Energy Levels of One Dimensional Anharmonic Oscillator via Neural Networks

Halil Mutuk*

Physics Department, Ondokuz Mayis University, 55139, Samsun, Turkey

In this work, we obtained energy levels of one dimensional quartic anharmonic oscillator by using neural network system. Quartic anharmonic oscillator is a very important tool in quantum mechanics and also in quantum field theory. Our results are in good agreement in high accuracy with the reference studies.

PACS numbers: 03.65.-w, 84.35.+i

I. INTRODUCTION

The theory of harmonic and anharmonic oscillators have an important applications in all areas of physics. Especially harmonic oscillator is an important analogy while modelling physical systems. Most quantum mechanical problems are tried to be solved by harmonic oscillator analogy. Many physical problems can be reduced to a harmonic oscillator problem with appropriate boundary conditions. This is because harmonic oscillator eigenvalue problem can be solved exactly, i.e. it has analytic solution. The Schrödinger equation with harmonic oscillator potential can be solved by using algebraic techniques, say using ladder operators.

Yet there is no pure harmonic oscillator in the nature. That is why anharmonic oscillator have been the focus of attention since the early days of quantum mechanics [1–11]. The general method to solve anharmonic oscillator problem is Rayleigh-Schrödinger perturbation theory but it is well known that the expansion of series in terms of eigenvalues, are convergent only small values for the coupling potential parameter. Moreover excited states can be problematic due to convergence problem. Overwhelming these difficulties is cumbersome: either solving a numerical difference equations [12] or summation of strongly divergent perturbation series [13, 14]. To overwhelm these difficulties some nonperturbative methods are also used [15, 16]. The particular feature of all these approaches is that, they have some additional restrictions on the field of their applications.

In recent years, considerable progress has been made to develop mathematical methods for calculating eigenvalues and eigenfunctions of anharmonic oscillators. In [17], the authors presented new perspective for the anharmonic oscillator problem based on the SU(2) group method (SGM). In [18], Popescu showed how the variational method, in which a variational global parameter is used, can be combined with the finite element method for the study of the generalized anharmonic oscillator in D dimensions. Koscik and Okopinska applied power series method to compute the spectrum of the Schrödinger equation for central potential [19]. Dong et al. in [20],

proposed a new anharmonic oscillator and present the exact solutions of the Schrödinger equation with this oscillator by constructing new ladder operators. Sous in [21], by utilizing an appropriate ansatz to the wave function, reproduced the exact bound-state solutions of the radial Schrödinger equation to various exactly solvable sextic anharmonic oscillator and confining perturbed Coulomb models in D dimensions. Ikhdair and Sever utilized an appropriate ansatz to the wave function and they reproduced the exact bound-state solutions of the radial Schrödinger equation to various exactly solvable sextic an-harmonic oscillator and confining perturbed Coulomb models in D-dimensions [22]. Ciftci studied quantum quartic anharmonic oscillator problem and obtained accurate eigenvalues for both small and large coupling parameters [23] via asymptotic iteration method. Liverts et al. solved Schrödinger equation with a certain potential by first casting the Schrödinger equation into a nonlinear Riccati form and then solving that nonlinear equation analytically in the first iteration of the quasilinearization method (QLM) [24]. In work of Nagy and Sailer [25], functional renormalization group methods formulated in the real-time formalism are applied to the O(N) symmetric quantum anharmonic oscillator, considered as a (0+1)dimensional quantum field-theoric model, in the next-toleading order of the gradient expansion of the one- and two-particle irreducible effective action. Maiz and Al-Faify applied Airy function approach to quantum anharmonic oscillator by setup to approach the real potential V(x) of the anharmonic oscillator system as a piecewise linear potential u(x) and to solve the Schrödinger equation of the system using the Airy function [26]. Fernandez showed the application of group theory to a quantummechanical three-dimensional quartic anharmonic oscillator with O-h symmetry [27].

All these methods above have their own shortcomings. For example, most of the usable approaches have no indication for the behaviour of the anharmonic oscillator wave functions in physically relevant ranges of their coordinates [11].

Artificial neural networks (ANNs) are being used since two decades for solving ordinary and partial differential equations. Traditional numerical techniques require discretization of domain by the number of finite domains or points where the solution functions are locally approximated. Thay are iterative methods and can contain com-

 $[*]Electronic \ address: \ halilmutuk@gmail.com$

putational complexity because of the repetition of iterations when the number of sampling points and dimensions of the problem increase. Compared to existing numerical techniques, ANNs provide some advantages such as, solution functions have a single independent variable regardless of the dimension of the problem and solutions are continuous over all the domain of integration. The computational complexity does not increase remarkably when the the number of sampling points and dimensions of the problem increase.

In the present work, we consider the following anharmonic oscillator Hamiltonian:

$$H(x) = \frac{p^2}{2m} + x^2 + \lambda x^4$$
 (1)

where λ is a parameter. The eigenvalues of this Hamiltonian was studied in [23, 28] and extensively in [29]. We obtained energy eigenvalues of this anharmonic oscillator potential via artificial neural network.

The paper is organized as follows. In Section II we give methodology of artificial neural network and in Section III, we give our numerical results. In Section IV, we discuss and conclude our work.

II. ARTIFICIAL NEURAL NETWORK FORMALISM

Artificial neural network systems (ANN) are simplified models of biological nervous systems. They are based on the systems of biological neurons that receive, process, and transmit information through electrical and chemical signals. In this manner artificial neural networks are made of artificial neurons and these neurons are imitations of biological neurons. A neuron has a dendrite and this can be excited by synapses of other neurons. As a result of this excitement, an electrical signal is produced and transmitted through its axon. This process repeat itself with dendrites of other neurons through its synapse. A biological neural network can be seen in Figure 1.

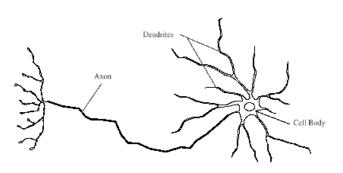
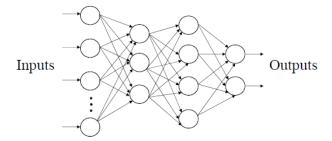


FIG. 1: A biological neural network picture

Being a mimicked version of biological neuron, artificial neurons are connected to each other and excite each other through these connections. Neural networks are

organized in layers. The input layers receive information from outside world and send them to the hidden layers. Generally, there is no process of information in input layers. A neural network diagram is shown in Figure 2.



Input Layers Hidden Layers Output Layers

FIG. 2: A neural network architecture

There is one in and one out of every process element. The output is being sent to all processing elements from input layers. The hidden layers process the outputs coming from input layers and process information. They send their outputs to the output layers. Output layers produce outputs according to the inputs from input layers and send to the outside world. Every process element is connected to the all process elements from hidden layers. The mathematical formulation of a single neuron is shown in Figure 3.

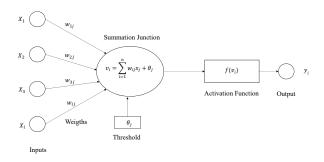


FIG. 3: A schematic diagram of single neuron

A neuron (perceptron in computerized systems) N_i accepts a set of n inputs which is an element of the set $S = \{x_j | j = 1, 2, \dots, n\}$. Each input is weighted before entrance of a neuron N_i by weight factor w_{ij} for $j = 1, 2, \dots, n$. Furthermore, it has bias term w_0 , a threshold value θ_k which has to be reached or exceeded

for the neuron to produce output signal. Mathematically, the output of the i-th neuron N_i is

$$O_i = f(w_0 + \sum_{j=1}^n w_{ij} x_j).$$
 (2)

The neuron's work condition can be defined as

$$w_0 + \sum_{j=1}^n w_{ij} x_j \ge \theta, \tag{3}$$

and the input signal of the *i*-th neuron N_i is

$$v_i = w_0 + \sum_{j=1}^n w_{ij} x_j. (4)$$

A function f(s) acts on the produced weighted signal. This function is called activation function. The output signal obtained by activation function is

$$O_i = f(v_i - \theta_i). (5)$$

All inputs are multiplied by their weights and added together to form the net input to the neuron. This is called net and can be written as

$$net = \sum_{j=1} w_{ij} x_j + \theta, \tag{6}$$

where θ is a threshold value which is added to the neuron. The neuron takes these inputs and produce an output y by mapping function f(net)

$$y = f(\text{net}) = f\left(\sum_{j=1}^{n} w_{ij} x_j + \theta\right)$$
 (7)

where f is the neuron activation function. Generally the neuron output function is proposed as a threshold function but linear, sign, sigmoid or step functions are widely used. We used a sigmoid activation function

$$f(x) = \frac{1}{1 + e^{-x}} \tag{8}$$

which is typical in multilayer perceptron neural networks. We used feed forward neural network. A feed forward neural network is the simplest form of the artifical neural network. The information moves only in one direction forward from the input nodes to the hidden and to the output nodes. If the connections between neurons are only in forward direction, the network is called a feed forward network. Connections between neurons that are in the same layer or in nonconsecutive layers are not allowed in feed forward neural networks. Figure 2 represents a feed forward neural network.

The learning procedure of neural network in this work is unsupervised learning. In this procedure, weight adjustments are not based on comparison with some target output but some guidelines for successful learning (for example, ground state energy eigenvalue in the harmonic oscillator) is required.

A. A warm up example: Harmonic oscillator

In this subsection, we obtained ground state harmonic oscillator energy eigenvalue. The oscillator potential $V(x)=\frac{1}{2}wx^2$ in the Schrödinger equation can be solved by using algebraic method, such as ladder operators. Many problems in physics can be reduced to a harmonic oscillator problem with appropriate initial/boundary conditions. The Schrödinger equation of harmonic oscillator potential can be written with $w=m=\hbar=1$ as

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}x^2\psi(x) = E\psi(x)$$
 (9)

where E is the eigenvalue. The wave function satisfies the boundary conditions $\psi(-\infty) = \psi(\infty) = 0$. The energy levels of the harmonic oscillator can be found by

$$E_n = (n + \frac{1}{2})\hbar w \tag{10}$$

where n is the principal quantum number and equals n=0 for the ground state. Once the neural network parameters (weights and biases) and a pretrain value for energy are defined, the neural network obtained the eigenvalue which is presented in Table I.

TABLE I: Comparison of ground state eigenvalue of harmonic oscillator

Eigenvalue	ANN	Exact
\overline{E}	0.502739612	0.5

Motivated from this evaluation, we obtained eigenvalues of the anharmonic oscillator in the following section.

III. NUMERICAL RESULTS

In this section we give numerical results of the anharmonic oscillator eigenvalues. In Table II, eigenvalues for the anharmonic oscillator are presented.

It can be seen from Table II that obtained eigenvalues for different λ values are in good agreement with the given references except than the results of Ref. [30], especially for large λ values. Note that the results of Ref. [30] are multiplied by 2 for correspondence.

TABLE II: Ground state eigenvalues for the quartic anharmonic oscillator with different λ values in one dimension.

λ	E_{present}	[23]	[28] Num.	[30]
0.025	1.0180097924545166	1.0180010006248	1.0180010006142	1.0180010006142
0.05	1.034240512816455	1.0347296978234	1.0347296972554	1.0347296972530
0.1	1.0654383929670153	1.0652855199	1.0652855096	1.0652854984
0.2	1.1131419947840997	1.1182927141	1.1182926544	1.1182887632
0.5	1.2430124818673798	1.2418546983	1.2418540597	1.2412579542
1.0	1.3929635377412355	1.3923519526	1.3923516416	1.3853951994
4.0	1.9029500973873372	1.9031372697	1.9031369454	1.769229616
100.0	4.9974247519017035	4.9991429	4.9994175452	4.9580018282
400.0	7.862963023360612	7.8620150257	7.8618626782	7.670735377
2000	13.382962917034375	13.388719667	13.388441701	12.7473822552
40000	36.2329683376409	36.275234713	36.274458146	33.30734404
2×10^{6}	133.6329668678526	133.6029981	133.6001252^{35}	120.199459212

TABLE III: First eight eigenvalues of the quartic anharmonic oscillator for $\lambda=0.1$ in one dimension

\overline{n}	E_{present}	[23]	[31]
0	1.0654383929670153	1.065286	1.065286
1	3.3019057811028074	3.306872	3.306872
2	5.749852350602235	5.747959	5.747959
3	8.358116291676646	8.352686	8.352678
4	11.09861795976142	11.09837	11.09860
5	13.968331266291228	13.96890	13.96993
6	16.95956005318641	16.95307	16.95479
7	20.000623087595994	20.00854	20.04386

In Table III, first eight eigenvalues of the quartic anharmonic oscillator are presented. Obtained eigenvalues are in good agreement with the reference studies.

IV. DISCUSSION AND CONCLUSION

Since two decades, machine learning technologies have been steadily developing and obtaining remarkable successes. Especially in particle physics and cosmology, large datasets are present and the current techniques can be insufficient to deal with them. Besides that, there are high energy physics researches by the neural networks [32–34].

The quartic anharmonic oscillator is a very important tool in quantum mechanics and also in quantum field theory. The importance of this anharmonic oscillator potential lyes in nuclear structure, quantum chemistry and quark confinement [5].

In this paper we have applied artificial neural network method to the quartic anharmonic oscillator in one dimension and have been able to find the energies. The results are in very good agreement with accurate numerical values in the literature. Our approach yielded highly accurate results for the energies of the ground state and of some excited states for this anharmonic oscillator.

D. M. Dennison and G. E. Uhlenbeck, The Two-Minima Problem and the Ammonia Molecule, Phys. Rev. 41, 313 (1932).

^[2] R. P. Bell, The occurrence and properties of molecular vibrations with $V(x) = ax^4$, Proc. Roy. Soc. A **183**, 328 (1944).

^[3] C. M. Bender and T. T. Wu, Anharmonic Oscillator, Phys. Rev. 184, 1231 (1969).

^[4] F. T. Hioe, D. MacMillen, and F. T. Montroll, Quantum theory of anharmonic oscillators: Energy levels of a single and a pair of coupled oscillators with quartic coupling, Phys. Rep. 43, 305 (1978).

^[5] P. M. Radmore, The Schrödinger equation with an anharmonic oscillator potential, J. Phys. A- Math. Gen. 13, 173-179 (1980).

^[6] E. Magyari, Exact Quantum Mechanical Solutions for Anharmonic Oscillator, Phys. Lett. A, 81(2-3), 116-118

⁽¹⁹⁸¹⁾

^[7] B. Simon, Large orders and summability of eigenvalue perturbation theory: A mathematical overview, Int. J. Quantum Chem. 21, 3 (1982).

^[8] F. Arias de Saavedra and E. Buendia, Perturbativevariational calculations in two-well anharmonic oscillators, Phys. Rev. A 42, 5073 (1990).

^[9] M. Lakshmanan, P. Kaliappan, K. Larsson, F. Karlsson, and P. O. Fröman, Phase-integral approach to quantal two- and three-dimensional isotropic anharmonic oscillators, Phys. Rev. A 49, 3296 (1994).

^[10] E. Delabaere and F. Pham, Unfolding the Quartic Oscillator, Ann. Phys-New York, 261, 180 (1997).

^[11] L. V. Chebotarev, On the Nature of Energy Levels of Anharmonic Oscillators, Ann. Phys-New York, 273, 114-145 (1999).

^[12] K. Bay and W. Lay, The spectrum of the quartic oscilla-

- tor, J. Math. Phys. 38, 2127 (1997).
- [13] R. Guardiola, M. A. Solis, and J. Ros, Strong-coupling expansion for the anharmonic oscillators $-d^2/dx^2 + x^2 + \lambda x^{2N}$, Nuovo Cim. B **107**, 713 (1992).
- [14] E.J. Weniger, Construction of the Strong Coupling Expansion for the Ground State Energy of the Quartic, Sextic, and Octic Anharmonic Oscillator via a Renormalized Strong Coupling Expansion, Phys. Rev. Lett. 77, 2859 (1996).
- [15] J.L. Chen, L.C. Kwek, C.H. Oh, Y. Liu, Solving the anharmonic oscillator problem with the SU(2) group, J. Phys. A- Math. Gen. **34**(42), 8889-8899 (2001).
- [16] C.R. Handy, Application of the eigenvalue moment method to the quartic anharmonic double-well oscillator, Phys. Rev. A 46, 1663 (1992).
- [17] T. Kunihiro, Renormalization-group resummation of a divergent series of the perturbative wave functions of the quantum anharmonic oscillator, Phys. Rev. D 57, R2035 (1998).
- [18] V. Popescu, Combination of the variational and finite element methods for the D-dimensional generalized anharmonic oscillator, Phys. Lett. A 297(5-6) 338-343 (2002).
- [19] P. Koscik, A. Okopinska, Application of the Frobenius method to the Schrödinger equation for a spherically symmetric potential: an anharmonic oscillator, J. Phys. A- Math. Gen. 38(35), 7743-7755 (2005).
- [20] S.H. Dong, G.H. Sun, M. Lozada-Cassou, Exact solutions and ladder operators for a new anharmonic oscillator, Phys. Lett. A 340(1-4), 94-103 (2005).
- [21] A. J. Sous, Solution for the eigenenergies of sextic anharmonic oscillator potential V(x) = A(6)x(6) + A(4)x(4) + A(2)x(2), Mod. Phys. Lett. A **21**(21), 1675-1682 (2006).
- [22] S.M. Ikhdair, R. Sever, An alternative simple solution of the sextic anharmonic oscillator and perturbed coulomb problems, Int. J. Mod. Phys. C 18(10), 1571-1581 (2007).
- [23] H. Çiftçi, Anharmonic Oscillator Energies by the Asymptotic Iteration Method, Mod. Phys. Lett. A 23(4) 261-267 (2008).

- [24] E.Z. Liverts, V.B. Mandelzweig, Approximate analytic solutions of the Schrödinger equation for the generalized anharmonic oscillator, Phys. Scripta 77(2), 025003 (2008).
- [25] S. Nagy, K. Sailer, Functional renormalization group for quantized anharmonic oscillator, Ann. Phys-New York, 326, 1839-1876 (2011).
- [26] F. Maiz, S. AlFaify, Quantum anharmonic oscillator: The airy function approach, Physica B 441, 17-20 (2014).
- [27] F. M. Fernandez, Group theoretical analysis of a quantum-mechanical three-dimensional quartic anharmonic oscillator, Ann. Phys-New York, 356, 149-157 (2015).
- [28] I. A. Ivanow, Reconstruction of the exact ground-state energy of the quartic anharmonic oscillator from the coefficients of its divergent perturbation expansion, Phys. Rev. A 54, 81 (1996).
- [29] B. Simon, Coupling constant analyticity for the anharmonic oscillator, Ann. Phys. (N.Y.) 58, 76 (1970).
- [30] G.F. Chen, Extended Rayleigh–Schrödinger perturbation theory for the quartic anharmonic oscillator, J. Phys. A-Math. Gen. 34(4), 757–769 (2001).
- [31] A. Mostafazadeh, Variational Sturmian approximation: A nonperturbative method of solving time-independent Schrödinger equation, J. Math. Phys. 42, 3372 (2001).
- [32] J. Barnard, E. N. Dawe, M. J. Dolan, and N. Rajcic, Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks, Phys. Rev. D 95, 014018 (2017).
- [33] P. Baldi, K. Cranmer, T. Faucett, P. Sadowski, and D. Whiteson, Parameterized neural networks for highenergy physics, Eur. Phys. J. C 76(5), 235 (2016).
- [34] M. Paganini, L. de Oliveira, and B. Nachman, CaloGAN: Simulating 3D high energy particle showers in multilayer electromagnetic calorimeters with generative adversarial networks, Phys. Rev. D 97, 014021 (2018).