

Convergent Behaviour of Morse-Feshbach Nonlinear Perturbation Series: Energy Levels of Anharmonic Oscillator

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Received: 28 March 2024

doi: <https://doi.org/10.55318/bgjp.2026.53.1.001>

Abstract. We make an extensive study on the convergent behaviour of the Morse-Feshbach nonlinear perturbation series (MFNPS) to find out the energy levels of an anharmonic oscillator (AHO) in both weak and strong coupling limits. We developed a new method of multi-step optimal splitting to get convergence in MFNPS for the ground state of AHO and found that two-step optimal splitting is sufficient to provide convergence in MFNPS. Unlike the ground state, the optimal splitting parameters for excited states were modified according to their state dependence to achieve convergence in MFNPS. We apply both single-step and two-step optimal splitting up to the 10th excited states of AHO in both weak and strong coupling limits and achieve a good level of convergence in MFNPS.

KEY WORDS: Morse-Feshbach, non-linear perturbation series, anharmonic oscillator, energy levels.

1 Introduction

In quantum mechanics, the exact solution of Schrödinger equation exist only for a few Hamiltonians. However for any arbitrary Hamiltonian, one has to use some sort of approximation. Perturbation theory is one of the few principal methods of approximation in finding solution to eigenvalue problems in quantum mechanics [1–11]. In perturbation theory, one needs to solve the Hamiltonian of the type

$$H = H_0 + \lambda\mathcal{H}, \quad (1)$$

where H_0 is the unperturbed Hamiltonian, which can be solved exactly and $\lambda\mathcal{H}$ is the perturbation term. If E corresponds to the energy of the total Hamiltonian H and $E_n^{(0)}$ to the unperturbed Hamiltonian H_0 , then one can obtain E in two different ways as

$$E = f(E_n^{(0)}, \lambda) \quad (2)$$

or

$$E = f(E, E_n^{(0)}, \lambda). \quad (3)$$

It is evident from the relation in Eq.2 that R.H.S is a function of known energy $E_n^{(0)}$ and coupling constant λ . This method of calculation is known as constant function perturbation theory as seen from the literature [1–6]. In Eq.3 both L.H.S and R.H.S are the function of unknown energy E . This type of perturbation series is known as a nonlinear series. The simplest nonlinear perturbation series is the Morse-Feshbach nonlinear perturbation series (MFNPS) [8, 9]. Further, it is observed that almost all attempts of perturbation theory reflect Eq.2 with AHO as an example [1, 2, 5, 6, 11–14]. The existing work on nonlinear series reflecting Eq.3 is meager [8, 9]. Because of its highly nonlinear nature MFNPS is extremely difficult to solve analytically and needs high computational skill to solve it numerically to achieve higher-order convergence. The solution encounters two major difficulties. First, there are always no small parameters allowing for the safe use of perturbation theory, and even when small parameters exist, the related perturbative series are strongly divergent. Second, such perturbative series in powers of these parameters are rather short, so that the standard resummation techniques yield bad approximations. The basic aim of this paper is to study the applicability of this series by calculating both ground state and excited state energy considering AHO as an example with weak and strong coupling limits.

2 Morse-Feshbach Nonlinear Perturbation Series (MFNPS)

In this section, an attempt has been made, as shown below, to write the MFNPS in a simplified language [8, 9]. Let us solve the unperturbed Hamiltonian

$$H_0 |n\rangle = E_n^{(0)} |n\rangle, \quad (4)$$

where $|n\rangle$ is the unperturbed eigenstate corresponding to energy eigenvalue $E_n^{(0)}$. According to MFNPS, the n^{th} state energy E_n for the total perturbed Hamiltonian H is given as

$$\begin{aligned} E_n = & E_n^{(0)} + \lambda \langle n | \mathcal{H} | n \rangle + \lambda^2 \sum_{m \neq n} \frac{\langle n | \mathcal{H} | m \rangle \langle m | \mathcal{H} | n \rangle}{(E_n - E_m^{(0)})} \\ & + \lambda^3 \sum_{m, k \neq n} \frac{\langle n | \mathcal{H} | m \rangle \langle m | \mathcal{H} | k \rangle \langle k | \mathcal{H} | n \rangle}{(E_n - E_m^{(0)})(E_n - E_k^{(0)})} \\ & + \lambda^4 \sum_{m, k, p \neq n} \frac{\langle n | \mathcal{H} | m \rangle \langle m | \mathcal{H} | k \rangle \langle k | \mathcal{H} | p \rangle \langle p | \mathcal{H} | n \rangle}{(E_n - E_m^{(0)})(E_n - E_k^{(0)})(E_n - E_p^{(0)})} \\ & + \lambda^5 \sum_{m, k, p, q \neq n} \frac{\langle n | \mathcal{H} | m \rangle \langle m | \mathcal{H} | k \rangle \langle k | \mathcal{H} | p \rangle \langle p | \mathcal{H} | q \rangle \langle q | \mathcal{H} | n \rangle}{(E_n - E_m^{(0)})(E_n - E_k^{(0)})(E_n - E_p^{(0)})(E_n - E_q^{(0)})} \\ & \dots + \lambda^K \sum_{m \dots z \neq n} \frac{\langle n | \mathcal{H} | m \rangle \dots \langle z | \mathcal{H} | n \rangle}{(E_n - E_m^{(0)}) \dots (E_n - E_z^{(0)})}. \end{aligned} \quad (5)$$

Here K is the order of terms in the perturbation series.

2.1 Convergence test for ground state using two-step optimal splitting

In this section, we test the convergence of the ground state energy of the AHO, whose Hamiltonian is given as

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x^4, \quad (6)$$

using two-step optimal splitting in higher-order calculation. The coordinates x and momentum p satisfy the relation

$$[x, p] = i. \quad (7)$$

Now we rewrite the Hamiltonian in Eq.6 as

$$H = \frac{p^2}{2} + w^2 \frac{x^2}{2} + \lambda x^4 - f(x), \quad (8)$$

where w is a parameter and

$$f(x) = \frac{6\lambda x^2}{2w}, \quad (9)$$

$$w^2 = 1 + \frac{6\lambda}{w}. \quad (10)$$

Further we rewrite the Eq.8 as

$$H = \frac{p^2}{2} + W_1^2 \frac{x^2}{2} + \lambda x^4 - f(x) - F_1(x), \quad (11)$$

where W_1 is another parameter and

$$F_1(x) = \frac{6\lambda x^2}{2W_1}, \quad (12)$$

$$W_1^2 = w^2 + \frac{6\lambda}{W_1}. \quad (13)$$

Now we rewrite the Hamiltonian as

$$H = H_D + H_N, \quad (14)$$

where H_D is the diagonal term considered as unperturbed Hamiltonian for the MFNPS in Eq. 4. Similarly, H_N is the non-diagonal term considered as a perturbation term for the MFNPS in Eq.5. Now to find the expression for H_D and H_N , we use the second quantization formalism, instead of coordinate representation. We use the transformation

$$x = \frac{a + a^\dagger}{\sqrt{2w}}, \quad (15)$$

$$p = -i\sqrt{\frac{w}{2}}(a - a^\dagger) \quad (16)$$

and the commutation relation

$$[a, a^\dagger] = 1. \quad (17)$$

The explicit expression for H_D in terms of creation operator a^\dagger and annihilation operator a is

$$H_D = \frac{\left(W_1 + \frac{1}{W_1}\right)(2a^\dagger a + 1)}{4} + \lambda \frac{3 + 12a^\dagger a + 6(a^\dagger)^2 a^2}{4W_1^2}. \quad (18)$$

Similarly the expression for H_N in terms of creation operator a^\dagger and annihilation operator a is

$$H_N = \lambda \left[\frac{a^4 + (a^\dagger)^4 + 4(a^\dagger)^3 a + 4a^\dagger a^3}{4W_1^2} - \frac{3(a^2 + (a^\dagger)^2)}{2wW_1} \right]. \quad (19)$$

The nonzero expectation values of the diagonal Hamiltonian H_D are given as

$$\langle n|H_D|n\rangle = \left(\frac{2n+1}{4}\right) \left(W_1 + \frac{1}{W_1}\right) + \frac{3\lambda}{4W_1^2}(2n^2 + 2n + 1). \quad (20)$$

The nonzero expectation values of the non-diagonal Hamiltonian H_N are given as

$$\langle n|H_N|n+2\rangle = \frac{\lambda\sqrt{(n+1)(n+2)}}{W_1} \left(\frac{n}{W_1} - \frac{3}{2w}\right), \quad (21)$$

$$\langle n|H_N|n+4\rangle = \frac{\lambda\sqrt{(n+1)(n+2)(n+3)(n+4)}}{4W_1^2}. \quad (22)$$

Table 1. Convergent value for ground state energy E_0 of an AHO with $\lambda = 1$ in MFNPS using two-step optimal splitting parameters. For comparison, results obtained by Caswell [1] are also given. The number in parenthesis is the estimate of the accuracy of the final digit obtained using 15 terms of perturbation series

Order K	Convergent value E_0 with $w = 2.0$ and $W_1 = 2.52510225481$	Order K	Convergent value E_0 with $w = 2.0$ and $W_1 = 2.52510225481$
0	0.847907429	8	0.8037708
1	0.847907429	9	0.8037707
2	0.8041	10	0.80377064
3	0.8039	11	0.80377063
4	0.80379	12	0.80377062
5	0.803779	13	0.80377063
6	0.803772	14	0.803770624
7	0.803771	15	0.803770628
Caswell [1]		0.8037706513 (7)	

The two step optimal splitting parameters w and W_1 are evaluated from the cubic equation Eq. 10 and Eq. 13 respectively and found to be $w = 2.0$ and $W_1 = 2.52510225481$. The MFNPS given in Eq. 5 has been solved numerically for the ground state energy of AHO using the above two step optimal splitting parameters w and W_1 . The convergent ground state energy values for different order of terms K in MFNPS with coupling constant $\lambda = 1$ is given in Table 1. Here we achieved a good level of convergence up to 8^{th} digits after decimal point for 15 order of terms in the perturbation series.

2.2 Convergence test for groundstate using multi-step optimal splitting

In this section, we introduce a multi-step optimal splitting approach on parameter calculation with an aim to improve the convergence. Following the previous procedure, we write the Hamiltonian H as

$$H = \frac{p^2}{2} + W_k^2 \frac{x^2}{2} + \lambda x^4 - f(x) - F_1(x) - \dots - F_k(x). \quad (23)$$

Now we write the expression for H_D as

$$H_D = \frac{\left(W_k + \frac{1}{W_k}\right)(2a^\dagger a + 1)}{4} + \lambda \frac{3 + 12a^\dagger a + 6(a^\dagger)^2 a^2}{4W_k^2}. \quad (24)$$

Similarly the expression for H_N is

$$H_N = \lambda \left[\frac{a^4 + (a^\dagger)^4 + 4(a^\dagger)^3 a + 4a^\dagger a^3}{4W_k^2} - \frac{3(a^2 + (a^\dagger)^2)}{2W_k} \left(\frac{1}{W_{k-1}} + \frac{1}{W_{k-2}} + \dots + \frac{1}{W_1} + \frac{1}{w} \right) \right], \quad (25)$$

where k is the order of multi-step optimal splitting. The optimal splitting parameters W_k are given by

$$W_k^2 = W_{k-1}^2 + \frac{6\lambda}{W_k} \quad (26)$$

with

$$W_1^2 = w^2 + \frac{6\lambda}{W_1}. \quad (27)$$

The nonzero expectation values of diagonal Hamiltonian H_D are given as

$$\langle n | H_D | n \rangle = \left(\frac{2n+1}{4} \right) \left(W_k + \frac{1}{W_k} \right) + \frac{3\lambda}{4W_k^2} (2n^2 + 2n + 1). \quad (28)$$

The non-zero expectation values of non diagonal Hamiltonian H_N are given as

$$\langle n|H_N|n+2\rangle = \frac{\lambda\sqrt{(n+1)(n+2)}}{W_k} \times \left[\frac{n}{W_k} - \frac{3}{2} \left(\frac{1}{W_{k-1}} + \frac{1}{W_{k-2}} + \cdots + \frac{1}{W_1} + \frac{1}{w} \right) \right], \quad (29)$$

$$\langle n|H_N|n+4\rangle = \frac{\lambda\sqrt{(n+1)(n+2)(n+3)(n+4)}}{4W_k^2}. \quad (30)$$

Here we evaluated the parameters of three-step, four-step and five-step optimal splitting from the cubic recurrence relation given in Eq. 26. The multi-step optimal splitting parameters are listed in Table 2. The convergent values of the ground state energy E_0 of AHO, with coupling constant $\lambda = 1$ is given in Table 2. The level of convergence achieved for ground state energy of AHO for different optimal splitting as a function of order of terms in MFNPS is illustrated in Fig. 1. From the above results we found that for the ground state, two step optimal splitting is sufficient to provide convergence in the perturbation series.

Table 2. Convergent value for ground state energy E_0 of an AHO with $\lambda = 1$ in MFNPS using multi step optimal splitting parameters

Order	Convergent value E_0	Convergent value E_0	Convergent value E_0
	$w = 2.0$	$w = 2.0$	$w = 2.0$
K	$W_1 = 2.52510225481$	$W_1 = 2.52510225481$	$W_1 = 2.52510225481$
	$W_2 = 2.90538656129$	$W_2 = 2.90538656129$	$W_2 = 2.90538656129$
		$W_3 = 3.21090388686$	$W_3 = 3.21090388686$
			$W_4 = 3.46974595594$
0	0.901242878	0.953331243	1.00178467
1	0.901242878	0.953331243	1.00178467
2	0.802	0.804	0.809
3	0.805	0.809	0.815
4	0.8037	0.803	0.803
5	0.8038	0.8040	0.804
6	0.803770	0.80374	0.803
7	0.803771	0.80378	0.8038
8	0.80377067	0.80376	0.80375
9	0.80377065	0.80377154	0.80378
10	0.803770634	0.80377053	0.803769
11	0.803770632	0.80377069	0.803771
12	0.8037706314	0.80377064	0.8037704
13	0.80377063129	0.80377065	0.8037707
14	0.803770631219	0.803770647	0.80377061
15	0.803770631216	0.803770648	0.80377064
Caswell [1]		0.8037706513 (7)	

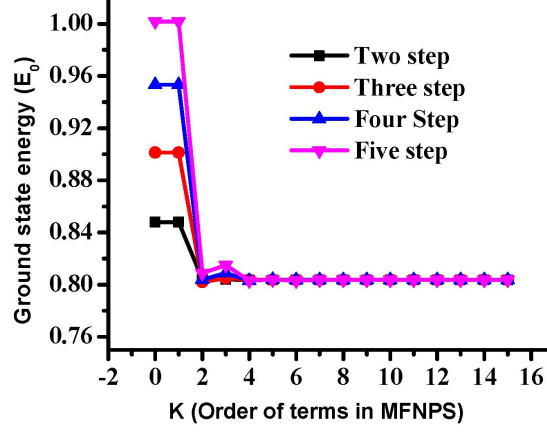


Figure 1. Ground state energy E_0 of an AHO with $\lambda = 1$ in MFNPS using two-step, three-step, four-step, and five-step optimal splitting parameters.

3 State-Dependent Parameter Calculation for Excited States Using Single Step Optimal Splitting

The state-dependent parameter W is determined in such a way that it will simultaneously make H_D and H_N as small as possible. One of the simplest ways is to determine W from H_D for the desired state, say n , using the variational principle

$$\frac{d\langle n|H_D|n\rangle}{dW} = 0. \quad (31)$$

W is determined from the cubic equation

$$W^3 - W - \frac{6\lambda(2n^2 + 2n + 1)}{(2n + 1)} = 0. \quad (32)$$

For ground state $n = 0$, the above equation gets reduced to the state-independent equation as discussed in Eq 10.

Now with this variational parameter, the non-zero expectation value of diagonal Hamiltonian H_D is given as

$$\langle n|H_D|n\rangle = \frac{2n + 1}{4} \left(W + \frac{1}{W} \right) + \frac{3\lambda}{4W^2} (2n^2 + 2n + 1). \quad (33)$$

The nonzero expectation value of nondiagonal Hamiltonian H_N is given as

$$\langle n|H_N|n+2\rangle = \left[\frac{1}{4} \left(-W + \frac{1}{W} \right) + \frac{\lambda}{W^2} \left(n + \frac{3}{2} \right) \right] \sqrt{(n+1)(n+2)}, \quad (34)$$

$$\langle n|H_N|n+4\rangle = \frac{\lambda \sqrt{(n+1)(n+2)(n+3)(n+4)}}{4W^2}. \quad (35)$$

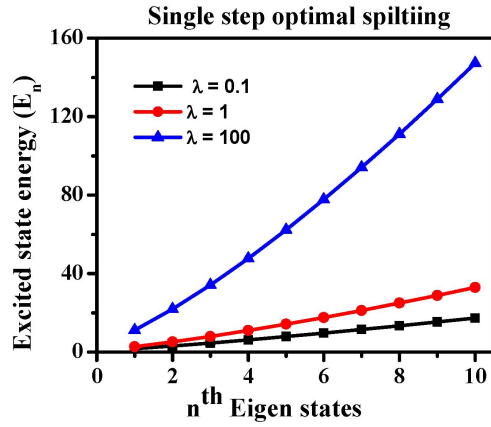


Figure 2. Convergent energy eigenvalues for different excited state for coupling constant $\lambda = 0.1, 1.0, 10$ with $K = 15$ order of terms in MFNPS using single-step optimal splitting variational parameters.

Table 3. The convergent eigenvalues for different excited state for coupling constant $\lambda = 0.1, 1.0, 10$ using single-step optimal splitting variational parameters. For comparison of convergence we gave the results for 14 and 15 order of terms in the perturbation series corresponding to different excited states $n = 1$ to $n = 10$

State n	Order K	E_n for coupling parameter $\lambda = 0.1$	E_n for coupling parameter $\lambda = 1$	E_n for coupling parameter $\lambda = 100$
1	14	1.7695025	2.737826568	11.185
1	15	1.7695027	2.737955961	11.188
2	14	3.1386242	5.1792031	21.906
2	15	3.1386243	5.1793031	21.907
3	14	4.6288827	7.942400664	34.1824
3	15	4.6288828	7.942406660	34.1825
4	14	6.2203008	10.963582	47.7071
4	15	6.2203009	10.963583	47.7072
5	14	7.89976725	14.203138	62.28123
5	15	7.89976726	14.203139	62.28124
6	14	9.657840024	17.634048	77.77076
6	15	9.657840029	17.634049	77.77077
7	14	11.487315622	21.2364354	94.0780479
7	15	11.487315625	21.2364355	94.0780494
8	14	13.3824749	24.99493650	111.1279601
8	15	13.3824748	24.99493657	111.1279607
9	14	15.33864203	28.89725106	128.8606294
9	15	15.33864207	28.89725105	128.8606296
10	14	17.351907678	32.9332631	147.226995
10	15	17.3519076	32.9332630	147.226994

The state-dependence single-step optimal splitting parameters for different excited states are evaluated from the cubic equation Eq. 32. The convergent eigenvalues for different excited states has been evaluated numerically and shown in Table 3 for both weak and strong coupling limit $\lambda = 0.1, 1.0, 100$. The convergent energy eigenvalues for different coupling constant $\lambda = 0.1, 1.0, 100$ as function of excited states is illustrated in Fig. 2.

4 State-Dependent Parameter Calculation for Excited States Using Two-Step Optimal Splitting

In this section, we introduce the state-dependent parameter using two-step optimal splitting procedure for the convergence test on excited states. The two optimal splitting parameters W and w are calculated from the cubic equation:

$$W^3 - w^2W - \frac{6\lambda(2n^2 + 2n + 1)}{(2n + 1)} = 0, \quad (36)$$

where

$$w^2 = 1 + \frac{6\lambda}{w}. \quad (37)$$

The nonzero expectation value diagonal Hamiltonian H_D is given as

$$\langle n|H_D|n\rangle = \left(\frac{2n+1}{4}\right)\left(W + \frac{1}{W}\right) + \frac{3\lambda}{4W^2}(2n^2 + 2n + 1), \quad (38)$$

$$\langle n|H_N|n+2\rangle = \sqrt{(n+1)(n+2)}\left[\frac{-W}{4} + \frac{1}{4W} + \frac{\lambda}{W^2}\left(n + \frac{3}{2}\right)\right]. \quad (39)$$

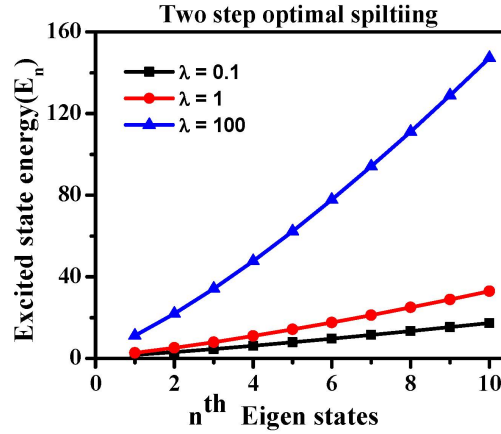


Figure 3. Convergent energy eigenvalues for different excited state for coupling constant $\lambda = 0.1, 1.0, 10$ with $K = 15$ order of terms in MFNPS using two-step optimal splitting variational parameters.

The nonzero expectation value nondiagonal Hamiltonian H_N is given as

$$\langle n|H_N|n+4\rangle = \frac{\lambda\sqrt{(n+1)(n+2)(n+3)(n+4)}}{4W^2}. \quad (40)$$

The convergent energy eigenvalues for different excited states up to $K = 14$ and $K = 15$ order of terms in the perturbation series for both weak and strong coupling limits $\lambda = 0.1, 1, 100$ are given in Table 4. Numbers in the parenthesis represent the degree of convergence achieved for $K = 14$ and $K = 15$ order of terms in the perturbation series. The convergent eigenvalues of different coupling constants $\lambda = 0.1, 1, 100$ for various excited states are illustrated in Fig. 3.

Table 4. Excited state energy levels E_n of the AHO using $K = 14$ order of terms in the MFNPS perturbation series using two-step optimal splitting variational parameters. Numbers in parentheses represent the convergent digits for 14 and 15 order terms in the perturbation series

State n	Order K	E_n for coupling parameter $\lambda = 0.1$	E_n for coupling parameter $\lambda = 1$	E_n for coupling parameter $\lambda = 100$
1	14	1.7695025954	2.73789228	11.18829
1	15	1.7695025957 (10)	2.73789229 (8)	11.18725 (4)
2	14	3.1386241977	5.179291722	21.90689767
2	15	3.1386241978 (10)	5.179291724 (9)	21.90689768 (9)
3	14	4.62888251162	7.942403919	34.1825234878
3	15	4.62888251166 (11)	7.942403920 (9)	34.1825234871 (11)
4	14	6.22030086313	10.9635829385	47.70720519
4	15	6.22030086314 (11)	10.9635829382 (11)	47.70720518 (9)
5	14	7.899767113294	14.203139252	62.2812382
5	15	7.899767113290 (12)	14.203139250 (10)	62.2812381 (8)
6	14	9.6578400597	17.63404889	77.770772
6	15	9.6578400596 (10)	17.63404886 (9)	77.770771 (7)
7	14	11.487315307	21.2364359	94.078057
7	15	11.487315305 (10)	21.2364355 (8)	94.078050 (7)
8	14	13.38247452	24.994939	111.12799
8	15	13.38247450 (9)	24.994935 (7)	111.12795 (7)
9	14	15.3386416	28.89726	128.860656
9	15	15.3386414 (8)	28.89724 (6)	128.860655 (8)
10	14	17.351907	32.933264	147.226984
10	15	17.351906 (7)	32.933265 (7)	147.226983 (8)

5 Results and Discussion

Now replacing $\lambda\mathcal{H}$ by H_N and H_0 by H_D in Eq.(1, 4, 5) we calculate the ground state energy of the AHO up to 15 order of terms in the MFNPS. Table 1 shows the convergent values for ground state energy E_0 of an AHO with $\lambda = 1$ for two-step optimal splitting parameters as discussed in Section 2.1. Here K is the

order of terms in the perturbation series. The higher the number of terms in the perturbation series, the higher the convergent digits. We obtained a convergency of 8 digits for a 15 order of terms. For comparison, we also given the result obtained for ground state by Caswell [1], which is exactly matching up to 8 digits.

We also calculate the groundstate energy E_0 for $\lambda = 1$ for multi-step splitting parameters as discussed in Section 2.2 and the results are given in Table 2. We notice that the two-step optimal splitting is sufficient to provide convergence in MFNPS for the ground state of AHO. Two-step optimal splitting approach is also applied to the ground state of AHO for the higher coupling parameter λ . Table 2 shows the last three higher-order convergent results for different coupling parameters λ . The results are matching with the results of Caswell [1]. We apply previously calculated optimal splitting parameters for the ground state of AHO to the excited state of AHO. The results are given in Table 5. We observe that for $n \geq 5$, the MFNPS is not giving any convergent value, and also for $n \leq 5$, the number of convergent digits decreases with the increase of state value n . Again the convergent results are not comparable for higher excited states with the results calculated previously by several authors [1–3]. This was expected as the excited state energy depends on the state value n . So the optimal splitting parameters have to be modified according to their state dependence. The state-dependent parameter W is determined using the variational technique as discussed in Section 3. We calculate the excited state energies of an AHO up to 14 order and 15 order terms in MFNPS using the single-step (two-step)

Table 5. Convergent value for excited state energy E_n of an AHO using 15 order of terms of the MFNPS using optimal splitting parameters for the ground state (NC-No Convergency)

State E_n	E_n for Coupling parameter $\lambda = 0.1$	E_n for Coupling parameter $\lambda = 1$	E_n for Coupling parameter $\lambda = 100$
1	1.769502633601580	2.737893473247960	11.18727013754662
2	3.138624640483820	5.179368610682413	21.90792389514790
3	4.628893580258386	7.944276200342911	34.20660264641097
4	6.220490587163873	10.98830903940391	48.00716948459711
5	7.901913609979696	14.41671095662173	65.17919098201246
6	9.674274270406038	NC	NC
7	11.58029965657092	NC	NC
8	NC	NC	NC
9	NC	NC	NC
10	NC	NC	NC

variational parameters and the results are given in Table 3 (Table 4). We achieve a convergence up to a minimum of 7 digits.

6 Conclusion

In this paper, we have taken a very fruitful approach to get convergence in MFNPS in order to get the energy levels of an AHO. The problem of energy levels of AHO has been analyzed from wide angles to achieve convergence in MFNPS. MFNPS seems to be one of the simplest nonlinear series to be used for energy levels of AHO. The optimal splitting method is found to be a very efficient technique to achieve convergence in MFNPS.

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