Anharmonic-oscillator energies with operator recursion mechanics*

C. A. Uzes
Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602
(Received 8 April 1976)

The procedure of the new Tamm-Dancoff method of Heisenberg *et al.* is considered in the context of the nonlinear oscillator. Recurrence equations which result from the operator algebra and equation of motion of the oscillator's displacement operator are converted into a meaningful characteristic energy eigenvalue problem via an infinite-dimensional basis transformation of the form SAT, where A is a matrix representing the recursion equation and where S is not the inverse of T. This procedure, appropriate to the situation where the recursive matrix A is not orthogonal or Hermitian, is numerically seen to lead to convergent approximation sequences for energy eigenvalues for several nonlinear oscillators. The matrix elements of SAT are defined by summable but nonconvergent infinite series. In each order of approximation eigenvalues exist which are locally independent of the single parameter upon which S and T depend, a fact which implies that this recursive method belongs to an as yet not defined variational principle. As the approximation order is increased the eigenvalues are numerically seen to converge to the proper limits for several different oscillators, the convergence being independent of the parameter.

I. INTRODUCTION

The equation of motion and quantum conditions imposed on the displacement operators of a system can be used to construct recursion relations for the operator products. In principle both spectral and scattering information can be obtained by analyzing the different matrix elements of these equations. Of concern here is the spectral problem, which is solved in practice by converting the recursive set into a meaningful set of characteristic equations. This nonperturbative approach was first developed by Heisenberg *et al.*[1,2] for use in the nonlinear spinor theory—the new Tamm-Dancoff (NTD) method. From a practical point of view the technique, suitably modified, is also of interest to other areas of physics, particularly in solid-state and particle field theories. The purpose of the present paper is to clarify some of the ground rules that should be considered in using NTD-type recursive methods.

The anharmonic oscillator serves as a convenient model through which the methods can be analyzed. The essence of the eigenvalue problem is not lost in this simple model, but other unrelated difficulties are avoided. As first shown by Stumpf, Wagner, and Wahl[3] for the quartic oscillator, the differential equation of motion and Hamiltonian lead to a recursive set which can be represented in the matrix form

$$A(E,\omega)\vec{\tau}=0, \tag{1}$$

where $A(E,\omega)$, $\omega=(E'-E)/\hbar$, is an infinite matrix and the components of the vector $\vec{\tau}$,

$$\tau^l=\langle E|Q^l|E'\rangle, \quad l=0,1,\ldots,\infty \tag{2}$$

are the exact-energy-eigenstate matrix elements of powers of the oscillator's displacement operator.[4] With the exact ground-state energy eigenvalue as input, a meaningful sequence of approximations for the ground-state–even-parity-eigenstate transition frequencies was derived from the characteristic equation

$$\det(C^{-1}AC)_N=0. \tag{3}$$

The elements of the matrix C were defined by the coefficients of the Wick transformation relating ordinary and normal products, while the subscript N denotes the $N\times N$ truncation of the matrix product.

An infinite number of other choices for C have also been found through which other characteristic equations having the form (3) can be defined.[5] Different sets of $\vec{\tau}$ eigenvector solutions to the harmonic-oscillator recursion equations can be used to define C; the Wick transformation is included in these as a special case. Use of the set of transformations permits a complete determination of an oscillator's spectra from low-order approximations. However, it was necessary that a proper choice be made for the C matrices' single parameter, Δ, and that a good value for the ground-state energy be used in each case. Further inspection also shows that the resulting transition frequency and energy eigenvalues can be seen not to be desirable or sufficiently stationary functions of Δ in low orders of approximation. This result is typical of all the approximations (3).

A reliable self-contained and self-consistent recursive approximation method should yield eigenvalues that are stationary and well-defined functions of any parameters involved. It is shown below that these criteria can be met for the calculation of energy eigenvalues by altering the definition

of the characteristic equation (3) to one of the form

$$\det(SAT)_N = 0. \tag{4}$$

In contrast to the previous procedures, S and T are not triangular and S is not the inverse of T. Rather the elements of S are associated with the covariant eigenvectors of A, which are related to the τ^l with $l<0$. The matrix elements of SAT are infinite nonconvergent series which are, however, summable with Euler's method. The resultant matrix is nonsymmetric but nevertheless numerically leads to well-defined and stationary energy eigenvalues in all orders of approximation.

II. THE CHARACTERISTIC MATRIX FOR THE ENERGY

Let $|E_a\rangle$ denote the exact energy eigenstates of the complete Hamiltonian

$$H = \frac{p^2}{2m} + \sum_{n=1} \frac{\lambda_n Q^{2n}}{2n} . \tag{5}$$

As an alternative to the previous[3,5] derivations one need only evaluate the matrix element

$$\langle E_a|[H,[H,Q^l]]|E_b\rangle = (E_a - E_b)^2 \tau^l_{ab} ,$$

using the equal-time commutation relation

$$[p, Q^l] = -i\hbar l Q^{l-1} \tag{6}$$

and

$$p Q^{l-1} = \frac{i}{2\hbar l}[p^2, Q^l] + \frac{\hbar}{2i}(l-1)Q^{l-2}, \tag{7}$$

which follows from (6). One obtains

$$\omega_{ba}^2 \tau^l_{ab} - \frac{1}{m}\sum_1 \lambda_n \frac{l(l+n-1)}{n} \tau^{l+2n-2}_{ab} + \frac{2\hbar}{m}\binom{l}{2}\left(\frac{2E_a}{\hbar} + \omega_{ba}\right)\tau^{l-2}_{ab} + \frac{6\hbar^2}{m^2}\binom{l}{4}\tau^{l-4}_{ab} = 0, \tag{8}$$

where

$$\hbar\omega_{ba} = E_b - E_a,$$

and τ^l is defined by (2). Note that (5) can be used to eliminate p^2 in (7).

The complete energy-eigenvalue problem is defined by (8) with

$$\omega_{ba} = 0, \quad b = a.$$

As a consequence of the parity-symmetric nature of the Hamiltonian only the even components of τ^l contribute. Then $A(E,0)$ of (1) has the matrix elements

$$A_{lj} = -\frac{1}{m}\sum_{n=1} \lambda_n \frac{(2l)(2l+n-1)}{n} \delta_{l,j-n+1} + 4\binom{2l}{2}\frac{E}{m}\delta_{l,j+1} + \frac{6\hbar^2}{m^2}\binom{2l}{4}\delta_{l,j+2}, \tag{9}$$

where here the indices have been changed so that the τ^l denotes the previous component τ^{2l}.

The approach to be followed below is justified by the following considerations. Let $\vec{\tau}_n$, $n = 0, 1, \ldots, \infty$ be a set of vectors for which

$$A(E_n)\vec{\tau}_n = 0, \tag{10}$$

and let the nth column of the matrix T be defined by the components of $\vec{\tau}_n$. Then the nth column of the matrix product AT must vanish at E_n, and in particular

$$\det[A(E_n)T]_N = 0, \tag{11}$$

where the subscript indicates that the determinant is constructed from only the first N rows and columns of the product matrix. If $\vec{\tau}_n$ only approximately satisfies (10) one still may expect that (11) leads to a well-defined characteristic equation in the sense that

$$\lim_{N\to\infty} E_n^{(N)} = E_n ,$$

where $E_n^{(N)}$ is the argument for which (11) vanishes.

Similarly one can consider covariant eigenvectors $\vec{\sigma}_n$ satisfying

$$\vec{\sigma}_n A(E_n) = 0. \tag{12}$$

Then if S is a matrix whose nth row is constructed from the components of $\vec{\sigma}_n$ the nth row of the product $SA(E)$ vanishes at E_n. If $\vec{\sigma}_n$ only approximately satisfies (12) then the characteristic equation

$$\det[SA(E_n^{(N)})]_N = 0 .$$

might also lead to a convergent sequence of roots in N.

It is clear that the best procedure should result from the matrix multiplication SAT, for when $\vec{\sigma}_n$ and $\vec{\tau}_n$ are both exact eigenvectors the nth row and column of the matrix product will vanish. This motivates (4). The procedure followed below will be to construct the matrices S and T from the known covariant and contravariant eigenvectors of the harmonic-oscillator recursion equation.

III. THE HARMONIC EIGENVECTORS

The eigenvectors $\vec{\tau}_H$ of the harmonic energy matrix $A(E)_H$ can be determined directly from normalized harmonic-oscillator wave functions via

$$\tau^l_{Ha} = \int_{-\infty}^{\infty} |\psi_a|^2 q^{2l}\, dq . \tag{13}$$

However, the recursion approach gives more insight into the problem of determining the covariant eigenvectors $\vec{\sigma}_{Hn}$, for which the analog to (13) is yet unknown.

Making in (9) the substitutions

$$\Delta = \frac{\hbar}{2m\omega_0}, \quad \lambda_n = m\omega_0{}^2\delta_{n1}, \qquad \tau^l_{Ha} = t^l_a \Delta^n, \quad E_a = \hbar\omega_0(a+\tfrac{1}{2}), \tag{14}$$

one obtains the recursion equation

$$l^2 t^l_a - (2a+1)\binom{2l}{2} t^{l-1}_a - 6\binom{2l}{4} t^{l-2}_a = 0. \tag{15}$$

Note that from a field-theoretic point of view the parameter Δ coincides with the harmonic oscillator's equal-time pairing function

$$\Delta = [Q^-(t), Q^+(t)],$$

where Q^+ (Q^-) is the positive- (negative-) frequency component of Q.

Direct iteration of the recursion equation leads to the ground-state eigenvector

$$t^l_0 = \frac{(2l)!}{2^l l!} = \frac{1}{2^l \pi^{1/2}}\,\Gamma(\tfrac{1}{2}+l), \tag{16}$$

a result which is consistent with (13). The eigenvector for the ath energy level is found through the substitution

$$t^l_a = \frac{1}{a!}\, g_{l,a}\, t^l_0. \tag{17}$$

One obtains the recursion equation

$$(l+1)g_{l+1,a} = (2a+1)g_{l,a} + l\, g_{l-1,a}. \tag{18}$$

The initial condition

$$g_{0,a} = a! \tag{19}$$

ensures via (17) that t^0_a is unity.

From (12) one finds that the covariant eigenvectors $\vec{\sigma}_a$ are determined by the recursion equation

$$6\binom{2l+4}{4} s^{l+2}_a + \binom{2l+2}{2}(2a+1)s^{l+1}_a - l^2 s^l_a = 0, \tag{20}$$

where

$$\sigma^l_a = s^l_a \alpha^l, \quad \alpha = \frac{2m\omega_0}{\hbar}. \tag{21}$$

It will be useful later to distinguish α from Δ^{-1}. Since only the components

$$A_{lj}, \quad l \geq 1, \quad j \geq 0$$

are needed to uniquely specify both the covariant and contravariant eigenvector sets, one finds from direct iteration the ground-state eigenvector

$$\sigma^l_0 = \frac{(-1)^{l-1}(l-1)!\,2^l\alpha^l}{(2l)!}, \quad l \geq 1, \quad \sigma^0_0 = 0. \tag{22}$$

In a manner similar to (17), the covariant eigenvectors for the nth energy level are determined by the substitution

$$s^l_a = s^l_0 h^l_a.$$

Then (20) implies that $h_{l,a}$ satisfies the recursion relation

$$(l+1)h^{l+2}_a - (2a+1)h^{l+1}_a - l\,h^l_a = 0,$$

which leads to the result that

$$h^l_a = g_{l-1,a}.$$

The general covariant eigenvector then has the components

$$\sigma^l_a = \frac{(-1)^{l-1}(l-1)!\,2^l\alpha^l}{(2l)!\,a!}\, g_{l-1,a}, \quad \sigma^0_a = 0. \tag{23}$$

Comparison of (23) with (16) and (20) with (15) leads to an interesting result. Evaluated in the limit $z = -l + \epsilon$, the Γ-function identity

$$2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2}) = \pi^{1/2}\Gamma(2z)$$

implies that

$$s^l_0 = -\frac{\pi^{-1/2}}{l2^l}\,\Gamma(-l+\tfrac{1}{2}),$$

which suggests in comparison with (16) that

$$s^l_a = -\frac{1}{l}\, t^{-l}_a, \quad l \geq 1. \tag{24}$$

Indeed one can easily verify that (24) takes (20) into (15). Thus the covariant eigenvectors are intimately connected with the matrix elements of Q^{-l}, as defined by the recursion equations. One can say that the recursion equations give meaning to (13) for negative l, and that these components of τ^l are needed in the definition of the characteristic equation.

Insight into the explicit form of $g_{l,a}$ is obtained by viewing (18) for large l as the differential equation

$$l\,\frac{d}{dl}\, g_{l,a} = a g_{l,a},$$

which implies that

$$g_{l,a} \to \text{const} \times l^a.$$

This result coupled to the invariance of (18) under the transformation

$$l \to -l, \quad g_{l,a} \to \pm g_{-(l+1),a}$$

suggests that $g_{l,a}$ is a polynomial of degree a which is either symmetric or antisymmetric in the variable $(2l+1)$.

Let

$$g_{l,a}=\sum_{s=1}^{a+1} G(a+1,s)(2l+1)^{s-1}. \tag{25}$$

Making use of the symmetry of $g_{l,a}$, direct evaluation of the recursion equation for $l=0,1,\ldots,a/2$ if a is even or $l=0,1,\ldots,(a+1)/2$ if a is odd defines with (19) the simultaneous linear equations from which the coefficients $G(r,s)$ can be determined. Table I lists the coefficients $G(r,s)$ for $r,s=1,\ldots,7$. The reader can verify by inspection that the $g_{l,a}$ also satisfy the recursion equation

$$g_{l,a}=(2l+1)g_{l,a-1}+(a-1)^2 g_{l,a-2}$$

in the index a, which is useful in determining higher order $G(r,s)$.

IV. DEFINITION OF THE CHARACTERISTIC EQUATION

In the following the eigenvectors' components (23) and (17) define the elements of the rows and columns of S and T, respectively. Since these harmonic eigenvectors have an infinite number of nonvanishing components the elements of the characteristic matrix are defined by infinite series. Letting x denote the product $(\alpha\Delta)$, the result of the matrix multiplication (4) can be expressed in the form

$$(SAT)_{lm}=\sum_n \beta_n A(n,l,m), \tag{30}$$

where

$$A(n,l,m)=\frac{2m}{l!m!}\sum_{s=1}^{m+1}\sum_{u=1}^{l+1}\sum_{q=1}^{n} f(n,q)G(m+1,s)G(l+1,u)\sum_{t=1}^{s}\binom{s-1}{t-1}(2n)^t S(s+u+q-t-2).$$

The sums $S(p)$ in (28) for small values of p are given in Table III. They are obtained by expressing $S(p)$ in terms of the geometric series

$$S(0,x)=\frac{1}{1+x},$$

as in Appendix A.

$$(SAT)_{lm}=\frac{2^m}{l!m!}\sum_{n=-1}\beta_n\sum_{k=0}^{\infty}(-1)^k F(k,n)g_{k,l}\,g_{k+n,m}\,x^k, \tag{26}$$

where from (9), (17), and (23),

$$F(k,-1)=2k,\quad F(k,0)=1,$$

$$F(k,n)=(2k+n+1)\prod_{q=1}^{n-1}(2k+2q+1), \tag{27}$$

$$\beta_{-1}=\frac{\alpha^2\hbar^2}{2xm^2},\quad \beta_0=\frac{4E\alpha}{m},\quad \beta_n=\frac{2\lambda_n x^n}{nm}\alpha^{1-n},\quad n\geq 1.$$

The coefficients of x^k in the infinite series in (26) are polynomials in k and thus diverge if x is unity. However, the matrix element (26) can be defined by evaluating sums of the form

$$S(p)=\lim_{x\to 1^-}\sum_{k=0}^{\infty}(-1)^k(2k+1)^p x^k. \tag{28}$$

Thus it is convenient to express all coefficient factors of $(\alpha\Delta)$ involving k in (26) as polynomials in $(2k+1)$. Writing

$$F(k,n)=\sum_{q=1}^{n} f(n,q)(2k+1)^{q-1}, \tag{29}$$

where the coefficients $f(n,q)$ for the oscillators studied below are given in Table II, and expanding $g_{k+n,m}$ as a function of $(2k+1)$ using the binomial expansion, one obtains

The diagonal elements of (SAT) are proportional to the diagonal elements of the Rayleigh-Ritz matrix, that is,

$$(SAT)_{ll}=\frac{(-1)^l\alpha 2^{l+1}}{m}\langle E_l|(H-E)|E_l\rangle,$$

where the $|E_l\rangle$ here are the harmonic-oscillator

TABLE I. The expansion coefficients $G(r,s)$ of the eigenvector polynomials $g_{l,r-1}$.

$r\backslash s$	1	2	3	4	5	6	7
1	1	0	0	0	0	0	0
2	0	1	0	0	0	0	0
3	1	0	1	0	0	0	0
4	0	5	0	1	0	0	0
5	9	0	14	0	1	0	0
6	0	89	0	30	0	1	0
7	225	0	439	0	55	0	1

TABLE II. The expansion coefficients $f(n,q)$ of the function $F(k,n)$ appearing in the characteristic matrix SAT, Eq. (29).

$n\backslash q$	1	2	3	4	5
−1	−1	1	0	0	0
0	1	0	0	0	0
1	1	1	0	0	0
2	4	4	1	0	0
4	192	224	92	16	1

energy eigenstates corresponding to α. However, the matrix SAT is not equivalent to the Rayleigh-Ritz matrix in the sense of a finite-dimensional similarity transformation. For nonlinear oscillators these results are independent of the oscillator potential. For example, one finds for the Hamiltonian

$$H=\frac{p^2}{2m}+m\omega_0^2\frac{Q^2}{2}+\frac{\lambda Q^4}{4}$$

the 4×4 truncated characteristic matrix

$$(SAT)_4=\begin{bmatrix} \frac{2E\alpha}{m}-\frac{\alpha^2\hbar^2}{4m^2}-\omega_0^2-\frac{3\lambda}{2m\alpha} & \frac{-8\lambda}{m\alpha}+\frac{\alpha^2\hbar^2}{2m^2}-2\omega_0^2 & \frac{-20\lambda}{m\alpha} & \frac{-48\lambda}{m\alpha} \\ \frac{2\lambda}{m\alpha}-\frac{\alpha^2\hbar^2}{4m^2}+\omega_0^2 & \frac{-4E\alpha}{m}+\frac{3\alpha^2\hbar^2}{2m^2}+\frac{15\lambda}{m\alpha}+6\omega_0^2 & \frac{40\lambda}{m\alpha}-\frac{2\alpha^2\hbar^2}{m^2}+8\omega_0^2 & \frac{56\lambda}{m\alpha} \\ \frac{-\lambda}{m\alpha} & \frac{-16\lambda}{m\alpha}+\frac{\alpha^2\hbar^2}{m^2}-4\omega_0^2 & \frac{8E\alpha}{m}-\frac{5\alpha^2\hbar^2}{m^2}-20\omega_0^2-\frac{78\lambda}{m\alpha} & \frac{-160\lambda}{m\alpha}+\frac{6\alpha^2\hbar^2}{m^2}-24\omega_0^2 \\ 0 & \frac{6\lambda}{m\alpha} & \frac{72\lambda}{m\alpha}-\frac{3\alpha^2\hbar^2}{m^2}+12\omega_0^2 & \frac{-16E\alpha}{m}+\frac{14\alpha^2\hbar^2}{m^2}+56\omega_0^2+\frac{300\lambda}{m\alpha} \end{bmatrix}$$

Attention is called to the nonsymmetric nature of (SAT) and to the fact that $\det(SAT)_N$ apparently cannot be factored into the product of two determinants giving separately the even- and odd-parity eigenvalues. This is in sharp contrast to the results of the Rayleigh-Ritz method.[6] The matrix $A(n, l, m)$ of (30) is tabulated in Appendix B.

V. NUMERICAL RESULTS AND COMPARISONS

A comparison of results for the quartic oscillator

$$H=\frac{p^2}{2}+\frac{Q^4}{4},$$

for which $\lambda_n=\delta_{n2}$, $m=1$ will clearly illustrate some of the differences between the LNTD method previously employed[5] and that used here, which will hereafter be referred to as the operator recursion mechanics (ORM) method. However, it should be pointed out that the C matrix used in the LNTD method in energy-eigenvalue calculations differs from that used here. With LNTD method, in order to make an invertible matrix, all but one of the column vectors of each of the C matrices employed were obtained from the harmonic eigenvectors of (8) with $\omega_{ba}\neq0$. Actually, there are several different ways in which energy eigenvalues can be obtained from (8) using (3), but with regard to a variation in the C matrix parameter these methods all have the same characteristic features. Thus the comparison is made here even though C and T are not the same matrix.

The first two approximations to the ground-state energy resulting from the LNTD method define the algebraic equations

TABLE III. The generalized geometric series sums $S(p)$ appearing in the matrix elements of SAT, Eq. (27).

p	$S(2p)$	$S(2p+1)$
0	0.5	0
1	− 0.5	0
2	2.5	0
3	−30.5	0
4	692.5	0
5	−25 260.5	0

$$E^{(1)}_{\mathrm{LNTD}}=9/4\alpha^2,$$

$$E^{(2)}_{\mathrm{LNTD}}=\frac{8.25}{\alpha^2}-\left(\frac{216}{\alpha^4}-\frac{4.5}{\alpha}\right)^{1/2}.$$

In the first approximation the ground-state energy is not stationary for any value of α. The second approximation contains one stationary point for which $(\partial E/\partial\alpha)=0$.

$$\bar{E}^{(2)}_{\mathrm{LNTD}}=0.354,\quad \bar{\alpha}=2.5. \tag{31}$$

However, for $\alpha>3.63$ the second-order energy eigenvalues become complex.

In contrast, the first two approximations to the ground-state energy resulting from the recursion mechanics method developed here define the eigenvalues

$$E^{(1)}_{\mathrm{RM}}=\frac{\alpha}{8}+\frac{3}{4\alpha^2},$$

$$E^{(2)}_{\mathrm{RM}}=\frac{\alpha}{4}+\frac{9}{4\alpha^2}-\frac{1}{2}\left(\frac{\alpha^2}{8}+\frac{17}{\alpha4}\right)^{1/2}.$$

The first approximation has one stationary point,

$$\bar{E}^{(1)}_{\mathrm{RM}}=0.4293,\quad \bar{\alpha}=2.29,$$

and the second approximation has three stationary points, approximately given by

$$\bar{E}^{(2,1)}=0.415,\quad \bar{\alpha}_1=1.28$$

$$\bar{E}^{(2,2)}=0.438,\quad \bar{\alpha}_2=2.10$$

$$\bar{E}^{(2,3)}=0.418,\quad \bar{\alpha}_3=3.5.$$

Figure 1 plots the eigenvalues obtained in the LNTD and ORM methods in the above orders as a function of α, the reciprocal pairing parameter. Note that in the second-order ORM approximation

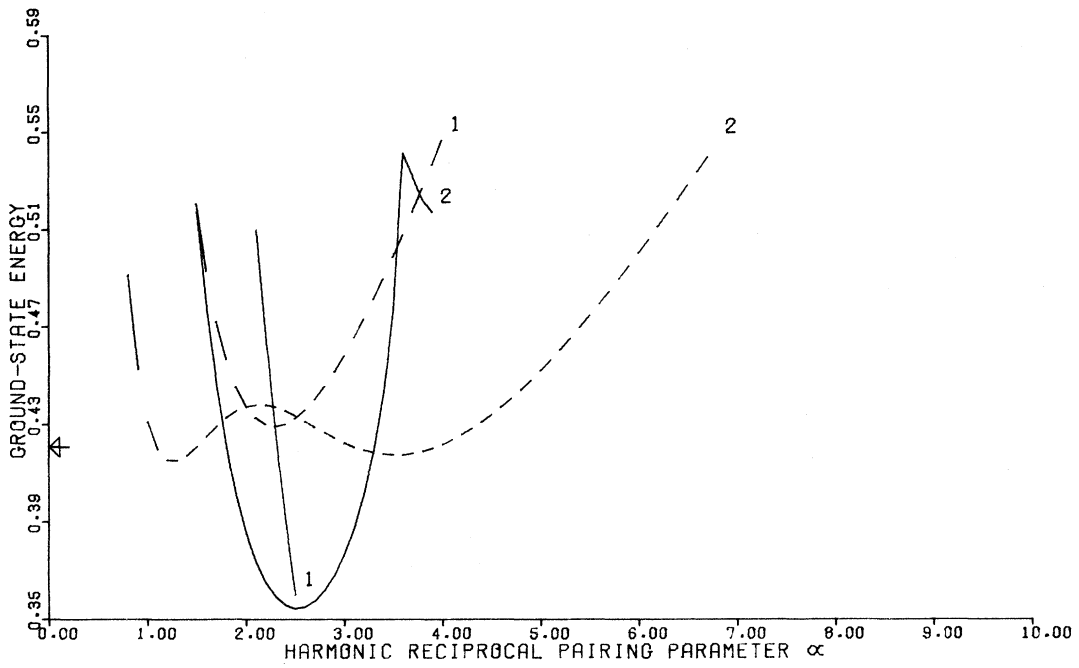

FIG. 1. Comparison of the LNTD (solid line) and operator-recursion-mechanics (dashed line) ground-state energy eigenvalue results for the quartic oscillator $H=p^2/2+Q^4/4$ as a function of the reciprocal pairing parameter α. $E^{(N)}_{\mathrm{LNTD}}$ and $E^{(N)}_{\mathrm{RM}}$ are illustrated for orders $N=1, 2$. The arrow indicates the correct energy.

$E^{(N)}_{(\alpha)}$ is real and positive for all values of α, and that all three energy stationary eigenvalues are a considerable improvement over the second-order result (31), in comparison with the "exact" numerical expression for the ground-state energy of 0.420 806.

Figure 2 gives the trend of convergence as one goes to higher orders in the ORM method. The abrupt tail on the two highest-order curves occurs when $E^{(N)}_{(\alpha)}$ jumps discontinuously to another correct eigenvalue, off-scale. Only in the operator-recursion-mechanics method is $E^{(N)}_{(\alpha)}$ always real. The fact that there may be more than one stationary value for the energy in a given order of approximation is typical in higher orders for both the LNTD and ORM methods. For this reason in doing an energy-eigenvalue calculation one has the problem of deciding which stationary values represent the best approximation to the true energy eigenvalue.

In a determination of the eigenvalues of a finite-dimensional matrix the results are completely independent of the choice of basis and of any parameter upon which the basis depends. Thus in our present calculation one may consider that the accuracy of the approximation is indicated by the degree of stationarity of the eigenvalue. The latter is indicated by the size of the second derivative of the eigenvalue with respect to the basis parameter evaluated at the stationary point. In the region of the ith stationary point

$$E=\bar{E}_i+\frac{1}{2}\left.\frac{\partial^2 E}{\partial\alpha^2}\right|_{\bar{\alpha}^i}(\alpha-\bar{\alpha}_i)^2.$$

Letting $y_i=|\partial^2 E/2\alpha^2|^{-1/2}$, a possible best approximation to an eigenvalue resulting from a given order of approximation can be defined by the weighted average

$$\bar{E}^{(N)}=\left(\sum_i \bar{E}^{(N)}_i y_i\right)\Big/\left(\sum_i y_i\right).$$

Note that the y_i can be changed by a scale factor without changing $\bar{E}^{(N)}$. Table IV illustrates the convergence of the "best" approximations to the quartic ground-state energy resulting from the ORM method.

The convergence of the ORM method results for several different nonlinear oscillators is illustrated in Table V for several energy levels. The convergence of the energy eigenvalues for the last two oscillators listed is in good agreement with that of the Rayleigh-Ritz method,[6] while that for the first is an improvement over the results of the LNTD convergence.

VI. DISCUSSION

Use of distinct basis transformations for the covariant and contravariant components of the $\vec{\tau}$-

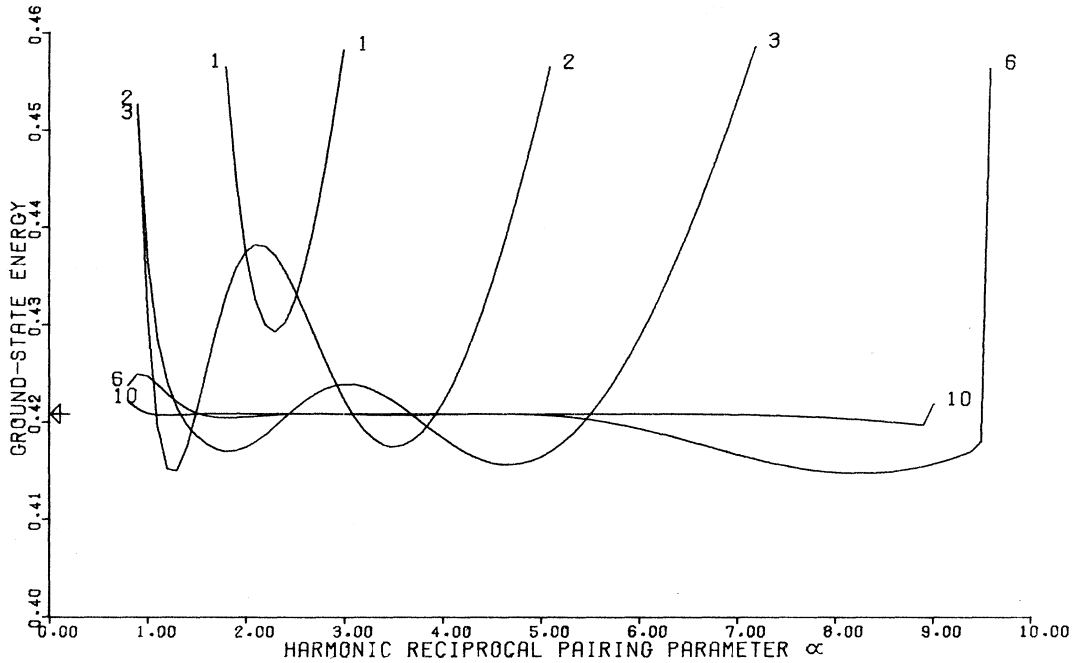

FIG. 2. Convergence in the operator-recursion-mechanics method of the quartic oscillator's ground-state energy eigenvalues as a function of the reciprocal pairing parameter α. The functions $E_{\alpha}^{(N)}$ are illustrated for orders $N=1,2,3,6,10$. The arrow indicates the correct energy.

function recursion matrices for anharmonic oscillators has been seen to lead to a marked improvement over the previous LNTD energy-eigenvalue approximations, wherein the characteristic equations are based upon similarity tranformations. Here every order of approximation yields energy eigenvalues which are real functions of the pairing parameter defining the transformations, and contains at least one stationary eigenvalue. As one goes to higher order progressively better approximations are obtained. This in particular is in contrast to the LNTD procedure used previously. Although a good result was obtained in first order through a proper choice of the pairing parameter, that consistent with an approximate solution to the canonical commutator sum rule, until a sufficiently high order was reached, poorer approximations than the first resulted from higher orders.

Results the same as those obtained here follow if (8) is regarded as an eigenvalue equation for the transition frequencies. This will be discussed in a sequel to this report, where a complete self-consistent and self-contained approximation procedure for the complete spectra of nonlinear oscillators will be developed. Heretofore, a very accurate value for an energy eigenvalue was required before good low-order results for transition frequencies could be obtained. One should keep in mind that a practical difference between the present method and those of the Rayleigh-Ritz and variational types is that with the present method both transition frequencies and energy eigenvalues can be calculated from the same basic set of equations, making a complete low-order determination of a system's spectra possible.

One has also gained something conceptually new from the current approach. First, a meaningful characteristic equation was defined via an infinite matrix multiplication where the matrix elements, infinite nonconvergent series, were determined

TABLE IV. Convergence of the weight ground-state energy eigenvalues belonging to the Nth order of approximation. $\mathfrak{D}$ is the difference between the weighted average and the "exact" value of E_0 obtained from numerical integration of the Schrödinger equation, 0.420 806.

N	$\overline{E}^{(N)}$	$\mathfrak{D}$
1	0.429 27	0.0085
2	0.4236	0.0028
3	0.4188	−0.002
4	0.4196	−0.0012
6	0.420 058	−0.000 75
8	0.420 786	0.000 02
10	0.420 803	−0.000 003

TABLE V. Sample convergence of energy eigenvalues of the ORM method for several nonlinear oscillators. The starred "exact" eigenvalues are those obtained from Ref. 6 in 28th order using the Rayleigh-Ritz method. The other exact eigenvalues were obtained from numerical integration of the Schrödinger equation and are believed correct to the figures given.

	$H=\frac{1}{2}p^2+\frac{1}{4}Q^4$ $m=1.0$ $\alpha=2.28$			$H=p^2+Q^2+Q^4$ $m=0.5$ $\alpha=3.33$			$H=p^2+Q^2+0.1Q^8$ $m=0.5$ $\alpha=4.6$		
N	E_0	E_1	E_3	E_0	E_2	E_4	E_0	E_2	E_4
1	0.420 28			1.4033			1.3908		
2	0.437 38	1.5683		1.4131			1.168 32		
3	0.419436	1.527 67		1.390 73	9.2627		1.183 318	8.32	
4	0.420 049	1.506 27	6.0764	1.391 47	8.6646		1.184 865	7.901	
5	0.421 291	1.509 40	4.7477	1.392 76	8.662 24	23.3546	1.168 301	7.7604	20.052
6	0.420 737	1.508 40	4.641 10	1.392 325	8.664 185	18.8396	1.165 305	7.6038	18.462
7	0.420 765	1.507 49	4.639 06	1.392 315	8.654 257	18.1518	1.169 398	7.6295	17.827
8	0.420 834	1.508 04	4.621 20	1.392 368	8.654 414	18.0842	1.169 95	7.5915	17.842
9	0.420 797	1.507 91	4.623 48	1.392 350	8.655 545	18.0623	1.168 647	7.640 95	17.884
10	0.420 804	1.507 87	4.621 23	1.392 350	8.654 934	18.065 16	1.168 755	7.633 88	17.733
12	0.420 804	1.507 90	4.621 53	1.392 351 4	8.655 082	18.057 71	1.168 978	7.641 38	17.785
Exact	0.420 806	1.507 90	4.621 22	1.392 352*	8.655 049*	18.057 56*	1.168 971*	7.6399*	17.76*

essentially by computing Padé-type sums. It seems likely that infinite matrix multiplication can frequently be carried out with this method, either approximately or exactly as was done here. In addition, one expects that, owing to the stationary nature of the eigenvalues obtained, the operator recursion mechanics method, based on good "eigenvector" basis transformations, must be derivable from a variational principle. One expects that this must proceed somewhat along the lines that Li, Klein, and Krejs[7] used to show that the iteration method,[7,8] based upon canonical commutation relation sum rules, is derivable from a variational principle.

Field theoretically the mass-eigenvalue calculation in the Heisenberg theory[1,2] is somewhat analogous to the NTD procedure (11), the mass in the two-point function corresponding to the parameter Δ. As with the LNTD anharmonic oscillator the calculated mass eigenvalues are not stationary functions of the two-point-function mass, which is identified in the earlier theory with the mass of the nucleon. But there, this approximation does not follow from the canonical commutation relation sum rule. There is as yet no field-theoretic analog to the present method, having two distinct basis transformations.

In solid-state theory the analog of the present method has been successfully applied to a one-dimensional band calculation, and the procedure seems to be a viable one for both energy and transition-frequency calculations.[9] The analogy of the τ functions there is the charge densities of the system or, more specifically, their Fourier coefficients.

ACKNOWLEDGMENT

The author is indebted to Donald Petcher for his assistance with the numerical calculations.

APPENDIX A: GENERALIZED GEOMETRIC SERIES

The infinite sums

$$S(p)=\lim_{x\to 1^-}\sum_0^\infty (-1)^k(2k+1)^p x^k$$

are evaluated in the following way. Letting $x=y^2$, one can write

$$S(p,y^2)=\lim_{y\to 1}\sum_0^\infty (-1)^k(2k+1)^p y^{2k}.$$

Then it is easily verified that these sums satisfy the recursive differential equation

$$S(p+1,y^2)=\frac{d}{dy}[yS(p,y^2)].$$

The ansatz

$$S(p,y^2)=\left(\sum_0^p (-1)^n a(p,n)y^{2n}\right)\Big/(1+y^2)^{p+1}$$

leads to the recursion equation

$$a(p+1,n)=(2n+1)a(p,n)+(2p-2n+3)a(p,n-1).$$

The sums $S(p)$ are then obtained from

$$S(p)=\frac{1}{2^{n+1}}\sum_{n=0}^p (-1)^n a(p,n).$$

APPENDIX B: THE (*SAT*) MATRIX ELEMENTS $A(n,l,m)$

The matrix elements $A(n,l,m)$ for $n=\mp 1$ are

$$A(\mp 1,l,m)=(-2)^{l-2}[-2(2l+1)\delta_{lm}\pm 4(l+1)\delta_{l,m-1}\pm l\delta_{l,m+1}].$$

For $n=2$ the 9×7 truncation of $[A(2,l,m)]$ is

$$[A(2,l,m)]=\begin{bmatrix} -1.5 & -8 & -20 & -48 & -128 & -320 & -768 \\ 2.0 & 15 & 40 & 56 & 96 & 256 & 640 \\ -1 & -16 & -78 & -160 & -160 & -192 & -512 \\ 0 & 6 & 72 & 300 & 544 & 448 & 384 \\ 0 & 0 & -24 & -256 & -984 & -1664 & -1216 \\ 0 & 0 & 0 & 80 & 800 & 2928 & 4736 \\ 0 & 0 & 0 & 0 & -240 & -2304 & -8160 \\ 0 & 0 & 0 & 0 & 0 & 672 & 6272 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1792 \end{bmatrix}$$

and for $n=4$ the 10×6 truncation of $[A(4,l,m)]$ is

$$[A(4,l,m)]=\begin{bmatrix} -52.5 & -696.0 & -4\,728.0 & -23\,136 & -93\,888 & -336\,000 \\ 72.0 & 945.0 & 4\,904 & 25\,680 & 96\,192 & 336\,768 \\ -78.0 & -1278.0 & -8\,610.0 & -35\,808 & -113\,472 & -342\,912 \\ 48.0 & 1140.0 & 10\,656.00 & 54\,180 & 176\,448 & 442\,752 \\ -12.0 & -576.0 & -8\,592.0 & -62\,976 & -269\,640 & -751\,488 \\ 0 & 120.0 & 3\,840.0 & 46\,560 & 297\,600 & 1\,144\,080 \\ 0 & 0 & -720.0 & -19\,200 & -206\,880 & -1\,211\,904 \\ 0 & 0 & 0 & 3\,360 & 80\,640 & 805\,056 \\ 0 & 0 & 0 & 0 & -13\,440 & -301\,056 \\ 0 & 0 & 0 & 0 & 0 & 38\,304 \end{bmatrix}$$

---

*Research supported in part by the Air Force Aerospace Research Laboratories, Air Force Systems Command, United States Air Force, under Contract No. F33615-75-C1177.

[1]W. Heisenberg, *Introduction to the Unified Field Theory of Elementary Particles* (Interscience, New York, 1966).

[2]H. P. Dürr, W. Heisenberg, H. Mitter, S. Schlieder, and K. Yamazaki, Z. Naturforsch. 14A, 441 (1959); H. P. Dürr, *ibid.* 16A, 327 (1961).

[3]H. Stumpf, F. Wagner, and F. Wahl, Z. Naturforsch. 19A, 1254 (1964); F. Wagner, Ph.D. dissertation, University of München, 1966 (unpublished).

[4]It should be pointed out that the implied recurrence relation here has a fundamentally different origin from those of the Rayleigh-Ritz and Hill determinantal methods. Here the same energy eigenstates define every term in the recurrence relation and the "recurrence" is in the operator appearing in the matrix element. In the Rayleigh-Ritz, Hill determinantal, and other related methods, the recurrence relation is generated by expanding the wave function in a complete linearly independent set of functions and by letting the energy-eigenstate condition imply a recurrence relation for the expansion coefficients. See for example S. N. Biswas *et al.*, J. Math. Phys. 14, 1190 (1973); F. T. Hioe and E. W. Montroll, *ibid.* 16, 1945 (1975), and Ref. 6 below.

[5]C. A. Uzes and J. H. Henkel, Phys. Rev. D 8, 1067 (1973).

[6]S. Graffi and V. Grecchi, Phys. Rev. D 8, 3487 (1973).

[7]C. Li, A. Klein, and F. Krejs, Phys. Rev. D 12, 2311 (1975).

[8]J. H. Henkel and C. A. Uzes, Phys. Rev. D 8, 4430 (1973).

[9]C. A. Uzes and D. N. Petcher (unpublished).