

A Study of Some Approximation Schemes in Quantum Mechanics*

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By means of numerical examples in one dimensional Hamiltonian problems, we study the behavior of the approximation scheme known as the New Tamm-Dancoff method. It is concluded that for good convergence of this, and other related methods, one should arrange to start with a symmetric set of equations.

INTRODUCTION

It has long been an outstanding problem to achieve effective solutions to the dynamical equations of quantum field theory and the non-relativistic many-body problem away from the limit of weak couplings. We here close our eyes to some famous and formidable difficulties in these theories (infrared and ultraviolet divergences, etc.) and simply consider how we might effectively calculate numbers when perturbation theory is not an acceptable answer. We have in mind that one will need to make good use of modern computing machines, but some appropriate analytical preparations must come first. For while one may expect to be able to handle several coupled integro-differential equations in several variables, the equations of interest are infinite in extent and the number of independent variables is likewise unlimited.

The general line of approximation we wish to study may be called the N -particle scheme. In quantum field theory we are referring to the Tamm-Dancoff approximation, in both its old form (OTD) and its new (NTD). In this paper we strip away many complicating aspects of the real problems and look at simple one-dimensional Hamiltonian problems. The question we wish to study is whether these above mentioned schemes do converge nicely to the correct answers as the order of approximation, N , is systematically advanced.

METHODS

The general problem is: given a Hamiltonian \mathcal{H} , defined in some Hilbert space, we want to find its spectrum (assumed discrete)

$$\mathcal{H} | \alpha \rangle = E_\alpha | \alpha \rangle, \quad \langle \alpha | \beta \rangle = \delta_{\alpha\beta}. \quad (1)$$

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Method I: This is the conventional variational approximation technique, which for field theory problems may be called the old Tamm-Dancoff (OTD) method. Take N members of some arbitrary complete (not necessarily orthonormal) set of basis vectors in the Hilbert space of \mathcal{H} ,

$$|i\rangle, \quad i = 1, 2, \dots, N \quad (2)$$

and construct the $N \times N$ matrix representation of (1).

$$\| \mathcal{H}C_{ij} - EI_{ij} \| = 0 \quad (3)$$

$$i, j = 1, 2, \dots, N,$$

$$\mathcal{H}C_{ij} = \langle i | \mathcal{H} | j \rangle, \quad I_{ij} = \langle i | j \rangle. \quad (4)$$

One then solves (3) numerically for the eigenvalue $E(N)$; and the question at hand is, "How rapidly does this sequence of approximate eigenvalues—arrived at by systematically increasing the set (2)—converge to the true value E_α ?"

Method II: The so-called New Tamm-Dancoff (NTD) method, invented by Dyson (1), is characterized by the fact that attention is focused not on a single eigenvalue of \mathcal{H} , but rather on the difference of some pair of these eigenvalues. (In quantum field theory the energy of every state has an infinite added constant, attributed to the infinite spatial domain of the vacuum, and this causes serious difficulties in the OTD method.)

Take some complete set of operators Θ_i which are functions of the operators appearing in \mathcal{H} (these were chosen by Dyson as ordered products of annihilation and creation operators of the field). Define as the variables of interest the set of matrix elements of these Θ_i between some chosen pair of eigenstates of \mathcal{H} .

$$A_i^{\alpha\beta} \equiv \langle \alpha | \Theta_i | \beta \rangle. \quad (5)$$

Now consider the commutator of Θ_i with \mathcal{H} :

$$[\Theta_i, \mathcal{H}] = \sum_j S_{ij} \Theta_j \quad (6)$$

where the expansion on the right, characterized by the numbers S_{ij} , is supposed to exist because the Θ_i are a complete set. Now taking the α, β matrix element of (6) we get the infinite set of coupled equations for the amplitudes A_i , (suppressing the labels α, β)

$$\Delta A_i = \sum_j S_{ij} A_j \quad (7)$$

where $\Delta \equiv E_\beta - E_\alpha$ is the "eigenvalue" being sought. While the system of equations (7) is less familiar than (3) it looks no more complicated at first glance; the important question is, "Can we find an accurate approximation scheme for reducing this infinite set of equations to some manageable size?". This question was considered by Symanzik (2) and, while he reached no definitive conclusion,

he suggested that the NTD method might have serious difficulty due to the following observation. The matrix (3) is symmetric (Hermitian) and this insures the convergence of the Ritz procedure; but if one solves (7) by successive truncations (set all $A_i = 0$ for $i > N$ and keep only the first N equations), the resulting $N \times N$ matrix S_{ij} is not symmetric and one knows nothing in general about the convergence of the computed results $\Delta(N)$ as N is increased.

In this paper we shall study, by simple numerical examples, just this question of the importance of the symmetry of truncated sets of infinite coupled equations. To this purpose we shall also define the following modifications of methods I and II.

Method I': We proceed much as in Method I but force the equations to become nonsymmetrical. Assume an expansion of the exact state in terms of the chosen basis

$$|\alpha\rangle = \sum_i C_i |i\rangle; \quad (8)$$

then insert this into the Schrödinger equation, multiply from the left by some function or operator W , then contract with one of the basis vectors to obtain

$$\sum_j (B_{ij} - EW_{ij})C_j = 0 \quad (9)$$

where

$$W_{ij} = \langle i | W | j \rangle \quad (10)$$

might easily be a symmetric matrix, but

$$B_{ij} = \langle i | WH | j \rangle \quad (11)$$

will not be symmetric, excepting a trivial choice of W .

Method II': We seek some special set of operators \mathcal{O}_i such that the matrix S_{ij} is symmetric.

EXAMPLES: METHOD I

We take as the object of study for almost all of our examples the one dimensional nonlinear oscillator

$$\mathcal{H} = \frac{p^2}{2} + \frac{x^4}{4}, \quad [p, x] = -i. \quad (12)$$

Parameters for the mass and coupling strength may be removed by appropriate scaling of length and energy, and we take (12) as our standard form. The basis for our solution will be in terms of the harmonic oscillator

$$\mathcal{H}_0 = \frac{p^2}{2} + \omega^2 \frac{x^2}{2} = \omega \left(a^+ a + \frac{1}{2} \right) \quad (13)$$

where

$$\begin{aligned} a &= (\omega/2)^{1/2}(x + ip/\omega) \\ a^+ &= (\omega/2)^{1/2}(x - ip/\omega) \\ [a, a^+] &= 1 \end{aligned} \quad (14)$$

and ω is some parameter to be determined.

The simplest variational calculation is to just use a single eigenstate of \mathcal{H}_0 and get a best fit to the corresponding state of \mathcal{H} by varying ω . For the ground state this yields

$$\begin{aligned} \omega &= (3/2)^{1/3} \\ E(0) &= \frac{3}{8}\omega; \end{aligned} \quad (15)$$

and in the subsequent calculations we keep ω fixed at this value and give the energy in units of $E(0)$:

$$E = \epsilon \frac{3}{8}\omega. \quad (16)$$

The required matrix elements are

$$\begin{aligned} \left\langle n \left| \frac{p^2}{2} \right| n \right\rangle &= \frac{2}{3} (2n + 1) \\ \left\langle n \left| \frac{x^4}{4} \right| n \right\rangle &= \frac{1}{3} (2n^2 + 2n + 1) \\ \left\langle n - 2 \left| \frac{p^2}{2} \right| n \right\rangle &= -\frac{2}{3} [n(n - 1)]^{1/2} \\ \left\langle n - 2 \left| \frac{x^4}{4} \right| n \right\rangle &= \frac{2}{9} (2n - 1)[n(n - 1)]^{1/2} \\ \left\langle n - 4 \left| \frac{x^4}{4} \right| n \right\rangle &= \frac{1}{9} [n(n - 1)(n - 2)(n - 3)]^{1/2}; \end{aligned} \quad (17)$$

and the solution of the matrix eigenvalue problem (3) is easily done by machine, yielding the results shown in Table I, for the ground state. The results obviously converge exceedingly fast. Similar calculations for the first and second excited states converged only slightly slower; the resulting values are

$$\begin{aligned} \epsilon_0 &= 0.98028535 \\ \epsilon_1 &= 3.5127282 \\ \epsilon_2 &= 6.892655, \end{aligned} \quad (18)$$

which we believe approximate the exact eigenvalues to the number of figures given.

(It may be of interest to compare these results with the WKB approximation. For the Hamiltonian

$$\mathcal{H}(l) = \frac{p^2}{2} + \frac{|x|^l}{l} \tag{19}$$

we get the WKB approximation for the energy of the n th quantum state

$$E_n(l) = [(n + \frac{1}{2})/\Lambda(l)]^{(2l/(l+2))} \tag{20}$$

$$\Lambda(l) = \frac{(8)^{1/2}}{\pi} l^{1/l} \int_0^1 dy (1 - y^l)^{1/2}, \tag{21}$$

which is the exact answer for $l = 2$ (harmonic oscillator). For $l = 4$ this gives the following numbers to be compared with (18): 0.80, 3.46, 6.86; and the indication is that WKB becomes very good away from the ground state.)

In conclusion we state that the convergence of Method I is generally known to be good, and in Table I we see how very good it is for this particular problem.

EXAMPLES: METHOD II

We shall attack the Hamiltonian (12) by the NTD method as originally conceived by Dyson, defining amplitudes

$$A_{m,n} = \langle \alpha | a^{+m} a^n | \beta \rangle. \tag{22}$$

$$m, n = 0, 1, 2, \dots$$

We shall use the operators a and a^+ defined by (14) with ω arbitrarily fixed at the value given in (15). It takes a fair amount of algebra to compute the matrix

TABLE I
 LOWEST EIGENVALUE OF (12) BY METHOD I

Maximum $n/2$	Size of matrix	ϵ_0	Error
0	1	1.00000000	1.97×10^{-2}
1	2	1.00000000	1.97×10^{-2}
2	3	0.98283858	2.55×10^{-3}
3	4	0.98037067	8.53×10^{-5}
4	5	0.98036642	8.10×10^{-5}
5	6	0.98030926	2.39×10^{-5}
6	7	0.98028737	1.98×10^{-6}
7	8	0.98028556	2.1×10^{-7}
8	9	0.98028555	2.0×10^{-7}
9	10	0.98028547	1.2×10^{-7}
10	11	0.98028540	$5. \times 10^{-8}$
11	12	0.98028536	$1. \times 10^{-8}$
12	13	0.98028535	—
13	14	0.98028535	—

S of (6), and we give here the resulting equation (7), using the abbreviation

$$(ij) = A_{m+i, n+j}, \quad (23)$$

$$\begin{aligned} & [-\frac{3}{2}\Delta + (n-m)(n+m+3)](00) + n(n-1)[2(1-1) + (2-2)] \\ & - m(m-1)[2(-1+1) + (-2+2)] \\ & + \frac{2}{3}n(n-1)(n-2)[(0-2) + (1-3)] \\ & - \frac{2}{3}m(m-1)(m-2)[(-20) + (-3+1)] \\ & + \frac{1}{6}n(n-1)(n-2)(n-3)(0-4) \\ & - \frac{1}{6}m(m-1)(m-2)(m-3)(-40) + \frac{2}{3}n(3-1) - \frac{2}{3}m(-1+3) \\ & + \frac{2}{3}(3n-m)(20) - \frac{2}{3}(3m-n)(0+2) + 2(n-m)(1+1) = 0 \end{aligned} \quad (24)$$

where

$$\Delta = (E_\beta - E_\alpha)/(3\omega/8)$$

is the difference of eigenvalues in the units (16).

This is an obviously complicated, nonsymmetrical recursion formula coupling sixteen terms mapped over a two-dimensional grid (m, n) . It is however still very simple to let the computer find eigenvalues Δ , once we fix a scheme for truncating the equations to finite (and not *too* big) size. We tried two schemes: keep only all amplitudes $A_{m,n}$ and corresponding equations (24) such that

$$(a) \quad m + n \leq 2L + 1 \quad L = 0, 1, 2, \dots \quad (\text{triangular}) \quad (25a)$$

$$(b) \quad m \leq L + 1 \quad \text{and} \quad n \leq L + 1 \quad L = 0, 1, 2, \dots \quad (\text{square}) \quad (25b).$$

We shall be looking only at the first interval, between the ground and first excited states, and the parity selection rule limits us to $m + n$ odd. The numerical results are shown jointly in Fig. 1, and the arrow there indicates the true value (from (18)).

The apparent conclusion is that Method II is very bad. Below $L = 7$ there seems to be fairly regular oscillation, with scheme (a) sort of converging and scheme (b) sort of diverging; but this is only a transient phenomenon since the points further to the right look more erratic. The best point (scheme (a) at $L = 6$) is in error by only one seventh of one per cent—but this must be considered a lucky accident; and after the first few points all the scheme (a) values err by no more than 2%—due perhaps to the propitious scaling given by the chosen value of ω . However there is clearly not any “good convergence” to be seen here (particularly when compared to the seven place accuracy achieved at the comparable stage of Method I); and we feel that Symanzik’s (2) conjecture has been realized true for this problem.

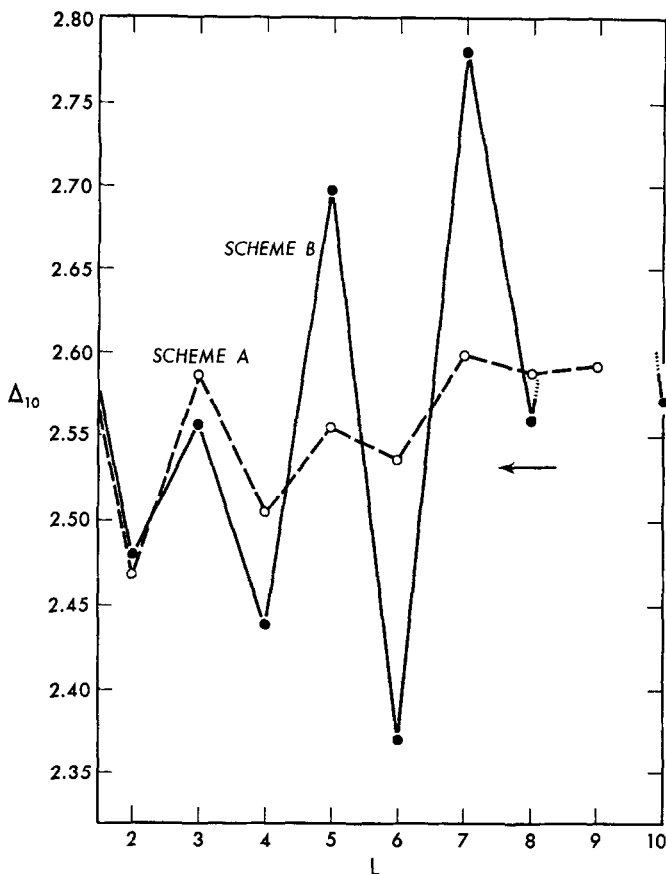


FIG. 1. Results of Method II (unsymmetrical NTD) for the lowest eigenvalue interval of the Hamiltonian (12). The arrow indicates the correct answer. We were unable to find the eigenvalue for scheme (b) at $L = 9$.

Even if the results of these calculations had converged reasonably well (as we shall make them do later), it is not likely that we would suggest Method II as a practical way to solve one-dimensional eigenvalue problems. Note that the matrix size, for the L th approximation in Method I was $L + 1$, while in Method II it is $(L + 1)(L + 2)$ for scheme (a) and $\frac{1}{2}(L + 2)^2$ for scheme (b). Thus the last scheme (a) point in Fig. 1 came from a matrix of dimension 110 which had to be manipulated in double precision arithmetic in order to give meaningful results; this was a more than trivial computer job. There is, in going from Method I to Method II, a doubling of the variables which seems unnecessary for simple quantum mechanical problems (the infinite set of equations (3) will yield the

singly infinite set of eigenvalues E_α while (7) will yield the doubly infinite set $E_\alpha - E_\beta$). However, in the realm of field theory, with its already numerous degrees of freedom, this deficiency may not be noticed; we should concentrate simply on the question of convergence, yes or no.

EXAMPLES: METHOD I'

We first studied the same Hamiltonian and basis as was used in the example for Method I, inserting for the weight function the positive operator

$$W = (a + a^+)^2. \quad (26)$$

The nonsymmetric eigenvalue problem (9) was solved in 30 successive approximations, and the results are shown in Fig. 2. Our conclusion is clearly: bad convergence behavior.

One might suggest that the poor behavior is not due to the symmetry problem,

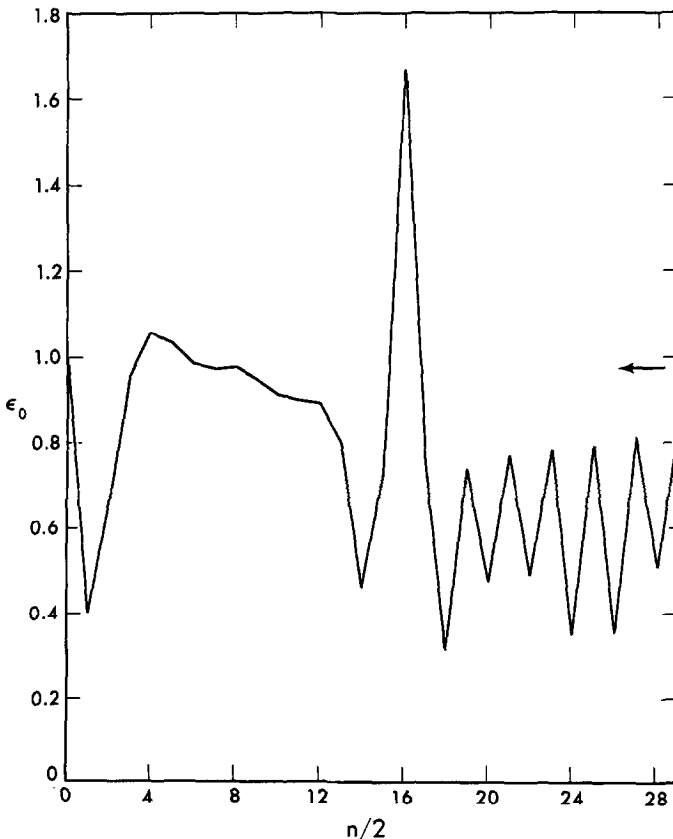


Fig. 2. Results of Method I' (unsymmetrized OTD) for the lowest eigenvalue of (12) using the weight function $W = x^2$. The arrow indicates the correct answer.

but rather to the fact that our weight function W vanishes at the origin (in the x -representation) and thus "wipes out" an important region of space for the determination of a good wave function. In order to overcome this objection we repeated the calculation with

$$W = 1 + (a + a^+)^2. \tag{27}$$

These results are shown in Fig. 3; and while the long wiggly tail is seen to stay much closer to the true value (about 1% off) than it did before (about 40% off), the convergence rate is still something painfully slow.

A second example of Method I' was also studied. The Hamiltonian here was the radial equation for s -waves in a Yukawa potential,

$$\mathcal{H} = -\frac{d^2}{dr^2} - g \frac{e^{-r}}{r}, \tag{28}$$

$$0 \leq r < \infty,$$

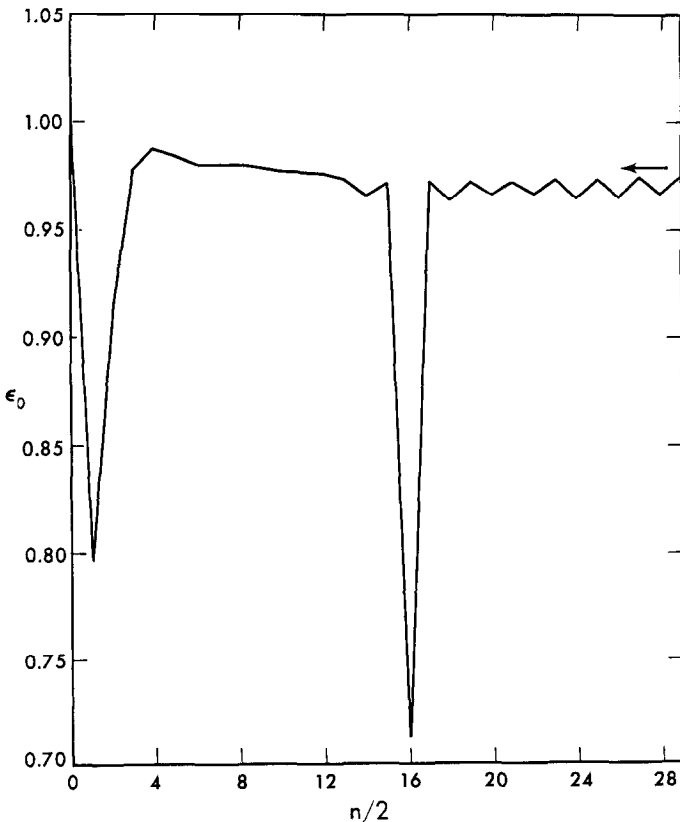


FIG. 3. Results of Method I' (unsymmetrized OTD) for the lowest eigenvalue of (12) using the weight function $W = x^2 + 1/(2\omega)$. The arrow indicates the correct answer.

with the boundary condition on the eigenfunction

$$u(0) = u(\infty) = 0.$$

The basis functions used for the calculation were chosen as the exponential-weighted Laguerre polynomials which satisfy the eigenvalue equation

$$\left(-\frac{d^2}{dr^2} + k^2\right)u_n = 2k(n+1)\frac{1}{r}u_n \quad (29)$$

and are orthonormal with respect to integrals with the weight function $1/r$. We considered the energy as fixed, $E = -k^2$, and then searched for the eigenvalue of the coupling parameter g . We calculated through 15 orders of approximation by Method I (for $k = 1/2$), and through 25 orders of Method I' using $W = 1/r$.¹ The two sets of results converged well at very nearly the same rate: the error decreasing by about a factor of two with each step. It was interesting to note that while $g(I)$ approached the true value (2.769226) monotonically from above, $g(I')$ approached at almost the same distance monotonically from below.

Thus we conclude that while Method I' (unsymmetrized Ritz variational procedure) *may*, as per our first example, be much worse than Method I (usual symmetric Ritz), it also *may*, as per our second example, prove to be just as good.

EXAMPLES: METHOD II'

Let us start by trying to guess why Method II (the New Tamm-Dancoff method) did not work. We will consider the variables p and x , which are just linear combinations of the operators a and a^+ used above. It is not hard to see that the truncation approximation,

$$A_i = 0 \quad \text{for } i > \text{some maximum,}$$

is absurd. (We are now considering the amplitudes

$$A_{mn} = \langle \alpha | p^m x^n | \beta \rangle \quad (30)$$

and let the index i stand for the pair of labels m, n .) For, thinking of the integral (30) in the x representation, we readily see that these amplitudes get *larger* as the indices m or n increase. What sort of operator functions \mathcal{O}_i can we think of whose matrix elements would *decrease* as we increased the index? Our answer, for functions rather than operators, would be a set of oscillating functions whose wavelengths get shorter as the index increases. (It is in this manner that we explain the good convergence of Method I.) We shall thus investigate the following

¹ This calculation may be seen as a prototype of the method used by Rotenberg (β) in his study of a three-body problem.

structure

$$\begin{aligned} \mathcal{O}_i &= u_m(p)v_n(x), \\ i &= (m, n) \end{aligned} \tag{31}$$

where u and v are some complete sets of functions, probably orthonormal in some sense to be determined.

Now let us see if we can make the matrix S_{ij} of (7) symmetric. We suppose that the Hamiltonian is a Hermitian operator built out of powers of p and x . The general term in the commutator (6) looks like

$$\begin{aligned} [u_m(p)v_n(x), p^s x^t] &= p^s [u_m(p), x^t] v_n(x) + u_m(p) [v_n(x), p^s] x^t \\ &= \sum_{\nu} \binom{s}{\nu} u_m(p) p^{s-\nu} x^t \left[\left(i \frac{\partial}{\partial x} \right)^{\nu} v_n(x) \right] \\ &\quad - \sum_{\mu} \binom{t}{\mu} p^s \left[\left(i \frac{\partial}{\partial p} \right)^{\mu} u_m(p) \right] x^{t-\mu} v_n(x); \end{aligned} \tag{32}$$

and we wish to re-express these terms as

$$\sum_{m'n'} S_{mn,m'n'} u_{m'}(p) v_{n'}(x) \tag{33}$$

with S a Hermitian matrix. This may clearly be achieved by choosing u and v to be orthonormal functions of the type $f(\xi)$, where the operators

$$\text{“multiply by } \xi \text{”} \tag{34}$$

$$\text{and } \pi = -i \frac{\partial}{\partial \xi} \tag{34}$$

are Hermitian. Equivalently we require

$$\int_a^b f_{n'}^*(\xi) f_n(\xi) d\xi = \delta_{nn'}$$

and

$$f_{n'}^*(b) f_n(b) - f_{n'}^*(a) f_n(a) = 0. \tag{35}$$

The variables p and x are real, with the range $-\infty$ to $+\infty$, and so we choose Hermite polynomials times a Gaussian as an appropriate basis.

$v_n(x) \rightarrow |n\rangle$: n th eigenstate of harmonic oscillator in ξ with frequency ω ,

$u_m(p) \rightarrow$ Fourier transform of the same thing with frequency ω' . (36)

$$m, n = 0, 1, 2, \dots$$

For the Hamiltonian (12) we then get the NTD equations (7)

$$\Delta A_{mn} = \sum_{m'n'} S_{mn,m'n'} A_{m'n'} \tag{37}$$

where we now have the *symmetric* matrix

$$\begin{aligned} S_{mn,m'n'} = & -\frac{1}{2} \langle m' | m \rangle \langle n' | \pi^2 | n \rangle + \omega' \langle m' | \xi | m \rangle \langle n' | \pi | n \rangle \\ & + \frac{1}{4\omega'^4} \langle m' | \pi^4 | m \rangle \langle n' | n \rangle - \frac{1}{\omega'^3} \langle m' | \pi^3 | m \rangle \langle n' | \xi | n \rangle \\ & + \frac{3}{2\omega'^2} \langle m' | \pi^2 | m \rangle \langle n' | \xi^2 | n \rangle - \frac{1}{\omega'} \langle m' | \pi | m \rangle \langle n' | \xi^3 | n \rangle. \end{aligned} \tag{38}$$

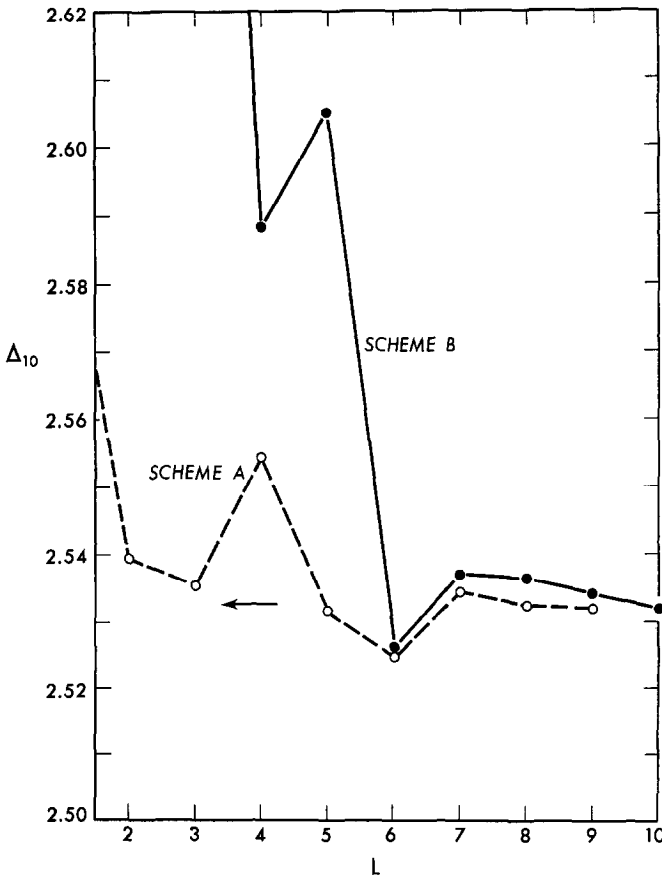


FIG. 4. Results of Method II' (symmetrized NTD) for the lowest eigenvalue interval of (12). The arrow indicates the correct answer. Compare with Fig. 1, noting change of scale of the ordinate.

We set $\omega = \omega' = (3/2)^{1/3}$ and let the machine grind out solutions. The results are shown in Fig. 4 for the same two truncation schemes (25) as were used for the nonsymmetrical Method II. The convergence looks fairly good (for as far as we have gone in the calculations). The rate of convergence is still a lot less than with Method I; but there is a vast improvement over the useless results of Method II. We have not tried to see if these results can be markedly improved by another choice of the scale parameters ω, ω' ; it seems sufficient that we have seen a significant gain upon transforming the NTD equations to a symmetric form.

In addition to the Hermiticity of \mathcal{H} , another feature which sometimes improves the convergence of the Ritz method is the fact that \mathcal{H} has a lower limit to its spectrum. The eigenvalue Δ of the NTD equations, on the other hand, clearly ranges from $+\infty$ to $-\infty$. It is possible to construct a second order NTD method by taking the commutator with \mathcal{H} twice. The resulting equations look like

$$\Delta^2 A_i = \sum_j T_{ij} A_j$$

where Δ^2 is clearly ≥ 0 , and the matrix $T = S^2$ now has all the nice properties of a Hamiltonian, if we have symmetrized S . We have made a quick try at this extension of the above calculations. The resulting eigenvalues do approach the correct value monotonically, to be compared with the points in Fig. 4, which oscillate. However, the magnitudes of the errors were much greater, and the method seemed too cumbersome to warrant closer study at this time.

CONCLUSIONS

Our chief interest is the validity of the Proposition: If one has an infinite system of equations to be solved by a sequence of truncations, then to insure (or at least to encourage) a good convergence of these approximations toward the true answer one should start with a symmetric system. Alternatively, one could say the approximations must follow from some variational principle.

Let us now review the results of the preceding numerical examples to see just how firmly this proposition has been supported.

Showing good results from symmetric systems:

Method I —definitely yes

Method II'—yes; certainly improved over Method II, but nowhere as good as Method I.

Showing bad results from nonsymmetrical systems:

Method II—yes

Method I'—yes, for first example; but definitely no, for the second (Yukawa potential problem).

We conclude that the evidence does not yield a resounding affirmation of the Proposition, but it does definitely point favorably in that direction. It should be

clear to the reader that our study has been very "experimental" in character; we cannot "prove" a proposition by numerical examples, and we would be happy to have any rigorous analysis possible for the elucidation of our questions. The problems we are really interested in solving are not simple one-dimensional Schrödinger equations, but the much more complex systems of field theory and many-body interactions. It is certainly a big step from the simple examples of this paper to those real problems, but we believe this principle of seeking a symmetric system of equations may prove to be useful.

APPENDIX

We shall show here how one may go from the NTD method back to the familiar Schrödinger equation. Recalling our earlier comments about the NTD method requiring twice the number of variables, let us see what happens when we try to work in only one variable, say x . Define the amplitudes

$$A_\alpha = \langle B | Q(x) | \alpha \rangle \quad (\text{A.1})$$

for some set of functionals $Q(x)$, between eigenfunctions of the given Hamiltonian

$$\mathcal{H} | \alpha \rangle = E_\alpha | \alpha \rangle \quad (\text{A.2})$$

$$\mathcal{H} = \frac{p^2}{2} + V(x). \quad (\text{A.3})$$

Taking the commutator with \mathcal{H} we get

$$(E_\beta - E_\alpha)A_\alpha = -\frac{i}{2} \langle \beta | pQ' + Q'p | \alpha \rangle \quad (\text{A.4})$$

which, because of the p operators, is a completely new quantity, not contained in the set of A_α . In order to remove the p 's, we take a second commutator with \mathcal{H} , rearrange the terms so that only p^2 appears, and then replace it by $2(\mathcal{H} - V)$, to arrive at

$$(E_\beta - E_\alpha)^2 A_\alpha = \langle \beta | \mathcal{F}(Q) | \alpha \rangle \quad (\text{A.5})$$

where the functional \mathcal{F} is given by

$$\mathcal{F}(Q) = -\frac{1}{4}Q'''' + (2V - E_\alpha - E_\beta)Q'' + V'Q'. \quad (\text{A.6})$$

We have eliminated the second variable from the NTD equations; and we now remove the corollary excess of eigenvalues ($E_\beta - E_\alpha$) by limiting our attention to the states $\alpha = \beta$. The left side of (A.5) is then zero, and so we set

$$\mathcal{F} = 0. \quad (\text{A.7})$$

One would like to recover from (A.7) the familiar Schrödinger equation,

$$-\frac{1}{2}\psi_\alpha''(x) + (V(x) - E_\alpha)\psi_\alpha(x) = 0; \quad (\text{A.8})$$

and indeed this may be done with the identification

$$Q(x) = \int^x dy \psi_\alpha^2(y). \quad (\text{A.9})$$

One can similarly see that choosing some fixed set of basis functions for the Q 's, Eq. (A.7) will be recognized as the equations of the OTD method.

We have not been able to extend this trick for Hamiltonians more general than the one-dimensional form (A.3).

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