Effective operator treatment of the anharmonic oscillator

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We analyze the one-dimensional anharmonic oscillator using effective operator methods in both the strong and weak coupling limits. We show that in the case of a one-dimensional model space, the similarity transformation needed to define the effective Hamiltonian is related to the coefficients in the expansion of the wave function in the unperturbed harmonic oscillator basis. We obtain an infinite system of equations which is equivalent to those obtained from the Hill determinant solution of the anharmonic oscillator. The analytic properties of the resulting equations reveal the nonperturbative features of the underlying problem. Thus, we demonstrate the utility of the effective operator method for solving a nonanalytic strong coupling problem.

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The effective operator method [1] has been used extensively and successfully within a cluster approximation scheme to obtain the low-lying spectroscopy of complex nuclei [2] with realistic nucleon-nucleon interactions. Central to the methodology of Ref. [1] is the iterative construction of a similarity transformation that transforms the original Hamiltonian to a new Hamiltonian having a two-component block diagonal structure where one component is finite dimensional and accommodates the low-lying spectroscopy. Diagonalizing this finite-dimensional block diagonal submatrix yields a finite number of eigenvalues to any desired precision corresponding to a subset of the exact solutions. In a sense, the similarity transformation is designed to decouple a finite-dimensional subspace from the rest of the spectrum, even in cases where the original Hamiltonian cannot be treated by perturbative methods. However, there are few rigorous results on the existence, or nonexistence [3], of the similarity transformation on which the utility of the method hinges, although several practical issues specific to strongly correlated nuclear systems are under investigation. Thus the formal properties of this effective operator approach require additional study, particularly within the framework of problems known to be nonperturbative in character. In addition to formal aspects, a deeper understanding of the errors associated with various approximations is required. For example, when a sequence of clusters is introduced as in the nuclear many body applications [2], we still need to understand how to optimize the convergence with increasing cluster size and/or with increasing model space size. In order to clarify the physical utility of the approach and refine our knowledge of its limitations and properties, we address a well-studied nonperturbative problem, the one-dimensional quartic oscillator in both the strong and weak coupling regime. In doing so, we shed light on the origins of the decoupling that plays such a crucial role.

The Hamiltonian H that we select, has the form H_0+V, where

$$H_0=\frac{p^2}{2m}+\frac{m\omega^2x^2}{2} \tag{1}$$

and $V=\lambda x^4$.

The perturbation expansion for energy eigenvalues is known not to converge, independent of the size of λ [4]. The divergent behavior of the expansion may be traced to the fact that, to large orders in perturbation theory, the growth in the number of contributions is sufficiently rapid to lead to a series that eventually diverges, even for arbitrarily small λ.

Various nonperturbative methods have been applied to extract the eigenvalues [5]. In this investigation we will construct an effective Hamiltonian using a similarity transformation along the lines proposed by Suzuki and Lee [1]. In addition to extracting energy eigenvalues from the effective Hamiltonian, the matrix elements of the generator of the similarity transformation will also be used to develop a system of equations equivalent to those obtained from the Hill determinant solution of the anharmonic oscillator.

We begin by establishing the following notation: let E denote a generic eigenvalue and $|\Psi\rangle$ the corresponding exact eigenstate of the Hamiltonian in Eq. (1). In that case we have

$$H|\Psi\rangle=E|\Psi\rangle. \tag{2}$$

Following Ref. [1], we define S, the generator of a similarity transformation such that $\tilde{H}=e^{-S}He^{S}$ and $|\tilde{\Psi}\rangle=e^{-S}|\Psi\rangle$. It then follows that

$$\tilde{H}|\tilde{\Psi}\rangle=E|\tilde{\Psi}\rangle. \tag{3}$$

For now, S is arbitrary, but subsequently, restrictions will be placed on S.

The next step in the treatment along the lines of Ref. [1] is the identification of a suitable model space (P space). We will use a one-dimensional model space containing the ground state of H_0 signified by $|0\rangle$. With this choice, P, the projection operator onto the model space is just $|0\rangle\langle 0|$. The Q space is then $\Sigma|i\rangle\langle i|$, where the sum over i runs over all states of the harmonic oscillator other than the ground state; P and Q are orthogonal and $P+Q=I$.

The first constraint we impose on S is that $S=QSP$. This leads to the identities

$$PS=SQ=0$$

and

$$S = SP = QS.$$

These identities will be used extensively later on. Since P and Q are orthogonal, $S^2 = 0$ leading to $e^{\pm S} = I \pm S$. With this choice of P and Q spaces and the restriction on S, S reduces to a column vector whose nonvanishing matrix elements are of the form $\langle i|S|0\rangle (i \neq 0)$, which will be denoted by S_i. The S_i will be seen to be related to the expansion coefficients of the true wave function in the unperturbed basis. The final condition we impose on S comes from the requirement that

$$\tilde{H}P|\tilde{\Psi}\rangle = EP|\tilde{\Psi}\rangle. \tag{4}$$

As in [1] we define the effective Hamiltonian H_{eff} to be $P\tilde{H}P$. In general, diagonalizing H_{eff} yields a subset of energy eigenvalues of the full Hamiltonian; since in our case H_{eff} is one dimensional, we will recover just one eigenvalue for any given S. Expanding H_{eff} in terms of S gives

$$H_{eff} = PHP + PVS. \tag{5}$$

From Eq. (4) and the fact that P and Q are projection operators, it follows that $Q\tilde{H}P = 0$, yielding

$$SHP + SVS = QVP + QHS, \tag{6}$$

which can be rewritten as

$$QVP + QHS = SH_{eff}.$$

After subtracting ΩS from both sides of the preceding equation (Ω is an arbitrary parameter), we obtain the following equation for S:

$$S = A[QVP - S(H_{eff} - \Omega)], \tag{7}$$

where

$$A = (\Omega - QHQ)^{-1}.$$

Note that since S and H_{eff} must be Ω independent, Ω is (strictly speaking) redundant. Nonetheless, the utility of Ω will soon be made clear. No use has been made of the fact that the P space is one dimensional, thus Eqs. (4)–(7) are perfectly general, and identical equations arise when treating more complex Hamiltonians along the lines of Ref. [1].

Since H_{eff} depends explicitly on S, Eq. (7) is a nonlinear operator equation for S potentially admitting more than one solution. In addition, A is ill defined in an infinite-dimensional Hilbert space. In applications to many body problems, it is customary to impose an arbitrary cutoff in the Q space, which leads to a well-defined A; in our case this amounts to neglecting all oscillator quanta above a certain energy. This also reduces S to a finite-dimensional column vector. Even with this simplification, Eq. (7) is still hard to solve exactly; in applications to many body Hamiltonians, iterative solutions are preferred. We propose the following sequence of iterations:

TABLE I. Energy eigenvalues by iteration.

Iteration (n)	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.3$	$\lambda = 1$	$\lambda = 2$	$\lambda = 3$
0	1.075	1.15	1.225	1.75	2.5	3.25
1	1.06792	1.12612	1.17806	1.45479	1.7359	1.95799
2	1.06603	1.12035	1.16752	1.40423	1.62662	1.79234
3	1.06551	1.11886	1.16495	1.39484	1.61088	1.77311
4	1.06535	1.11845	1.16429	1.3929	1.60819	1.77022
5	1.06531	1.11834	1.16411	1.39248	1.60768	1.76971
6	1.06529	1.11831	1.16407	1.39238	1.60757	1.76962

$$S^{(n)} = A[QVP - S^{(n-1)}({H^{(n)}}_{eff} - \Omega)], \tag{8}$$

$${H^{(n+1)}}_{eff} = PHP + PVS^{(n)}, \tag{9}$$

with $S^{(0)} = 0$ as the starting point in the sequence. After a suitable number of iterations the sequence is terminated. Since the P space is one dimensional, the final H_{eff} is simply the energy eigenvalue, and no diagonalization is necessary. On the other hand, it is necessary to check the cutoff independence of the energy eigenvalues and the convergence of the iterations, this can be done by varying both the cutoff and Ω. As a check, we calculate the eigenvalues emerging from this procedure after a total of seven iterations. We retain only the first ten harmonic oscillator eigenstates of even parity in calculating A; since V does not mix eigenstates of even and odd parity, it is adequate to consider only even parity states in calculating A. As in Ref. [6], we use $\hbar = 1$, $\omega = 2$, and $m = 0.5$ and allow λ to vary. Our results (setting $\Omega = -1$) are given in Table I.

These results (obtained using Mathematica) are in excellent agreement with the ground state energies in Ref. [6]; extending the size of the Q space used to obtain A changes the eigenvalues (if at all) only at the fifth significant figure or beyond. Furthermore, allowing Ω to vary between -2 and $+2$ leads to a similarly small change in the obtained eigenvalues. As in Ref. [7] we can access different solutions for S and thus different eigenvalues, by choosing a different range of values for Ω.

Given that the Hamiltonian is nonperturbative, the convergence of the sequence of iterations is nonperturbative in character; furthermore, the error induced by truncating the Q space to construct A is small. Since truncation of the Q space in the manner just described is a key ingredient in the application of effective operator methods in many body Hamiltonians, we will attempt to understand why this procedure is valid. More precisely, we will show that at least for the purposes of calculating low-lying eigenvalues, S may be accurately approximated by a column vector of finite dimension; since $S = QSP$, it then follows that the Q space needed to define A is effectively finite dimensional, which justifies the truncation we employ.

We start by expanding Eq. (4) in terms of S and H, leading to

$$(H - SH + HS - SHS)P|\Psi\rangle = EP|\Psi\rangle. \tag{10}$$

In order to derive an identity for E in terms of the S_i, we expand $|\Psi\rangle$ in terms of the eigenstates of H_0 as follows:

$$|\Psi\rangle = \sum \alpha_n |n\rangle. \tag{11}$$

The sum in Eq. (11) begins from zero and runs over all positive integers. For the sake of future notational convenience, we will denote $\langle n|A|m\rangle$ by A_{nm}, where A is any operator. Inserting the form of $|\Psi\rangle$ from Eq. (11) into Eq. (10) and operating with $\langle 0|$ on both sides yields

$$E = \langle 0|H|0\rangle + \langle 0|HS|0\rangle, \tag{12}$$

assuming that α_0 is nonvanishing. Inserting a complete set of states yields

$$E = H_{00} + V_{02}S_2 + V_{04}S_4 \tag{13}$$

exploiting the fact that the quartic perturbation connects the ground state only to states $|2\rangle$ and $|4\rangle$. Equation (13) is a special case of a more general expression for the exact eigenenergy resulting from an effective Hamiltonian in a one-dimensional model space derived in Ref. [7].

Equations for the remaining S_i may be obtained by sandwiching Eq. (6) between $|0\rangle$ and $\langle n|$, where $n \neq 0$. Doing so and using the fact that P and Q are projection operators gives

$$\langle n|SH|0\rangle + \langle n|SVS|0\rangle = \langle n|V|0\rangle + \langle n|HS|0\rangle. \tag{14}$$

By judicious insertions of complete sets of states, the left hand side of Eq. (14) can be reduced to

$$S_n(H_{00} + V_{02}S_2 + V_{04}S_4).$$

The term within brackets is just E from Eq. (13). Thus Eq. (14) may be written as

$$S_n E = \langle n|V|0\rangle + \langle n|HS|0\rangle. \tag{15}$$

Inserting a complete set of states yields

$$S_n E = V_{n0} + \sum_m H_{nm}S_m. \tag{16}$$

As before, we will assume that n to be even, the extension to include odd n is straightforward. Inserting different values of n into Eq. (16) leads to a system of coupled equations for the S_n. For $n=2$, we have

$$V_{20} + (H_{22} - E)S_2 + V_{24}S_4 + V_{26}S_6 = 0. \tag{17}$$

For $n=4$, we have

$$V_{40} + V_{42}S_2 + (H_{44} - E)S_4 + V_{46}S_6 + V_{48}S_8 = 0. \tag{18}$$

For $n=i$ and $i>4$, there is no term independent of S. The equation takes the form

$$V_{ii-4}S_{i-4} + V_{ii-2}S_{i-2} + (H_{ii} - E)S_i + V_{ii+2}S_{i+2} + V_{ii+4}S_{i+4} = 0. \tag{19}$$

We can make all the preceding equations homogenous with the generic substitution

$$S_i = \frac{\beta_i}{\beta_0}.$$

With this substitution, Eqs. (13), (17), and (18) read

$$(H_{00} - E)\beta_0 + V_{02}\beta_2 + V_{04}\beta_4 = 0, \tag{20}$$

$$V_{20}\beta_0 + (H_{22} - E)\beta_2 + V_{24}\beta_4 + V_{26}\beta_6 = 0, \tag{21}$$

$$V_{40}\beta_0 + V_{42}\beta_2 + (H_{44} - E)\beta_4 + V_{46}\beta_6 + V_{48}\beta_8 = 0. \tag{22}$$

For larger values of n, it is adequate to replace S_i by β_i in Eq. (19), giving

$$V_{ii-4}\beta_{i-4} + V_{ii-2}\beta_{i-2} + (H_{ii} - E)\beta_i + V_{ii+2}\beta_{i+2} + V_{ii+4}\beta_{i+4} = 0. \tag{23}$$

For the sake of comparison, we substitute the expansion from Eq. (11) into Eq. (2). Restricting ourselves to α_i with i even yields

$$(H_{00} - E)\alpha_0 + V_{02}\alpha_2 + V_{04}\alpha_4 = 0, \tag{24}$$

$$V_{20}\alpha_0 + (H_{22} - E)\alpha_2 + V_{24}\alpha_4 + V_{26}\alpha_6 = 0, \tag{25}$$

$$V_{40}\alpha_0 + V_{42}\alpha_2 + (H_{44} - E)\alpha_4 + V_{46}\alpha_6 + V_{48}\alpha_8 = 0, \tag{26}$$

and for larger values of i, we have

$$V_{ii-4}\alpha_{i-4} + V_{ii-2}\alpha_{i-2} + (H_{ii} - E)\alpha_i + V_{ii+2}\alpha_{i+2} + V_{ii+4}\alpha_{i+4} = 0. \tag{27}$$

It is clear that α_i and β_i satisfy the same set of equations. However, solving for α_i is equivalent to solving the Hill determinant for the quartic oscillator [6]. Since S_i are proportional to β_i, S_i may also be obtained from solving the Hill determinant. Furthermore, the physical significance of S_i is apparent, S_i may be taken equal (up to an overall constant) to the coefficients arising in the expansion of the true wave function in the unperturbed basis. As far as we are aware, this is the first instance where a connection between S and the expansion of the wave function in unperturbed basis has been established.

The α_i may be independently determined by the requirement that

$$\det(H - EI) = 0$$

for an invertible H. It can be shown that this requirement is equivalent to the more general statement in Ref. [7], of which Eq. (13) is a special case [8]. This provides an independent cross-check of our results.

There are additional constraints on S_i for large i, which arise from the behavior of the matrix elements V_{ij} at large i. To derive these constraints, let us rewrite Eq. (19) as follows:

$$V_{ii-4}S_{i-4}+V_{ii-2}S_{i-2}+H_{ii}S_i+V_{ii+2}S_{i+2}+V_{ii+4}S_{i+4}=ES_i. \quad (28)$$

For large i, the matrix elements appearing in Eq. (28) have the approximate form

$$\langle i|x^4|(i+4)\rangle=\left(\frac{\hbar}{m\omega}\right)^2\left(\frac{1}{4}\right)i^2(1+5/i)+\cdots, \quad (29)$$

$$\langle i|x^4|(i+2)\rangle=\left(\frac{\hbar}{m\omega}\right)^2 i^2(1+3/i)+\cdots, \quad (30)$$

$$\langle i|x^4|i\rangle=\left(\frac{\hbar}{m\omega}\right)^2\left(\frac{3}{4}\right)(2i^2+2i+1), \quad (31)$$

$$\langle i|x^4|(i-2)\rangle=\left(\frac{\hbar}{m\omega}\right)^2 i^2(1-1/i)+\cdots, \quad (32)$$

$$\langle i|x^4|(i-4)\rangle=\left(\frac{\hbar}{m\omega}\right)^2\left(\frac{1}{4}\right)i^2(1-5/i)+\cdots, \quad (33)$$

$$\langle i|x^2|(i+2)\rangle=\left(\frac{\hbar}{2m\omega}\right)i+\cdots, \quad (34)$$

$$\langle i|x^2|(i-2)\rangle=\left(\frac{\hbar}{2m\omega}\right)i+\cdots, \quad (35)$$

$$\langle i|x^2|i\rangle=\left(\frac{\hbar}{2m\omega}\right)(2i+1), \quad (36)$$

where higher order finite terms in the expansion have been neglected. As can be seen from the above equations, the left hand side of Eq. (28) contains both quadratic and linear divergences in i at large i, and no such divergences appear on the right. Equation (28) will be consistent only if S_i fall off rapidly for large i, aided by possible cancellations due to sign differences between the various S_i appearing on the left. As a consequence of the S_i falling off rapidly, low energy eigenvalues of the full Hamiltonian are expected to be only weakly dependent on high energy eigenstates of the unperturbed Hamiltonian. As a check, we allow i in Eq. (28) to run over a limited range of even values beginning at 0, and compute the lowest energy eigenvalues from the resulting equations. We use the same numerical values for the parameters as before and allow λ to vary over the same range. The results are summarized in Table II.

The entries in the table are the lowest energy eigenvalues obtained from sets of not more than 20 equations, and are in excellent agreement with the results obtained by our iterative procedure and with Ref. [6]. This is in strong support of our earlier claim that low energy eigenvalues of the full Hamiltonian are only weakly dependent on high energy states of the unperturbed Hamiltonian. It is now clear why the truncation of the Q space, which was implemented in order to facilitate the iterative procedure, is justified. The decoupling of high energy states in a toy model has been independently studied in Ref. [9]; however, unlike the quartic oscillator, the Hamiltonian in Ref. [9] can be analytically inverted, permitting the use of methods very different from the ones we employ in this paper.

As an additional analytical check on the decoupling of S_i for large i, we consider the following ansatz for large i:

$$\frac{S_{i+j}}{S_i}\sim(-1)^{j/2}\left(1-\frac{jf(j/2)}{i}\frac{m^2\omega^3}{\lambda\hbar}\right), \quad (37)$$

where f is some arbitrary unspecified function. Inserting this ansatz into Eq. (28) and using the asymptotic forms of the matrix elements given earlier, we see that Eq. (28) is free of divergences in i, provided

$$f(-2)-f(2)+2f(1)-2f(-1)+1=0. \quad (38)$$

The utility of Eqs. (38) and (37) will become apparent when we investigate what happens when λ is so large that it dominates the quadratic term in the potential. In that case the Hamiltonian may be conveniently expressed as

$$\frac{p^2}{2m}+\frac{m\omega^2x^2}{2}+\lambda x^4-\frac{m\omega^2x^2}{2}.$$

Following the same procedure as before but with $V=\lambda x^4-(m\omega^2x^2/2)$ gives an equation identical to Eq. (28) but with different values of H_{ii}, and $V_{ii\pm2}$. This is not surprising as the structure of Eq. (28) does not rely on the precise form of V, but on the fact that the only nonvanishing matrix elements V_{ij} have $|(i-j)|\leqslant 4$, which is the case for both forms of V which we consider.

Once again, consistency requires that all divergences quadratic and linear in i cancel on the left-hand side of Eq. (28), with V modified to study the strong coupling limit. Using the approximate forms of the relevant matrix elements given earlier, it is straightforward to verify that the recursion relation in Eq. (37) originally derived to analyze finite coupling is sufficient to guarantee the cancellations in the strong coupling limit as well. The only difference between the two cases lies presumably only in the $O(1/i^2)$ term, which plays

TABLE II. Energy eigenvalues by truncation.

i max/2↓	$\lambda\rightarrow$	0.1	0.2	0.3	1	2	3
5		1.06529	1.11829	1.16406	1.39337	1.61123	1.77481
10		1.06529	1.11829	1.16405	1.39235	1.60755	1.76963
15		1.06529	1.11829	1.16405	1.39235	1.60754	1.76959
20		1.06529	1.11829	1.16405	1.39235	1.60754	1.76959

no role in cancellation of divergences. This is a further indication of the nonperturbative nature of the effective operator method.

To conclude, we have implemented an effective operator treatment of the anharmonic oscillator on the lines of Ref. [1]. We have analyzed the validity of a key simplification made in the treatment of the nuclear many body problem. The role of the expansion of the exact eigenfunction in the basis of the unperturbed Hamiltonian in defining *S*, the generator of the similarity transformation has been emphasized. Both the strong and weak coupling cases may be treated along the same lines, underscoring the nonperturbative nature of the formulation. Our numerical application demonstrates rapid convergence to known results with modest effort.

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