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Approximate Energy Spectra of the Quantum Gaussian Well: A Four-parameter Potential Fitting

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Abstract: In this work, we present a detailed study of a one-dimensional Schrödinger equation in the presence of quantum Gaussian well interaction. Further, we investigate the approximate solutions by using the harmonic oscillator approximation, variational principle, four-parameter potential fitting and numerical solution using the finite-difference method. The parabolic approximation yields an excellent energy value compared with the numerical solution of the Gaussian system only for the ground state, while for the excited states, it provides a higher approximation. Also, the analytical bound-state energies of the four-parameter potential under the framework of the Nikiforov-Uvarov (NU) method have been used after getting the suitable values of the potential parameters using numerical fitting. The present results of the system states are found to be in high agreement with the well-known numerical results of the Gaussian potential.

Keywords: Gaussian potential, One-dimensional Schrödinger equation, Nikiforov- Uvarov (NU) method, Four-parameter potential.

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1. Introduction

The exact and approximate solutions of the Schrödinger wave equation with various potential models have attracted much interest since the beginning of quantum mechanics and are being increased due to the fabrication of nanodevices. Recently, one-dimensional potential wells have been commonly used to illustrate many quantum-mechanical phenomena due to their high relevance in nanophysics [1]. It is interesting to investigate the Schrödinger Hamiltonian with attractive Gaussian potential for its typical properties of short-range potentials [2]. Since these Gaussian potentials have no exact analytical solutions, many authors have made an approximation with parabolic harmonic oscillators, especially near the bottom of the well [3, 4]. Further, in some other works [5], many authors approximated the Gaussian potential to the so-called modified Gaussian using a hyperbolic function. Other authors [6] have discussed the existence and the number of bound states in a Gaussian well, tunneling through a Gaussian barrier, as well as the spectrum of a Gaussian double well. Also, the variational parameters of the Gaussian potential have been presented for the ground state as well as for the first and higher excited states [7].

Very recently, the exact solution of the Schrödinger equation for spectral problems with some solvable potential models has been the subject of many investigations [8-10]. Some of these exactly solvable potentials are exponential

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or hyperbolic potentials of the spatial coordinates. These exponential potentials are widely used in many branches of physics, such as nuclear physics, atomic physics and chemical physics [11-13].

Here, in general, we seek to choose the proposed appropriate four-parameter exponential-type potential [14] which may be reduced to the Rosen–Morse potential [15] as well as to the Hulthen-like effective potential [16]. With a special choice of parameters, the Eckart potential [17] may also turn to become the Hulthen potential and the generalized Morse potential.[18]. On the other hand, using numerical fitting for many-parameter potential would give an acceptable solution for our desired potential model.

In this study, we consider solutions to the one-dimensional Schrödinger equation with an attractive Gaussian potential and discuss our results for the parabolic approximation and variational methods. Further, we compare our results with numerical solution along with a numerical fitting of the Gaussian potential with four-parameter potential (FPP), which has an exact analytical solution.

This work is structured as follows. In Section 2, we discuss the solution of the Schrödinger equation using an approximation of a Gaussian potential as a parabolic potential, use harmonic oscillator wave functions as trial wave functions in the variational method and review the Nikiforov- Uvarov (NU) solution to the FPP. In Section 3, we emphasize the numerical comparisons and results for parabolic, Gaussian and solvable four-parameter potential. We also use numerical fitting to find the fitting-parameter values to calculate the bound-state solutions of the Gaussian potential model. Finally, Section 4 is devoted to our results and conclusions.

2. Theory and Method

We begin by solving the time-independent one-dimensional Schrödinger equation taking the simple form:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\,\psi(x), \tag{1}$$

where $\hbar$ is the reduced Planck constant, m denotes the mass of the particle, $\psi(x)$ stands for the wave function and $V(x)$ returns to the confining potential which is to be taken as the Gaussian potential (GP) form,

$$V(x)=-V_0\,e^{-\frac{x^2}{R_0^2}}, \tag{2}$$

where $V_0>0$. For the sake of simplicity, we choose units such that $\hbar$ = 2m = 1. It is well-known that the condition on $V(x)$ is to have at least one bound state

$$\int_{-\infty}^{\infty}V(x)\,dx<0, \tag{3}$$

which mainly depends on the shape of the potential and not on its strength. Thus, Eq. (3) is a sufficient condition for a potential to have a bound state, but it is not a necessary condition as in the case of harmonic oscillator potential. The main results in Ref. [6], such as the number of bound states, depend only on $V_0\times R_0^2$.

2.1 Parabolic Potential

Taking the Taylor expansion for the Gaussian potential (GP), see Eq. (2), it becomes:

$$V(x)=-V_0+V_0\frac{x^2}{R_0^2}-V_0\frac{x^4}{2!\,R_0^4}+\ \dots\dots \tag{4}$$

Hence, in the literature, it is sufficient to use the first two terms of the above expansion to have an adequate approximation form for the GP as called the Harmonic oscillator. Here, the first term in the expansion (4) is an additional constant, whereas the second term is a parabolic potential. Comparing with the harmonic oscillator, one solves:

$$V_0\frac{x^2}{R_0^2}=\frac{1}{2}\,m\,\omega^2\,x^2. \tag{5}$$

We obtain the angular frequency as:

$$\omega=\sqrt{2\frac{V_0}{m\,R_0^2}}. \tag{6}$$

Therefore, the energy of the harmonic oscillator becomes:

$$E_n=-V_0+\left(n+\frac{1}{2}\right)\hbar\,\omega. \tag{7}$$

To have more accuracy, we can consider the third and high-order terms of the above expansion (4) as a perturbation to the potential, which would somewhat improve the spectra result for excited states.

If we take the mathematical point of view for this comparison, we notice that the GP is always negative, while the parabolic potential may flip to positive values at large x; so, it is expected to give a good result for low-order states only, at the classical limit of small x.

2.2 Variational Technique

To obtain various upper bounds of the ground-state energy, we can calculate the average value of the Hamiltonian $\langle H \rangle$ for suitably chosen trial functions. The existence of a variational parameter β enables to minimize the upper bounds as much as possible. To do that, we shall choose normalized trial wave functions $\psi_0(x)$ and $\psi_1(x)$ for the ground state and the first excited state, respectively, with some adjustable parameters β and γ, defined as follows:

$$\psi_0(x) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} e^{-\beta x^2}, \tag{8}$$

and

$$\psi_1(x) = \left(\frac{2^5\gamma^3}{\pi}\right)^{1/4} x\, e^{-\gamma x^2}. \tag{9}$$

After calculating the energies as functions of the variational parameters, one obtains:

$$\langle \psi_0(x)|H|\psi_0(x)\rangle = \beta - \frac{\sqrt{2\,\beta}\,\mathrm{V}_0}{\left(2\beta + \frac{1}{R_0^2}\right)^{\frac{1}{2}}}, \tag{10}$$

and

$$\langle \psi_1(x)|H|\psi_1(x)\rangle = 3\gamma - \frac{\sqrt{8\,\gamma^3}\,V_0}{\left(2\,\gamma + \frac{1}{R_0^2}\right)^{\frac{3}{2}}}, \tag{11}$$

for the ground and first excited states, respectively, which can be minimized numerically to find the upper approximated energy.

2.3 Four-Parameter Potential Fitting

To have an approximation of the GP energy, we will apply a numerical fitting to find suitable parameters for the four parameter-potential (FPP) in the following form:

$$V(x) = \frac{V_0 e^{\alpha x}}{C + q e^{\alpha x}} - \frac{V_1 e^{\alpha x}}{(C + q e^{\alpha x})^2}. \tag{12}$$

This potential makes Schrödinger equation analytically solvable by using the Nikiforov-Uvarov (NU) method. To make the potential analytically solvable by the NU method, we have to write the Schrödinger equation in the following standard general form:

$$\frac{d^2\psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)}\frac{d\psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \tag{13}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most of second-degree, $\tilde{\tau}(s)$ is a first-degree polynomial. For more details, see Ref. [19].

For the potential given in (12), the Schrödinger equation reads:

$$\psi''(x) + \frac{2m}{\hbar^2}\left[E - \frac{V_0 e^{\alpha x}}{C + q e^{\alpha x}} + \frac{V_1 e^{\alpha x}}{(C + q e^{\alpha x})^2}\right]\psi(x) = 0. \tag{14}$$

After changing the independent variable s = $C + q e^{\alpha x}$ and following the procedures given in Ref. [20], one gets the bound-state energies as follows:

$$E_n = -\frac{\hbar^2\alpha^2}{2m}\varepsilon_n^2, \tag{15}$$

where n = 0, 1, 2, 3, … and

$$\varepsilon_n = \frac{\frac{2mV_0 1}{\hbar^2\alpha^2\, q}}{\left[-(2n+1) + \sqrt{1 + \frac{8mV_1}{\hbar^2\alpha^2}\frac{1}{qC}}\right]} - \frac{1}{4}\left[-(2n+1) + \sqrt{1 + \frac{8mV_1}{\hbar^2\alpha^2}\frac{1}{qC}}\right] \tag{16}$$

and the wave function

$$\psi_{nq}(s) = B_n s^{-(2\delta-1)}(C - s)^{2\varepsilon}\frac{d^n}{ds^n}\left[s^{n+(2\delta-1)}(C - s)^{n-2\varepsilon}\right] \tag{17}$$

where

$$\delta = \frac{1}{2}\left[1 - \sqrt{1 + \frac{4\gamma^2}{C}}\right], \gamma^2 = \frac{2mV_1}{\hbar^2\alpha^2 q}. \tag{18}$$

3. Results and Discussion

In this section, we display our calculated results for energy spectra and the wave function for the Gaussian potential. We also compare the present approximated results with the exact ones which have already been obtained by numerically solving the Schrödinger equation using the finite-difference method. Knowing that all, the parameters have been arbitrarily unit-scaled for the pre-assumption $\hbar = 2m = 1$.

In Fig. 1, we have plotted the GP, FPP and parabolic potential as functions of the coordinate x, for a fixed value of V_0 and different values of R_0. This figure shows the high agreement between the Gaussian and parabolic potentials for small values of |x| (near the bottom of the curves), while we have noticed some difference as |x| tends to become larger. This result supports our arguments on the use of the parabolic model as an approximation-scheme model for GP. By comparing the GP and FPP, one can see the agreement between both curves for a larger range of x compared with the parabolic approximation.

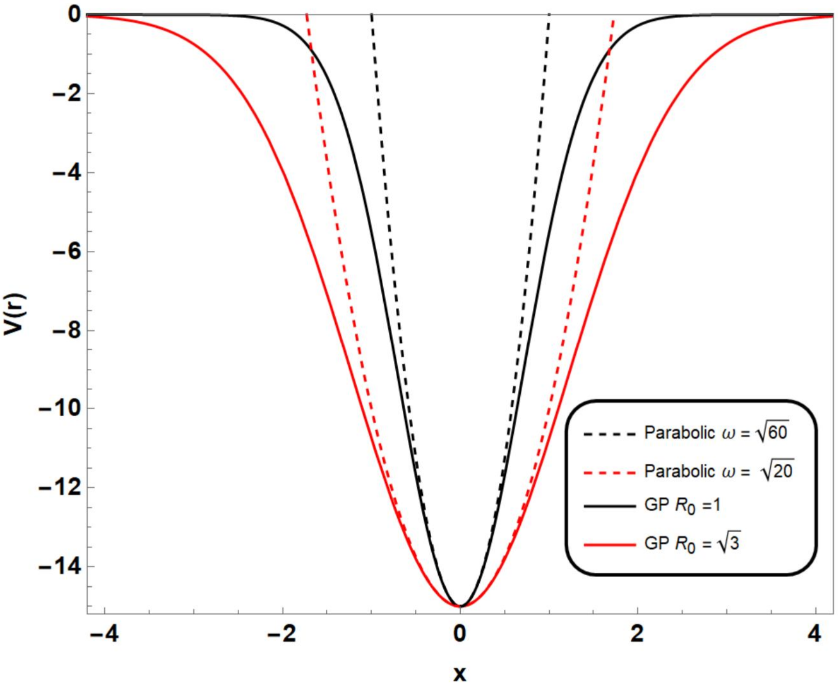


FIG. 1. GP, FPP and parabolic potential against the spatial coordinate x for a fixed value of $V_0 = 15$ and different values of R_0, Here, ω is given by Eq. (6).

In Table 1, we have shown the ground-state and first excited-state energies of the GP system compared with the variational result and parabolic approximation. These results in Table 1 show that the variational energies are in close agreement with the exact ones for the low-lying states (ground and first excited states) and with the corresponding variational parameters.

TABLE 1. Low-lying states in comparison with GP using parabolic approximation, the variation of parameter method and finite-difference numerical solution.

	$V_0 = 15, R_0 = \sqrt{3}, \omega = \sqrt{20}$			$V_0 = 15, R_0 = \sqrt{1}, \omega = \sqrt{60}$		
	E_{bar}	E_{var}	E_{num}	E_{bar}	E_{var}	E_{num}
E_0	-12.7639	-12.8873	-12.8896	-11.12701	-11.4934	-11.5046
E_1	-8.29179	-8.92558	-8.93837	-3.38105	-5.30696	-5.37760

For $R_0 = \sqrt{3}$ (1), the corresponding values of various parameters, $\beta = 0.995$ (1.574) and $\gamma = 0.905(1.283)$, agree with the fact that for a larger value of R_0 (smaller for ω), the parabolic approximation is found to be more accurate with the trial wave function as it goes to be the same as the solution of the harmonic oscillator. On the other hand, for smaller values of R_0, the parabolic deviates more and hence, the difference becomes more significant.

Moreover, in Fig. 2, we plot the low-lying state wave functions for the three cases: the numerical solution, the parabolic approximation and the variational technique. Here, we can notice the slight difference between GP and parabolic approximation.

In Table 2, we have presented the numerical values of the parameters of (FPP) concerning GP. If we look back to the (FPP), we can notice five parameters, but there is a close relation between these parameters (i.e., not independent parameters), so we used the numerical fitting to get their values.

To ensure the agreement, we have plotted the two potentials in the same graph in Fig. 3. We found similarities in their behaviors and asymptotes. On the other hand, there is a slight difference at the bottom of the curves, which is expected to yield a small difference in the ground-state energy.

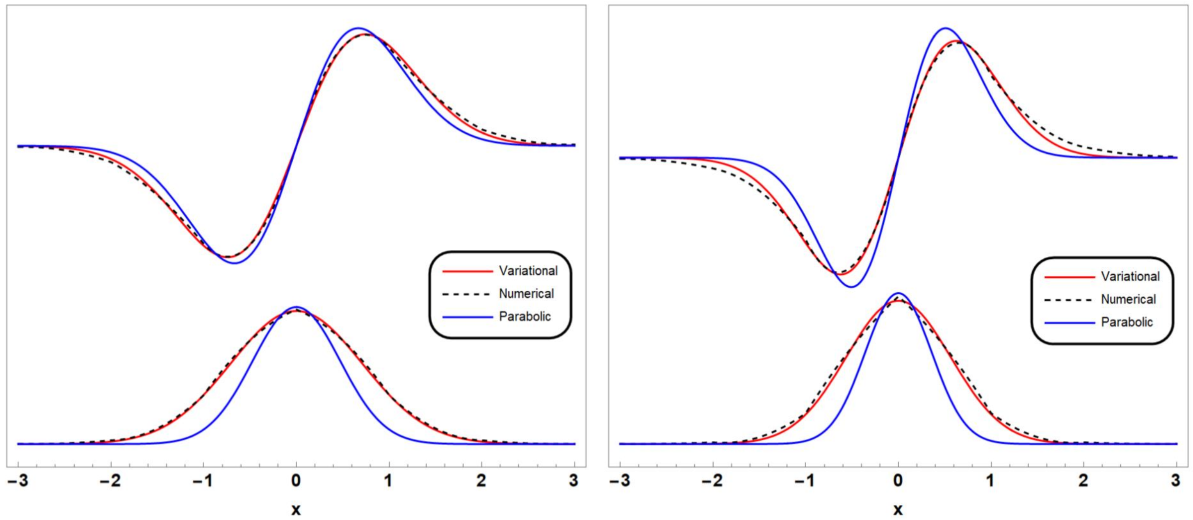


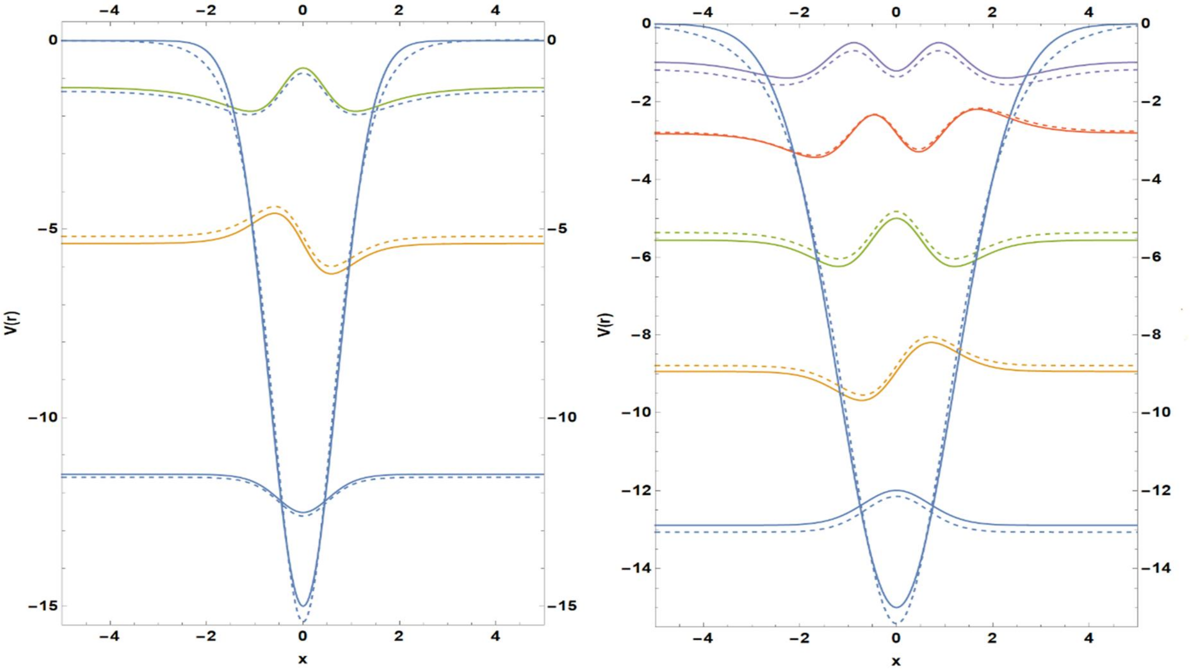
FIG. 2. The wave functions for the ground and first excited states as functions of the position for a) $V_0 = 15, R = \sqrt{3}$ and b) $V_0 = 15, R = 1$, corresponding to energies reported in Table 1.

TABLE 2. Numerical values for the fitted parameters of FPP at given values for Gaussian parameters.

	V_1	V_2	α	q	C
$V_0 = 20$ $R_0 = \sqrt{3}$	0.018137	9.275333	-1.29788	0.33512	0.336243
$V_0 = 35$ $R_0 = \sqrt{5}$	0.022753	4.470902	-1.00451	0.17574	0.17654

Also, we have displayed the spectra and wave function of GP and FPP in the same graph for different values of V_0 and R_0 in parts a, b, c and d. Here, we also see the good agreement between both potentials in their solutions.

Further, in Table 3, we have numerically listed our results of Fig. 3 to show the differences in energy. We notice the significant differences at small values of R_0 for higher excited states. This is mainly attributed to the significant role of larger values of |x| due to the behavior of the potential.



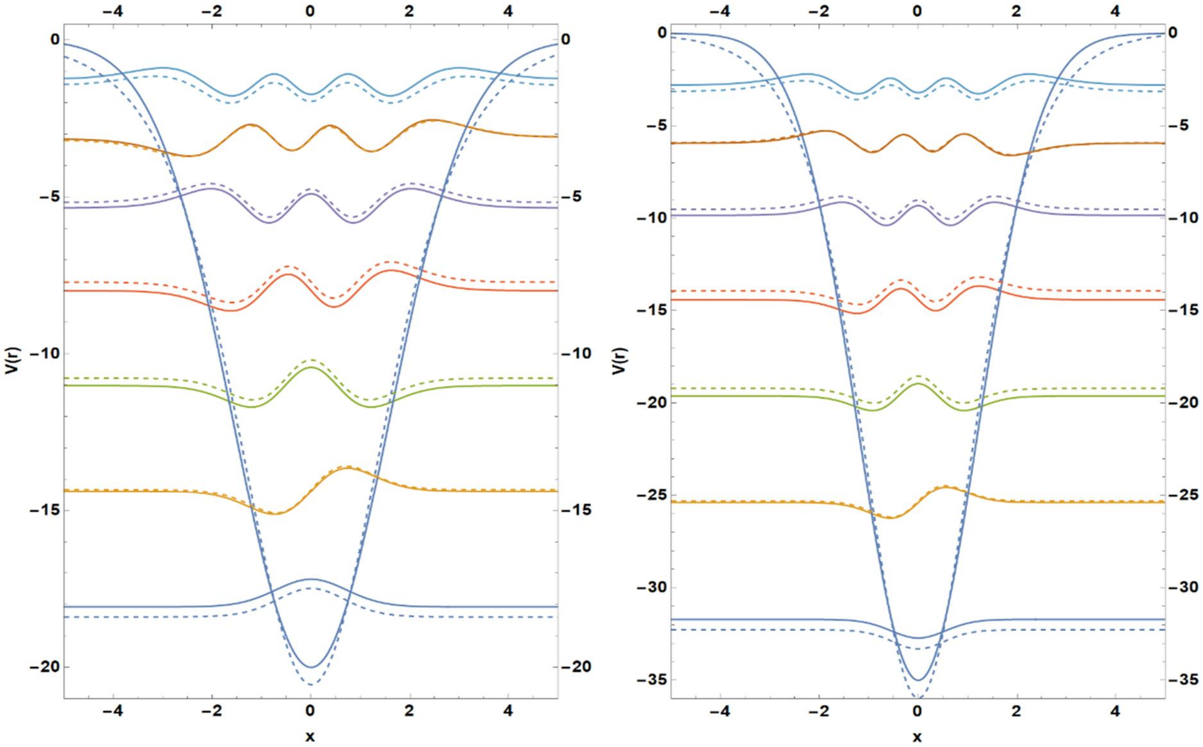


FIG. 3. The energy eigenfunctions and the corresponding eigenvalues for (V_0, R_0) taken to be in a, b, c and d, $(15, 1)$, $(15, \sqrt{3})$, $(20, \sqrt{5})$ and $(35, \sqrt{3})$ respectively. The solid (dashed) lines return to GP (FPP).

TABLE 3. The energy spectra of the GP and FPP for various values of the potential parameters.

	$R_0 = 1$		$R_0 = \sqrt{3}$		$R_0 = \sqrt{5}$	
	Gaussian	FPP	Gaussian	FPP	Gaussian	FPP
$V_0 = 15$	-11.5046	11.5852	-12.8896	-13.0659	-13.3433	-13.5595
	-5.3776	-5.18818	-8.93837	-8.79198	-10.1886	-10.109
	-1.2209	-1.32315	-5.55479	-5.36029	-7.36325	-7.16311
	---	---	-2.81231	-2.77086	-4.8946	-4.72171
	---	---	-0.85774	-1.02372	-2.82405	-2.78485
$V_0 = 20$	-15.9053	-16.0464	-17.5436	-17.8105	-18.0753	-18.3917
	-8.56120	-8.29402	-12.8974	-12.7501	-14.3834	-14.3317
	-3.08391	-3.0736	-8.80737	-8.53193	-11.016	-10.7763
	-0.15052	-0.38525	-5.32892	-5.15602	-7.9950	-7.72536
	---	---	-2.54899	-2.62238	-5.34937	-5.17897
$V_0 = 35$	-29.4610	-29.825	-31.7098	-32.2753	-32.4295	-33.0677
	-19.2012	-18.7962	-25.3917	-25.3176	-27.444	-27.5379
	-10.6823	-10.2995	-19.6133	-19.2021	-22.7762	-22.5126
	-4.19329	-4.33473	-14.4095	-13.9289	-18.4406	-17.9919
	-0.38543	-0.90205	-9.82653	-9.49795	-14.4548	-13.9757

Finally, Fig. 4 plots the vibrational bound-state energy E_n *versus* the principal quantum number n, where we have shown the three cases of GP, FPP and parabolic approximation for the sake of comparison. As percentage errors, the parabolic approximation ground-state energy is 0.23% higher than the numerical solution of GP, where the FPP yields 1.97% lower as previously mentioned, for the first excited state (n = 1). The parabolic potential (FPP) result is 1.39% higher (0.34% lower) and by comparing the 4th excited state (n = 4), the parabolic energy is 22% and FPP is 3.32% and both potentials give a higher approximation for the energy.

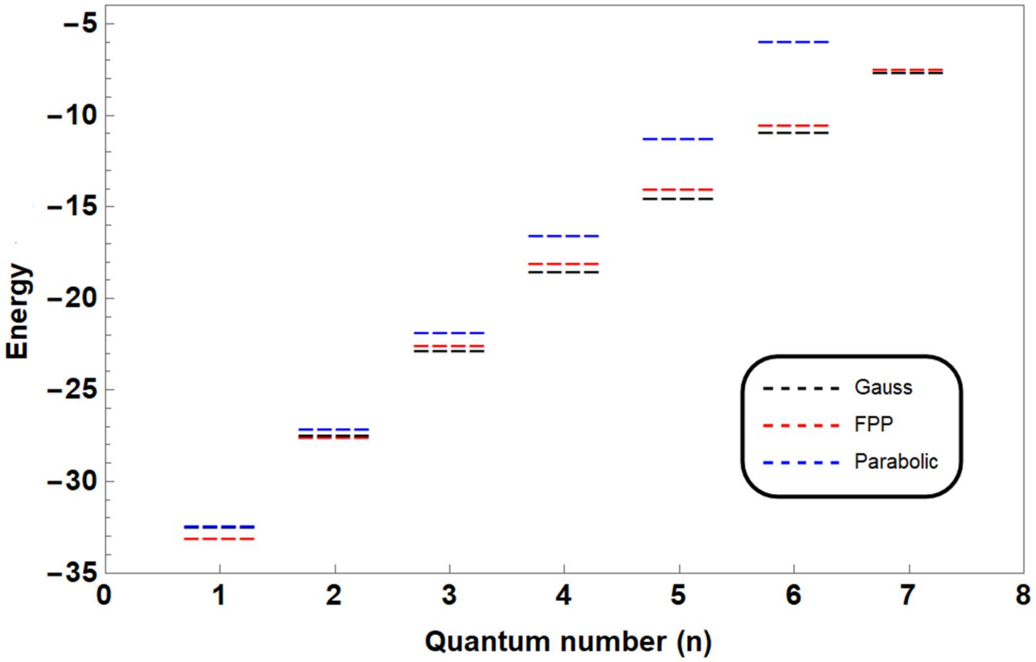


FIG. 4. The energy eigenvalues for different states (n) obtained for GP, parabolic approximation and FPP.

4. Conclusions

In this work, we have solved the one-dimensional Schrödinger equation to obtain the solutions of the bound states for the Gaussian well potential. Further, the wave functions as well as the vibrational eigenvalues are obtained by various methods. The parabolic approximation of the Gaussian potential is in excellent agreement with the exact energy for low-order states only. However, for higher states, it exhibits a significant difference. Using the well-known solution of the harmonic oscillator as a wave function with an undetermined parameter provides a very close result to the exact solution. On the other hand, the four-parameter potential having an analytical solution is also used as screening potential to be fitted using Gaussian information. Besides, the analytical solution of FPP was obtained using the Nikiforov Uvarov (NU) method. Finally, the presented results show that the fitting method provides a chance to compare with the available numerical energies and wave functions within an acceptable accuracy.

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