements fall off faster than $1/n$. Thus, if N is sufficiently large it is approximately true that

$$QUQ=PUQ=QUP=0; \tag{9}$$

in other words the potential has no nonzero matrix elements out of the space being considered. (In other applications these equations may be exactly satisfied, possibly by the definition of the appropriate U.) Given these properties of U one obtains from Eq. (7), by multiplying by P,

$$(\epsilon_\lambda-PhP)P|\lambda\rangle=PtQ|\lambda\rangle \tag{10}$$

and, by multiplying by Q,

$$(\epsilon_\lambda-QtQ)Q|\lambda\rangle=QtP|\lambda\rangle\,. \tag{11}$$

The last equation can be solved, formally, for $Q|\lambda\rangle$ and the result substituted into Eq. (10):

$$Q|\lambda\rangle=\frac{1}{\epsilon_\lambda-QtQ}QtP|\lambda\rangle\,, \tag{12}$$

$$(\epsilon_\lambda-PhP)P|\lambda\rangle=PtQ\frac{1}{\epsilon_\lambda-QtQ}QtP|\lambda\rangle\,. \tag{13}$$

At this point the advantage of using this particular basis becomes apparent. As is well known, the matrix elements of the kinetic energy operator in the harmonic oscillator representation vanish unless all quantum numbers except the principle quantum number n are the same in the bra and ket and the two principle quantum numbers must either be equal or differ by 1. Thus the only nonzero matrix elements of the kinetic energy are

$$\begin{aligned}\langle nljm\tau_z|t|nljm\tau_z\rangle &\equiv t_{nn}(l)=[2(n-1)+l+\tfrac{3}{2}]\hbar\omega\\ \langle nljm\tau_z|t|n+1ljm\tau_z\rangle &=\langle n+1ljm\tau_z|t|nljm\tau_z\rangle\\ &\equiv t_{n,n+1}(l)=[n(n+l+\tfrac{1}{2})]^{1/2}\hbar\omega\end{aligned} \tag{14}$$

where ω is the oscillator parameter.

Using this property, the right side of Eq. (13),

$$\sum_{\alpha\beta=1}^{N}\sum_{\gamma\delta=N+1}^{\infty}|\alpha\rangle\langle\alpha|t|\gamma\rangle\langle\gamma|\frac{1}{\epsilon_\lambda-QtQ}|\delta\rangle\langle\delta|t|\beta\rangle\langle\beta|\lambda\rangle,$$

TABLE I. The Hartree-Fock matrix in the harmonic oscillator representation (MeV). For those elements containing potential and kinetic energy contributions the potential matrix element is given in parentheses. It is, then, apparent that the potential is well represented in this truncated space. (The oscillator parameter used was $\hbar/m\omega=3.7$ fm^2.)

	1s	2s	3s	4s	5s	6s
1s	−42.75 (−51.16)	−15.07 (−21.93)	−7.92	−1.82	+0.62	+1.41
2s		−0.83 (−20.44)	−0.16 (−12.37)	−6.42	−2.87	−0.94
3s			+19.80 (−11.02)	+10.38 (−7.78)	−4.99	−2.81
4s				+35.34 (−6.69)	18.77 (−5.01)	−3.50
5s					49.08 (−4.14)	26.10 (−3.29)
6s						61.80 (−2.65)

becomes

$$|N\rangle t_{N,N+1}(l)\langle N+1|\,\frac{1}{\epsilon_\lambda - QtQ}\,|N+1\rangle t_{N,N+1}(l)\langle N|\lambda\rangle\,. \tag{15}$$

The needed matrix element of $(\epsilon_\lambda - QtQ)^{-1}$ can be evaluated by expanding $(\epsilon_\lambda - QtQ)^{-1}|N+1\rangle$ in a complete set of states, $|i\rangle$:

$$(\epsilon_\lambda - QtQ)^{-1}|N+1\rangle = \sum_i a_i |i\rangle\,. \tag{16}$$

Then

$$|N+1\rangle = \epsilon_\lambda \sum_{i=1}^{\infty} a_i |i\rangle - \sum_{i,j=N+1}^{\infty} a_i |j\rangle\langle j|t|i\rangle \tag{17}$$

and, for any state $|k\rangle$,

$$\delta_{k,N+1} = \epsilon_\lambda a_k - \sum_{i=N+1}^{\infty} a_i \langle k|t|i\rangle\,(1-\delta_{k,N}). \tag{18}$$

To obtain the desired matrix element it is necessary to determine only the coefficient a_{N+1}. This is, unfortunately, coupled to all the other a_i, with $i>N$, through the above set of equations:

$$\begin{aligned}
1 &= a_{N+1}(\epsilon_\lambda - t_{N+1,N+1}) - a_{N+2}t_{N+1,N+2}\,,\\
0 &= a_{N+2}(\epsilon_\lambda - t_{N+2,N+2}) - a_{N+1}t_{N+2,N+1} - a_{N+3}t_{N+2,N+3}\,,\\
0 &= a_{N+3}(\epsilon_\lambda - t_{N+3,N+3}) - a_{N+2}t_{N+3,N+2} - a_{N+4}t_{N+3,N+4}\,,\\
&\cdots\,.
\end{aligned} \tag{19}$$

One can obtain a sequence of approximate solutions for a_{N+1} by terminating this infinite set of equations at some point and setting the last a_i equal to zero. This sequence is

$$\begin{aligned}
a_{N+1}^{(0)} &= \frac{1}{\epsilon_\lambda - t_{N+1,N+1}}\,,\\
a_{N+1}^{(1)} &= \frac{1}{\epsilon_\lambda - t_{N+1,N+1} - \dfrac{t_{N+1,N+2}^2}{\epsilon_\lambda - t_{N+2,N+2}}}\,,\\
a_{N+1}^{(2)} &= \frac{1}{\epsilon_\lambda - t_{N+1,N+1} - \dfrac{t_{N+1,N+2}^2}{\epsilon_\lambda - t_{N+2,N+2} - \dfrac{t_{N+2,N+3}^2}{\epsilon_\lambda - t_{N+3,N+3}}}}\,.
\end{aligned} \tag{20}$$

This sequence converges quite rapidly for $\epsilon_\lambda \lesssim 0$, which is the region of interest, so that one may readily compute $a_{N+1}(\epsilon_\lambda)$ to arbitrary accuracy.

Equation (13) can now be written as

$$(\epsilon_\lambda - PhP)P|\lambda\rangle = |N\rangle t_{N,N+1}^2 a_{N+1}(\epsilon_\lambda)\langle N|\lambda\rangle \tag{21}$$

or, in matrix notation,

$$\sum_{\beta=1}^{N}\langle\alpha|(h+\Delta_N)|\beta\rangle\langle\beta|P\lambda\rangle = \epsilon_\lambda\langle\alpha|P\lambda\rangle\,,\quad \alpha=1,N \tag{22}$$

with

$$\langle\alpha|\Delta_N|\beta\rangle = \delta_{\alpha N}\delta_{\beta N} t_{N,N+1}^2 a_{N+1}(\epsilon_\lambda)\,. \tag{23}$$

This is not a simple eigenvalue problem because of the dependence of a_{N+1} on the eigenvalue. One method of solution is to form Δ_N for some ϵ_λ, diagonalize $h+\Delta_N$ and then vary the input ϵ_λ until an eigenvalue of $h+\Delta_N$ coincides with the input ϵ_λ. Since this only involves diagonalization of small matrices, the calculations can be carried out in a very short time. The accuracy of the resultant ϵ_λ's is determined by the accuracy of a_{N+1} and since the error in a_{N+1} can be made arbitrarily small, the negative energy eigenvalues of the infinite dimensional matrix can be determined, to any desired accuracy, in the N-dimension space.

The method will be applied here to the s-state Hartree-Fock matrix calculated for ^{16}O using the Tabakin nucleon-nucleon interaction.[3] The calculations were performed using six harmonic oscillator states for the s-state space and the resulting 6×6 Hartree-Fock matrix is shown in Table I. The eigenvalues of this matrix are given in Table II. Only the negative energy state, at -48.51 MeV, corresponds to an occupied orbital. The other eigenvalues are of use in numerous other types of calculations of such quantities as excited state spectra, perturbation corrections, etc. The fact that the second lowest eigenvalue has a positive value, $+1.22$ MeV, has been considered a deficiency of the Tabakin interaction. This manifests itself, in scattering calculations, in the difference between the phase shift at zero and infinite energy, which is, according to Levinson's theorem, equal to the number of bound states times π. It was, therefore, disturbing when this difference was actually calculated[4] and found to be 2π, rather than π.

To study this it was necessary to write a computer program to solve the bound-state Schrödinger equation. It was then found that, defining

$$U(\vec{r},\vec{r}') = \sum_{n,n'=1}^{6}\phi_n^*(\vec{r})\langle n|U|n'\rangle\phi_{n'}(\vec{r}')\,, \tag{24}$$

there were, in fact, two bound states. The ener-

TABLE II. Hartree-Fock eigenvalues (MeV). The fact that only one has negative energy does not mean there is only one bound state. In fact, there are two.

1s	2s	3s	4s	5s	6s
−48.51	+1.22	+9.62	+25.22	+50.38	+84.52

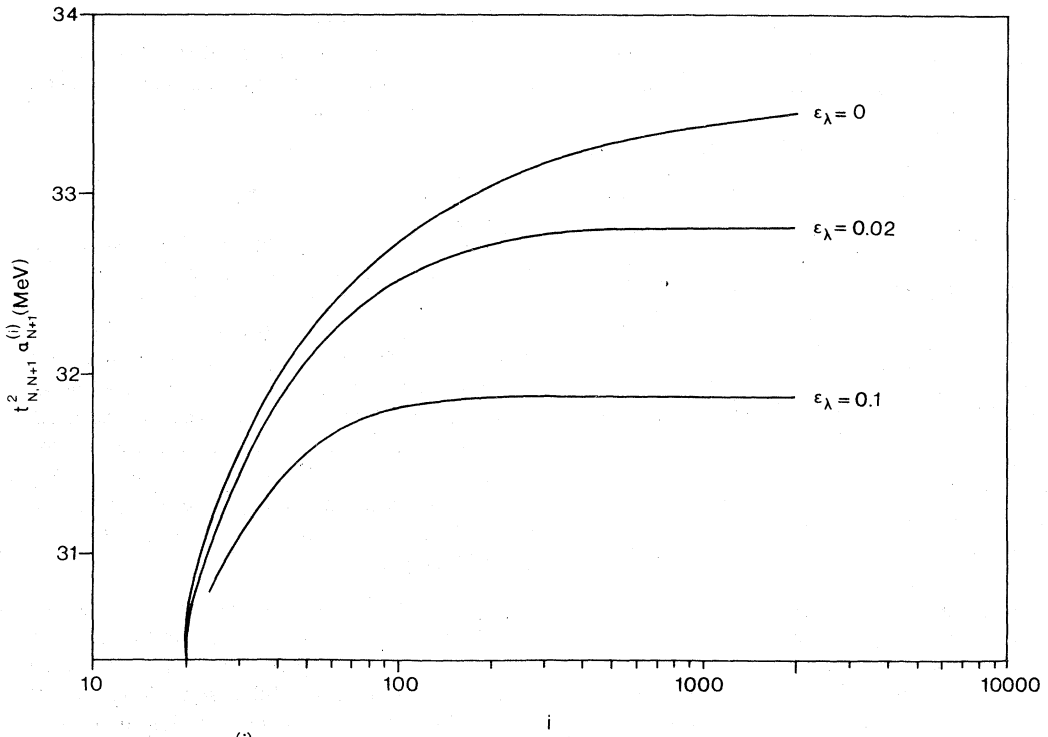

FIG. 1. The convergence of $a^{(i)}_{N+1}$. The continued fraction can be terminated at the ith term to obtain an approximation for a_{N+1}. The convergence is sufficiently rapid for any energy not positive because even the 5000th approximation can be calculated in a fraction of a second.

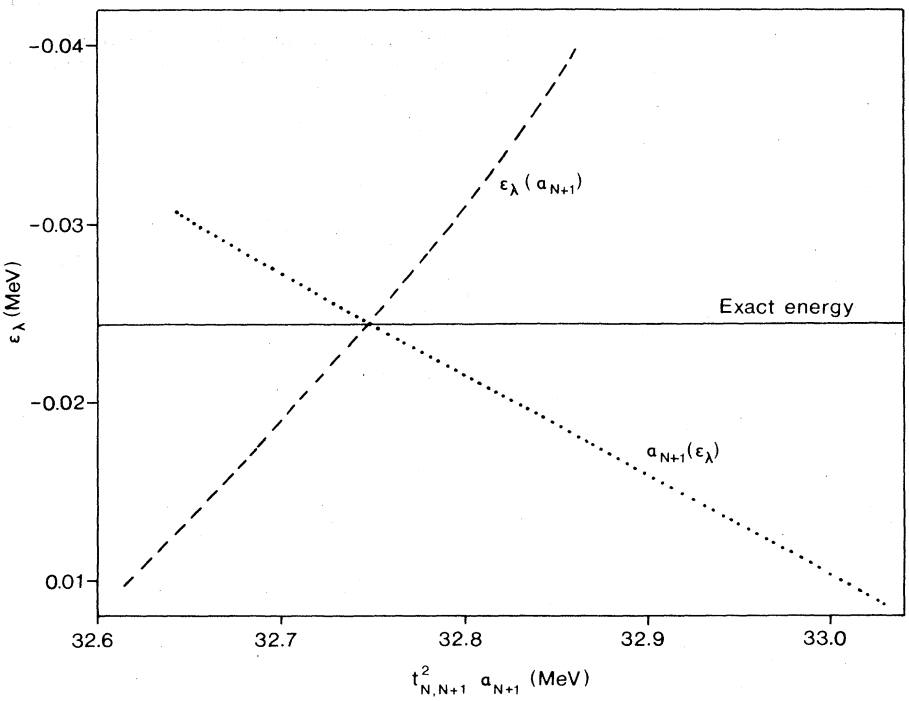

FIG. 2. Graphical solution of the non-linear matrix equation. The intersection of the dotted and dashed lines is at the energy of a true bound state, according to the method developed here. The solid line is drawn at the eigenenergy resulting from a numerical solution of the full Schrödinger equation. Any difference between the exact and approximate energy can be reduced by using more terms in the calculation of a_{N+1}. The error for the case shown above is less than $\frac{1}{10}$ of 1%.

gies of these states were found to be −48.514 and −0.0244 MeV, so that the lowest energy was very well approximated in the 6×6 space but the second lowest was not.

Thus the quantity $t^2_{N,N+1}a^{(i)}_{N+1}$ was calculated, for various values of ϵ_λ, for i large enough to obtain convergence. The results are shown in Fig. 1 for three values of ϵ_λ. The slowest convergence is for the case $\epsilon_\lambda = 0$ but since the evaluation, even for $i = 4000$, takes only fractions of a second this presents no problem. For $\epsilon_\lambda = -48$, on the other hand, a_{N+1} is determined to within one part in a million with just $i = 20$. With these various estimates of Δ_N, the matrix $h+\Delta_N$ is diagonalized in the 6×6 space. One then plots the resulting eigenvalue as a function of a_{N+1} and on the same graph plots the a_{N+1} as a function of the input ϵ_λ. The intersection of these two curves represents the value of ϵ_λ for which the input to a_{N+1} will match the eigenvalue of $h+\Delta_N$. This plot is shown in Fig. 2 along with the exact solution of the Schrödinger equation. As is apparent from the figure, the method reproduces the exact energy −0.0244 MeV quite well. The lowest s-state energy was also well reproduced by the method and agrees with the 6×6 answer.

The method was also tested for the p-state and d-state Hartree-Fock matrices and it works equally well in those cases.

Summary

A method has been suggested for obtaining the "exact" negative eigenvalues of an infinitely dimensioned matrix in a truncated basis. The only requirement for applicability is that the full matrix differ from the truncated matrix by a tridiagonal matrix, at most. As an example, the bound states in a Hartree-Fock potential were calculated using the method and they coincided quite precisely with the eigenvalues of the full Schrödinger equation. In addition to the accuracy of the results, the method has the advantage of only involving small computations.

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