Approximation to Expectation Value of Non-Selfadjoint Operator in Anharmonic Exponential Oscillator System With Use of Two-Sided Rayleigh Quotient

SEMRA BAYAT ÖZDEMİR
Istanbul Technical University
Informatics Institute
Maslak, 34469 İstanbul
TÜRKİYE
bayat@itu.edu.tr

METİN DEMİRALP
Istanbul Technical University
Informatics Institute
Maslak, 34469 İstanbul
TÜRKİYE
metin.demiralp@gmail.com

Abstract: This work focuses on the derivation of a solution methodology to exponential anharmonic oscillator system based on the expectation values. A differential-difference equation is constructed from the second derivative of expectation value of the exponential analytic function. Rearranging the equation gives us an eigenvalue problem. But the derived operator is not self-adjoint. This makes it impossible to use classical definition of Rayleigh Quotient for expectation value of the operator. Two-sided Rayleigh (or Ostrowski) Quotient considers both left and right eigenfunction of the non-selfadjoint operator and this definition of expectation value gives the energy value of the corresponding system. For the approximate eigenfunctions, the energy value is approximate. We construct the final expectation value equation for the operator. But the optimization process for finding the minimum approximate energy value isn't analytically solvable. To validate the methodology, harmonic oscillator is studied at the end and an acceptable result is found with elementary approximations of eigenfuctions. Improvement of the approximations and solution to exponential anharmonic oscillator system are left as future work.

Key–Words: Anharmonic Exponential Oscillator, Differential-Difference Equation, Variational Approximation, Two-sided Rayleigh (Ostrowski) Quotient.

1 Introduction

The motion of a quantum system is fully described by the Schrödinger Equation [1] which is a parabolic partial differential equations whose time variable is responsible for the system's evolution while the position variables describe the spatial behavior of the system. The position variables are in fact the eigenvalues of the position operators and they vary on the entire real axis or an interval semi-infinite or finite depending on how the system under consideration is modelled. The number of the independent position variables is the degree of the freedom for the system.

The solution of the Schrödinger equation gives the wave function whose complex modulus square defines the probability of the system under consideration, that is, the probability of the system's presence at a specific position in the space and at a specified time instance. Hence, the wave function should have a unit norm over the domain of its position variables. Of course, this brings the integrability condition on the wave function. On the other hand, in many certain cases the modelling does not permit the wave function to be normalized since the equal or almost equal probability density everywhere may be countered. In those cases not the unit norm condition but normalizability to Dirac delta function is considered.

The Schrödinger equation can be written in the following form

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = \widehat{H}\psi(\mathbf{x},t), \quad \psi(\mathbf{x},0) = \psi_0(\mathbf{x}) \tag{1}$$

where $\mathbf{x}$ denotes the set of independent position variables while ψ symbolizes the wave function of the system under consideration. On the other hand, the symbol $\widehat{H}$ stands for the system's Hamiltonian or Hamilton operator. It depends on the momentum and position operators and perhaps on time variable. Hence we can write

$$\widehat{H} = H(\widehat{\mathbf{p}}, \widehat{\mathbf{q}}, t) \tag{2}$$

where $\mathbf{p}$ and $\mathbf{q}$ stand for the momentum and position operator vectors respectively. Beyond these, H stands for the Hamilton function which defines the dependence of the Hamiltonian on these operators and on time. If we denote the degree of the system by n_{df}

then we can write

$$\widehat{\mathbf{p}} \equiv \left[\widehat{p}_1 \ \ldots \ \widehat{p}_{n_{df}} \right]^T \tag{3}$$

$$\widehat{\mathbf{q}} \equiv \left[\widehat{p}_1 \ \ldots \ \widehat{q}_{n_{df}} \right]^T. \tag{4}$$

Each element of these vectors corresponds to a different direction in the system's phase space defined by the expectation values of these elements. To be more specific we need to give the explicit 5 definitions. They are as follows

$$\begin{aligned} \widehat{q}_j f(x_j) &= x_j f(x_j), \qquad x_j \in [a_j, b_j], \\ & \qquad j = 1, 2, ..., n_{df} \end{aligned} \tag{5}$$

$$\begin{aligned} \widehat{p}_j f(x_j) &= -i\hbar \frac{\partial f(x_j)}{\partial x_j}, \qquad x_j \in [a_j, b_j], \\ & \qquad j = 1, 2, ..., n_{df} \end{aligned} \tag{6}$$

where f stands a continuous and differentiable at least once univariate function. Until now we have used $\hbar$ to denote the reduced Planck constant defined as the ratio of the Planck's universal constant h to 2π and we are going to do so from now on.

In the study of the quantum motions, operators stands as rather abstract entities and not themselves but their expectation values give informations about the system's observable properties. The expectation value of a given operator, say $\widehat{o}$ is defined as follows

$$\langle \widehat{o} \rangle (t) \equiv \int_V dV \psi(\mathbf{x}, t)^* \, \widehat{o} \psi(\mathbf{x}, t) \tag{7}$$

where V stands for the integration domain of the modelled system while dV is the product of the position variables (x_js).

Any operator defined to investigate a given quantum system may depend on the fundamental operators of the quantum mechanics. Even though the time and energy pair can be related fundamental components, the most basic motion related entities are momenta and positions and therefore the related operators, namely, momentum and position operators. Hence we can assume the momentum and position dependences of all operators, even though they exist or do not exist. These dependences may or may not change in time. If it does not change we can then mention autonomy (time independence) or otherwise nonautonomy (time dependence). Thus for the most general case we can write.

$$\widehat{o} = o(\widehat{\mathbf{p}}, \widehat{\mathbf{q}}, t) \tag{8}$$

where o stands for the so-called operator function defining the dependence of the operator $\widehat{o}$ on the momentum and position operators and on time. Thus, the time dependence of the expectation value of the operator $\widehat{o}$ comes from two origins: (i) from the motion of the system described by the wave function, (ii) from the nonautonomy of the operator's itself.

The autonomus operators have spectra remaining unchanged during the motion because of their time independences. Their eigenvalues and eigenfunctions are all time independent. That is, their value are preserved during the motion. On the other hand, only instantaneous spectral properties can be defined for the nonautonomous operator. Their spectral entities, eigenvalues and eigenfunctions must be time variant.

Since the observables of a quantum systems must be measurable entities, the operators, whose expectation values correspond to observables, must also be self-adjoint or in other statement Hermitian. The spectra of the Hermitian operators are located on the real axis and the eigenfunctions corresponding to different eigenvalues must be orthogonal. If the operator under consideration for measurable entity evaluation is Hermitian and nonautonomous. Then its Hermiticity must be conserved during the system's evolution. However, the orthogonality amongst the eigenfunctions remains instantaneous.

As being an operator, the system's Hamilton operator may be autonomous or nonautonomous. The case of autonomy corresponds to the time independent expectation value of the Hamilton operator. Since its eigenvalues are known as the system's energy, the time-independent Hamilton operator having systems have energies remaining constant during their evolution. However, this conservation is not automatic. The constancy of the Hamilton operator expectation value requres specifications on the initial form of the wave function. This initial value function must be one of the eigenfunctions of the Hamilton operator to get energy conservation. Otherwise, some oscillations are observed amongst different energy states [2, 3].

1.1 Anharmonic Exponential Oscillator

A one-dimensional anharmonic exponential oscillator system can be defined with the following Hamilton operator

$$\widehat{H} \equiv \frac{1}{2\mu}\widehat{p}^2 + \alpha\left(\mathrm{e}^{\frac{\kappa}{2}\widehat{q}^{\,2}} - \widehat{I}\right) \qquad \alpha, \kappa > 0 \tag{9}$$

where μ,α,κ denotes the mass of particle, harmonicty and anharmonicty constants respectively. An the operators are defined as

$$\begin{aligned} \widehat{p}g(x) \equiv -i\hbar g'(x), \ \ \widehat{q}g(x) \equiv xg(x), \ \ \widehat{I}g(x) \equiv g(x) \\ x \in (-\infty, \infty) \end{aligned} \tag{10}$$

Various studies were performed about this equation (9) in our previous works [4–7]. But the developed methodologies were inadequate to give an acceptable result.

For convenience when dealing with that Hamiltonian we can convert it to a dimensionless equation. To do this we have to define dimensionless time ($\bar{t}$) and position ($\bar{x}$) variable as

$$\bar{t} \equiv \frac{t}{t_{dv}}, \qquad \overline{x} \equiv \frac{x}{x_{dv}} \tag{11}$$

and put them into the Schrödinger equation.

$$\begin{aligned} i\frac{\partial\overline{\psi}\left(\overline{x},\bar{t}\right)}{\partial\bar{t}} =& -\frac{1}{2}\left(\frac{\hbar t_{dv}}{\mu x_{dv}^2}\right)\frac{\partial^2\overline{\psi}\left(\overline{x},\bar{t}\right)}{\partial\overline{x}^2} \\ &+\left(\frac{\alpha t_{dv}}{\hbar}\right)\left(\mathrm{e}^{\kappa x_{dv}^2\overline{x}^2}-1\right)\overline{\psi}\left(\overline{x},\bar{t}\right) \end{aligned} \tag{12}$$

Without loss of generality, we can choose the values in the brackets as

$$\frac{\hbar t_{dv}}{\mu x_{dv}^2}=1, \qquad \epsilon=\kappa^2 x_{dv}^2, \qquad \frac{\alpha t_{dv}}{\hbar}=\frac{1}{2\epsilon} \tag{13}$$

and write all other variables without bar($^-$) throughout the paper. After all, we obtained the potential energy for that system as

$$V(x)=\frac{\mathrm{e}^{\epsilon x^2}-1}{2\epsilon} \tag{14}$$

Here, ϵ is an exponential variable which defines the harmonic oscillator potential energy when $\epsilon \to 0$.

2 Differential-Difference Equation

To obtain an ordinary differential equation by using the definition of expectation values we take an analytic function that depends on the position operator $f\left(\widehat{q}\right)$. For any $f\left(\widehat{q}\right)$

$$\frac{d^2}{dt^2}\left\langle f(\widehat{q})\right\rangle = 0 \tag{15}$$

is correct at stationary state. For the E energy state, the explict form of (15) can be written as below.

$$\begin{aligned} &-\left\langle V'\left(\widehat{q}\right)f'\left(\widehat{q}\right)\right\rangle - 2\left\langle V\left(\widehat{q}\right)f''\left(\widehat{q}\right)\right\rangle \\ &+\frac{1}{4}\left\langle f^{(4)}\left(\widehat{q}\right)\right\rangle + 2E\left\langle f''\left(\widehat{q}\right)\right\rangle = 0 \end{aligned} \tag{16}$$

An analytic function for the system defined at (9) can be chosen as in exponential form and its expectation value labeled with $\sigma(\nu,\epsilon)$ is given below.

$$\begin{aligned} f\left(\widehat{q}\right) &\equiv \mathrm{e}^{-\nu\widehat{q}} \\ \sigma(\nu,\epsilon) &\equiv \left\langle f\left(\widehat{q}\right)\right\rangle \end{aligned} \tag{17}$$

By replacing the given $V(\widehat{q})$ (14) and chosen $f\left(\widehat{q}\right)$, the equation (16) can be rewriten. The obtained equation is called difference-differential equation in the literature [8–13].

$$\begin{aligned} &4\nu^4\sigma''\left(\nu,\epsilon\right)+12\nu^3\sigma'\left(\nu,\epsilon\right)+3\nu^2\sigma(\nu,\epsilon) \\ &-4\nu^2\frac{\sigma'\left(\nu,\epsilon\right)-\sigma'\left(\nu-\epsilon,\epsilon\right)}{\epsilon}-2\nu\sigma'\left(\nu-\epsilon,\epsilon\right) \\ &-2\nu\frac{\sigma\left(\nu,\epsilon\right)-\sigma\left(\nu-\epsilon,\epsilon\right)}{\epsilon} \\ &=E(\epsilon)\left[\,8\nu^2\sigma'(\nu,\epsilon)+4\nu\sigma(\nu,\epsilon)\,\right] \end{aligned} \tag{18}$$

To cope with such a complex equation we need to rearrange it and write in an eigenvalue problem form.

$$\widehat{\mathcal{L}}\sigma(\nu,\epsilon)=E(\epsilon)\sigma(\nu,\epsilon) \tag{19}$$

$\widehat{\mathcal{L}}$ is an operator where its expectaion value gives the energy of the system. Without giving the intermediate steps, basically the above form of the equation can be written by first obtaining differential identicals of appropriate group of terms in (18), then multiplying both sides with suitable terms to do simplification and finally by taking the integral of both sides from 0 to ν. We ended up with the following eigen-equation of $\widehat{\mathcal{L}}$.

$$\begin{aligned} &\frac{\nu^{\frac{3}{2}}}{2}\frac{d}{d\nu}\left(\nu^{\frac{1}{2}}\sigma(\nu,\epsilon)\right)-\frac{1}{2}\frac{\sigma(\nu,\epsilon)-\sigma(\nu-\epsilon,\epsilon)}{\epsilon} \\ &-\frac{\nu^{-\frac{1}{2}}}{4}\int_0^\nu d\eta\eta^{-\frac{1}{2}}\frac{d\sigma}{d\eta}\left(\eta-\epsilon,\epsilon\right) \\ &\equiv\widehat{\mathcal{L}}\sigma(\nu,\epsilon)=E(\epsilon)\sigma(\nu,\epsilon) \end{aligned} \tag{20}$$

3 Variational Computational Approximation

The equation (20) is ensured if both $\sigma(\nu,\epsilon)$ and $E(\epsilon)$ is a solution pair. But if we choose an approximation to $\sigma(\nu,\epsilon)$, we get an approximate $E(\epsilon)$ value. We can call them "Variational Computational Approximation" [3, 14].

For self-adjoint $\widehat{\mathcal{L}}$, the expectation value of the operator can be described with a ratio called "Rayleigh Quotient" [15, 16] as given below.

$$E(\epsilon)=\frac{\int_0^\infty d\nu\sigma(\nu,\epsilon)\widehat{\mathcal{L}}\sigma(\nu,\epsilon)}{\int_0^\infty d\nu\sigma(\nu,\epsilon)^2}\equiv\left\langle\widehat{\mathcal{L}}\right\rangle(\sigma) \tag{21}$$

But for the case defined in (20), the operator is not self-adjoint. So the approach and the definition of expectation value of $\widehat{\mathcal{L}}$ must be different [17–19]

For any operator $\widehat{\mathcal{L}}$, both right and left eigenequations can be written as

$$\widehat{\mathcal{L}}\sigma(\nu,\epsilon) = E(\epsilon)\sigma(\nu,\epsilon)$$
$$\widehat{\mathcal{L}}^{\dagger}\rho(\nu,\epsilon) = E(\epsilon)\rho(\nu,\epsilon) \quad (22)$$

respectively. $\sigma(\nu,\epsilon)$ is the right eigenfunction and $\rho(\nu,\epsilon)$ is the left eigenfunction and they are different for non-selfadjoint operator $\widehat{\mathcal{L}}$. The expectation value of $\widehat{\mathcal{L}}$ can be defined by "Two-Sided Rayleigh (Ostrowski) Quotient" [20–22] as given in the following equation.

$$E(\epsilon) = \frac{\int_0^\infty d\nu \rho(\nu,\epsilon)\widehat{\mathcal{L}}\sigma(\nu,\epsilon)}{\int_0^\infty d\nu \rho(\nu,\epsilon)\sigma(\nu,\epsilon)} \equiv \left\langle \widehat{\mathcal{L}} \right\rangle (\rho,\sigma) \quad (23)$$

First of all, we can start the calculations by suggesting very basic above approximations for right and left eigenfunctions.

$$\sigma_{app}(\nu,\epsilon) \equiv \mathrm{e}^{-\gamma_1\nu}, \qquad \rho_{app}(\nu,\epsilon) \equiv \mathrm{e}^{-\gamma_2\nu} \quad (24)$$

By using these approximations with (20) in Ostrowski quotient (23), the following expectaion value is derived.

$$\left\langle \widehat{\mathcal{L}} \right\rangle (\sigma,\rho) = \frac{1}{4(\gamma_1+\gamma_2)} + \frac{\gamma_1(\gamma_1+\gamma_2)}{4\sqrt{\gamma_1\gamma_2}} \arctan\left(\sqrt{\frac{\gamma_1}{\gamma_2}}\right) - \frac{\gamma_2}{(\gamma_1+\gamma_2)^2} + \left(1 + \frac{\gamma_1(\gamma_1+\gamma_2)}{2\sqrt{\gamma_1\gamma_2}}\epsilon \arctan\left(\sqrt{\frac{\gamma_1}{\gamma_2}}\right)\right)\frac{\mathrm{e}^{\gamma_1\epsilon}-1}{2\epsilon} \quad (25)$$

When $\gamma_1 > 3\gamma_2$, the energy value stays always positive. With proper choices of γ_1 and γ_2 this is always true.

To facilitate the analysis, polar coordinates can be used with the following definitions.

$$\gamma_1 \equiv r\sin(\varphi)^2, \qquad \gamma_2 \equiv r\cos(\varphi)^2, \quad (26)$$

Here φ varies from 0 to $\pi/2$ and r must be nonnegative to guarantee nonnegative γ values. Replacing γ's with their transformations in (25) gives us the following equation.

$$\left\langle \widehat{\mathcal{L}} \right\rangle (\sigma,\rho) = \left(\frac{1}{4} - \cos(\varphi)^2\right)\frac{1}{r} + \frac{\mathrm{e}^{r\cos(\varphi)^2\epsilon}-1}{\epsilon} + \frac{\varphi}{2}\tan(\varphi)\left(\mathrm{e}^{r\cos(\varphi)^2\epsilon} - \frac{1}{2}\right) r \quad (27)$$

Another condition is revealed from the above equation that for all nonnegative r values, $\varphi > \pi/3$ must be provided to verify the positivity of right-hand side and there must be a minimum value for it. To find the minimum, we have to take the derivative with respect to r and solve as it equals to zero. But unless ϵ is not equal to 0, analytical solution is not available.

For $\epsilon = 0$, the equation becomes the governing equation for energy value of harmonic oscillator.

$$E_{ho} = \left\langle \widehat{\mathcal{L}} \right\rangle (\sigma,\rho)\Big|_{\epsilon=0} = \left(\frac{1}{4} - \cos(\varphi)^2\right)\frac{1}{r} + \left(\frac{\varphi}{4}\tan(\varphi) + \cos(\varphi)^2\right) r \quad (28)$$

We take the derivative wrt r and equate it to zero. Then the optimal r_{opt} is found after solving the equation.

$$r_{opt} = \sqrt{\frac{1 - 4\cos(\varphi)^2}{\varphi\tan(\varphi) + 4\cos(\varphi)^2}} \quad (29)$$

The optimized energy value E_{opt} is found by replacing r with r_{opt} in (28) as

$$E_{opt} = \frac{1}{2}\sqrt{1 - 4\cos(\varphi)^2}\sqrt{\varphi\tan(\varphi) + 4\cos(\varphi)^2} \quad (30)$$

E_{opt} has a minimum in the range of $\pi/3 < \varphi < \pi/2$. This can be determined by focusing on the behaviour of r_{opt} in that range. $r_{opt} = 0$ where $\varphi = \pi/3$ and $\varphi = \pi/2$ and r_{opt} has a local maximum between these values since it is continuous. This value can be used to determine the optimal φ.

3.1 Flatness - Robustness Principle

The value of E_{opt} is monotonically increasing when φ varies from $\pi/3$ to $\pi/2$. This doesn't give information for determining φ. But as mentioned before, the behaviour of r_{opt} in that range gives a clue for the calculation.

r_{opt} is a minimum value and it is desirable that any small change in that value leads small changes in the E_{ho} value. This property defines the possible flatness (or robustness) of E_{ho}.

The less change in the second derivative of E_{ho} wrt r at r_{opt} gives the more flattened E_{ho} according to r. So taking the second derivative and then optimizing that equation wrt φ gives the sought values.

$$\frac{\partial^2 E_{ho}}{\partial r^2}(r_{opt},\varphi) = \frac{1}{2}\left(1-4\cos(\varphi)^2\right)^{-\frac{1}{2}}\left(\varphi\tan(\varphi)+4\cos(\varphi)^2\right)^{\frac{3}{2}} \quad (31)$$

The φ value that cause the smallest change while varying through $\pi/3$ to $\pi/2$, gives the flatness of robustness status of E_{ho}

$$0 = \frac{\partial}{\partial\varphi}\left(\frac{\partial^2 E_{ho}}{\partial r^2}(r_{opt},\varphi)\right) = \left(1-4\cos(\varphi)^2\right)^{-\frac{3}{2}}\left(\varphi\tan(\varphi)+4\cos(\varphi)^2\right)^{\frac{1}{2}}\Phi(\varphi) \quad (32)$$

where

$$\Phi(\varphi) = -\sin(2\varphi)\left(\varphi\tan(\varphi)+4\cos(\varphi)^2\right) + \frac{3}{4}\left(1-4\cos(\varphi)^2\right) \times\left(\tan(\varphi)+\varphi+\varphi\tan(\varphi)^2-4\sin(2\varphi)\right) \quad (33)$$

It is expected that the right-hand side (32) is 0 in a value between $\varphi=\pi/3$ and $\varphi=\pi/2$. It is just provided if and only if $\Phi(\varphi)=0$. Although $\Phi(\varphi)=0$ has a real solution, it is hard to determine analytically. So we can write basic scripts/codes in a symbolic or numerical computation programs to calculate it. We prefer to use MuPAD with 20 decimal sensitivity and get $\varphi = 1.179713302$. At same level, corresponding energy value for harmonic oscillator is found as $E_{ho} = 0.600330425$. That values is not a bad approximation to the the exact value $E_{ho} = 1/2$.

4 Concluding Remarks

This work is the early step of variational approximation to the anharmonic exponential oscillator system energy. The second derivative of expectation value of analytic function ($f(\widehat{q})$) wrt t is our primary equation. Its explicit form is differential-difference equation which is very complex to handle with common solution methods. So we need to rearrage it to define as an eigenvalue problem. The defined operator $\widehat{\mathcal{L}}$ in this step is non-selfadjoint. So basic Rayleigh Quotient gives false expectation value. An improved version for non-selfadjoint operators is defined Two-sided Rayleigh (Ostrowski) Quotient in the literature and we performed it for our case.

The validation is one of the important stage, so we choose very known harmonic oscillator system. The equations of desired system approximate harmonic oscillator when $\epsilon \to 0$. With very basic suggestions to the approximation of eigenfunctions, we get promising result in energy value. The approximations can be enhanced by adding enough parameters to the eigenfunctions. It is expected that with this enhancement, the E values can approximate the exact value more.

The second and more important step will be applying this methodology to the case where $\epsilon \neq 0$. Thus, the energy values of the desired system (anharmonic exponential oscillator) will be calculated. All these are left as future work for this study.

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