

# A Semi-Analytical Solution to the Schrödinger Equation with Gaussian Well

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## ABSTRACT

This paper proposes a new semi-analytical solution of the Schrödinger equation with Gaussian well. The approach is based on the harmonic oscillator and yields both the energy and the wave function for any specific eigenstate. Furthermore, the semi-analytical solution is compared to methods found in the literature and the Split-Operator method and deemed accurate.

## Keywords

Schrödinger equation, Gaussian well, harmonic oscillator

## INTRODUCTION

The Schrödinger equation (SE) is an important tool in quantum mechanics to determine the behavior of particles as a result of their surroundings. Its most commonly used variation, the time-independent SE is

$$\hat{H}\psi = E\psi, \quad (1)$$

where  $E$  is the energy of the particle,  $\psi$  its wave function, and  $\hat{H}$  is the Hamiltonian.  $E$  and  $\psi$  describe the particle itself, and are usually the unknown quantities. While the wave function itself is a rather abstract concept, the wave function squared  $|\psi|^2$  gives the probability density of the particle. The Hamiltonian depends on the system around the particle. For a single particle in one dimension

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x), \quad (2)$$

where  $\hbar$  is Planck's constant divided by  $2\pi$ ,  $m$  is the mass of the particle and  $V(x)$  is the potential energy as a function of position  $x$ . Insert the Hamiltonian into Equation (1) to obtain the full expression

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \quad (3)$$

Now, the SE can be solved by defining the potential  $V(x)$ . However, not for all potentials  $V(x)$  the SE will be analytically solvable. Then, physicists require numerical methods and approximations to obtain solutions. One of these cases is the Gaussian well potential, given by

$$V(x) = -V_0 e^{-\alpha x^2}, \quad (4)$$

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where  $V_0, \alpha > 0$ . The two parameters  $V_0$  and  $\alpha$  define the depth and the width of the well, respectively. One application of the Gaussian well is in the research of quantum dots, which are desired for their unique optical properties [1, 10]. This potential well is the focus of this paper. The literature presents various methods for the Gaussian well: Variational method with harmonic oscillator trial function [7, 9], WKB approximation [8], deep-well approximation perturbation theory [4] and Wronskian method [6, 5]. Furthermore, the Split-Operator method that will also be used in this work is based on papers by Bandrauk and Shen [3, 2].

In order to simplify the discussion, transform the Schrödinger equation into a unitless eigenvalue problem. For this purpose, define a new coordinate  $q = x\sqrt{\alpha}$  and appropriate wave function  $\psi_q(q) = \frac{1}{\sqrt{\alpha}}\psi\left(q\frac{1}{\sqrt{\alpha}}\right)$ . Then, the SE follows as

$$-\frac{1}{2} \frac{d^2}{dq^2} \psi_q(q) + V_q(q)\psi_q(q) = E_q\psi_q(q), \quad (5)$$

where

$$V_q(q) = -V_{q,0}e^{-q^2}, \quad (6)$$

with  $V_{q,0} = \frac{mV_0}{\hbar^2\alpha}$  and  $E_q = \frac{mE}{\hbar^2\alpha}$ . Evidently, every Gaussian well is equivalent to a Gaussian well with  $\alpha = 1$ , as long as the ratio  $V_0/\alpha$  is constant and the energy is adjusted accordingly. Finally, relabel  $q$  as  $x$  to obtain the unitless SE of the Gaussian well:

$$-\frac{1}{2} \frac{d^2}{dx^2} \psi(x) - V_0 e^{-x^2} \psi(x) = E\psi(x). \quad (7)$$

## SEMI-ANALYTICAL SOLUTION

### The Proposed Solution

One feature of the Gaussian well is its similarity to the harmonic oscillator close to the center of the well. Indeed, the Taylor series of the Gaussian well is

$$\begin{aligned} -V_0 e^{-\alpha x^2} &= -V_0 \sum_{k=0}^{\infty} \frac{(-\alpha x^2)^k}{k!} \\ &= -V_0 \left( 1 - \alpha x^2 + \frac{1}{2} \alpha^2 x^4 + \dots \right), \end{aligned} \quad (8)$$

such that the second term corresponds to the harmonic oscillator and the first is simply an irrelevant energy offset. Therefore, it is reasonable to assume that the groundstate solution of the Gaussian well is similar to the solution of the harmonic oscillator, which is

$$\psi_h(x) = C \exp(-b_1 x^2) = \exp(b_0 - b_1 x^2). \quad (9)$$

Since the Gaussian well contains all positive, even powers of  $x$ , try substituting the polynomial in the exponent of  $\psi_h$  with an infinite sum of even powers of  $x$ . Thus, suppose the ground state wavefunction associated with the time-independent SE in Equation (7) is given by the semi-analytical solution (SAS)

$$\psi(x) = e^{f(x)} = \exp\left(\sum_{i=0}^{\infty} b_n x^{2n}\right), \quad (10)$$

where  $b_n$  are coefficients to be determined.

Next, consider the excited states of the harmonic oscillator. The excited states are related to the ground state wave function by a multiplication with an even or odd polynomial. Similarly, suppose that the excited states  $\psi_n$  of the Gaussian well are also of the form

$$\psi_n(x) = P_n(x)\psi_0(x), \quad (11)$$

where  $P_n(x)$  is an even polynomial for even excited states and odd for odd excited states. For example, for the first three excited states, the polynomials are

$$P_1(x) = x, P_2(x) = (p_2 x^2 + 1), P_3(x) = (p_3 x^3 + x), \quad (12)$$

where  $p_n$  are some constants.

### Solving for the Coefficients

For the groundstate, the only variables to solve for are the coefficients  $b_n$  and the energy  $E$ . For this purpose, insert the wavefunction from Equation (10) back into the Schrödinger equation in Equation (7) obtain

$$\begin{aligned} -\frac{1}{2} \frac{d^2}{dx^2} \exp\left(\sum_{i=0}^{\infty} b_n x^{2n}\right) + (V_0 e^{-\alpha x^2}) \exp\left(\sum_{i=0}^{\infty} b_n x^{2n}\right) \\ = E \exp\left(\sum_{i=0}^{\infty} b_n x^{2n}\right). \end{aligned} \quad (13)$$

Seeing that the wavefunction is of the form  $\psi(x) = \exp(f(x))$ , find the second derivative by applying the chain and product rule:

$$\frac{d^2 \psi}{dx^2} = \frac{d}{dx} \left( f'(x) e^{f(x)} \right) = f''(x) e^{f(x)} + (f'(x))^2 e^{f(x)}. \quad (14)$$

Inserting this back into Equation (13) and subtracting  $E\psi$  from both sides yields

$$-\frac{1}{2} (f''(x)\psi + (f'(x))^2 \psi) - V_0 e^{-\alpha x^2} \psi - E\psi = 0. \quad (15)$$

Now, recall that the Taylor expansion of  $e^{-\alpha x^2}$  is an infinitely long, even polynomial. Thus, Equation (15) can be written as a polynomial equation after dividing by  $-\psi$ :

$$\frac{1}{2} f''(x) + \frac{1}{2} (f'(x))^2 + V_0 \sum_{k=0}^{\infty} \frac{(-\alpha x^2)^k}{k!} + E = 0. \quad (16)$$

Since all terms are even polynomials, Equation (16) amounts to another even polynomial:

$$0 = c_0 + c_1 x^2 + c_2 x^4 + \dots = \sum_{n=0}^{\infty} c_n x^{2n}, \quad (17)$$

with some  $c_n$ . In order to solve this equation for the  $b_n$  coefficients of the wavefunction, realize that the above equation must hold for all values of  $x$ . Thus,  $c_n = 0$  for all  $n \in \mathbb{Z}^+$ . All  $c_n$  are functions of the coefficients  $b_n$  of the wavefunction. To verify this, write Equation (16) up to  $x^2$ :

$$0 = (b_1 + E + V_0) + (12b_2 + 4b_1^2 - V_0\alpha)x^2 + \mathcal{O}(x^4). \quad (18)$$

Obviously,  $c_0$  depends on  $b_1$ , while  $c_1$  depends on both  $b_1$  and  $b_2$ , etc.. Since  $c_n$  is 0 for all  $n$ , this yields a set of algebraic equations, which can be solved one-by-one to obtain all  $b_n$ . For example,  $b_1 = -(E + V_0)$  and inserting this in  $c_2$  yields  $b_2 = \frac{1}{12} (V_0\alpha - 4b_1^2)$ . This way, all  $b_n$  will be expressed in terms of  $\alpha, V_0$  and  $E$ .

To find the energy  $E$ , exploit the fact that  $\psi$  will only be computed up to a certain number of terms  $n + 1$ . Then, the largest order term in  $\psi$  is  $b_n x^{2n}$ . Consequently,  $n$  equations are necessary to find all  $b_n$ , which implies there are  $n$  terms in the Schrödinger equation that need to be equated to zero. However, due to the  $(f'(x))^2$  component, the largest term in the Schrödinger equation is  $c_{2n-1} x^{2(2n-1)}$ , thus there are  $2n-1$  terms. As a consequence, there are  $2n-1-n = n-1$  possibly non-zero terms left after the  $b_n$  have been found in terms of  $E$ . Therefore, to find  $E$ , insert the  $b_n$  into the coefficient of the first non-zero term and set it equal to zero. Since the resulting equation is a high ordered polynomial in  $E$ , there will be multiple roots and therefore multiple possible wavefunctions. Empirically, only the largest energy  $E$  is associated with an acceptable wavefunction. The reason for this is currently unknown.

Excited states introduce new coefficients, because the wave function is multiplied by a polynomial, e.g.  $1 + p_2 x^2, x + p_3 x^3$ , and so forth. The coefficients  $b_n$  are then expressed in terms of  $V_0, \alpha, E$  and some  $p_k$ . Solve for the  $p_n$  in the same way as for the energy, i.e. by setting additional terms in the Schrödinger equation equal to zero. Every two excited states, an additional coefficient  $p$  has to be included in the set of equations, i.e. for  $\psi_2, \psi_4$ , etc.. The accuracy of the coefficients decreases for higher states, as the terms of high order in the SE suffer the most from the truncation of the wave function.

## RESULTS

With a short Mathematica program, one can easily compute the coefficients and the energy associated to some well depth. Table 1 shows the energy of the ground state and first excited state of the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$  for multiple numbers of coefficients in the wavefunction. At first, the results converge for increasing number of coefficients, but for high number of terms, the results do not seem to become more accurate. Table 2 gives the coefficients of the wavefunction when taking 15 terms. Higher powers of  $x$  correspond to smaller coefficients.

In addition, Table 3 compares the SAS to the methods from the literature by giving the energies of the ground state and first two excited states for the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$ . Clearly, the values from the SAS agree with the other methods, especially with the Split-Operator, Per-

Table 1: The energies of the ground state ( $E_0$ ) and first excited state ( $E_1$ ) of the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$  for different numbers of terms included in the wave function of the semi-analytical solution, up to  $x^{2n}$

| $2n$ | $E_0$            | $E_1$            |
|------|------------------|------------------|
| 2    | -35.527864045000 | -26.583592135001 |
| 4    | -35.728688856466 | -27.643351214170 |
| 6    | -35.715298957308 | -27.535814387300 |
| 8    | -35.716186011007 | -27.545456105583 |
| 10   | -35.716129721255 | -27.544652343279 |
| 12   | -35.716133241189 | -27.544718188878 |
| 14   | -35.716132971357 | -27.544711615698 |
| 16   | -35.716132997117 | -27.544712337292 |
| 18   | -35.716132995912 | -27.544712311159 |
| 20   | -35.716132995725 | -27.544712306110 |
| 22   | -35.716132995685 | -27.544712301447 |
| 24   | -35.716132995715 | -27.544712302886 |
| 26   | -35.716132995720 | -27.544712303961 |
| 28   | -35.716132995715 | -27.544712303617 |

Table 2: The 15 coefficients  $b_n$  of the (unnormalized) groundstate wavefunction for the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$ . The values include 4 significant figures

| $x^{2n}$ | $b_n$        | $x^{2n}$ | $b_n$                    |
|----------|--------------|----------|--------------------------|
| 1        | 1            | $x^{16}$ | $2.950 \times 10^{-7}$   |
| $x^2$    | -4.284       | $x^{18}$ | $-1.168 \times 10^{-8}$  |
| $x^4$    | 0.5495       | $x^{20}$ | $-9.788 \times 10^{-10}$ |
| $x^6$    | -0.07789     | $x^{22}$ | $-2.709 \times 10^{-11}$ |
| $x^8$    | 0.008829     | $x^{24}$ | $3.606 \times 10^{-11}$  |
| $x^{10}$ | -0.0007634   | $x^{26}$ | $-1.121 \times 10^{-13}$ |
| $x^{12}$ | 0.00005282   | $x^{28}$ | $-9.328 \times 10^{-13}$ |
| $x^{14}$ | -0.000003719 |          |                          |

Table 3: The energies of the ground state ( $E_0$ ) and first two excited states ( $E_1, E_2$ ) of the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$ . Apart from the semi-analytical solution, the values are based on several methods from the literature: Variational method with harmonic oscillator trial function [7, 9], WKB approximation [8], deep-well approximation perturbation theory [4], Wronskian method [6, 5] and Split-Operator method [3, 2]

| Method          | $E_0$    | $E_1$    | $E_2$    |
|-----------------|----------|----------|----------|
| Variational     | -35.7135 | -27.5306 |          |
| WKB             | -35.6220 | -27.4510 | -20.1000 |
| Perturbation    | -35.7161 | -27.5447 | -20.1930 |
| Wronskian       | -35.7165 | -27.5445 | -20.1935 |
| Split-Operator  | -35.7161 | -27.5447 | -20.1935 |
| Semi-Analytical | -35.7161 | -27.5447 | -20.1935 |

turbation and Wronskian approaches. In general, these three methods are more accurate than the Variational method or WKB approximation. Therefore, the small discrepancies between SAS, Variational method and WKB are negligible.

For a variety of other well-depths, Table 4 gives the SAS energies of the ground state and first excited state, computed

Table 4: The energies of the ground state  $E_0$  and first excited state  $E_1$  for various well depths and  $\alpha = 1$ , computed with the SAS including 15 coefficients and the SOM

| $V_0$ | $E_0^{SAS}$ | $E_0^{SOM}$ | $E_1^{SAS}$ | $E_1^{SOM}$ |
|-------|-------------|-------------|-------------|-------------|
| 0.2   |             |             |             |             |
| 0.5   | -0.0957453  |             |             |             |
| 1     | -0.556199   |             |             |             |
| 2     | -1.21914    | -1.18833    | -0.0682015  |             |
| 3     | -1.96325    | -1.96722    | -0.207038   |             |
| 4     | -2.77351    | -2.77449    | -0.709764   | -0.783701   |
| 5     | -3.60721    | -3.60768    | -1.23976    | -1.27221    |
| 10    | -7.95266    | -7.95267    | -4.27988    | 4.28060     |
| 15    | -12.4499    | -12.4500    | -7.78653    | -7.76229    |
| 20    | -17.0262    | -17.0262    | -11.4852    | -11.4852    |
| 25    | -21.6528    | -21.6529    | -15.3614    | -15.3614    |
| 30    | -26.3153    | -26.4154    | -19.3461    | -19.3462    |

by taking 15 coefficients in the wavefunction, in comparison to the energies found by the Split-Operator method. The two methods agree very well for most of the results, especially for deep wells. For shallow wells the values disagree slightly, possibly because the SOM results are unreliable for small  $V_0$ . This is supported by the fact, that the SOM does not produce any energies for  $V_0 = 0.5$  or  $V_0 = 1$ , while the SAS does.

To investigate the accuracy of the SAS groundstate wavefunction for  $V_0 = 40$  and  $\alpha = 1$ , consider Figures 1, 2, and 3. The coefficients of this wavefunction are listed in Table 2. Figure 1 shows the normalized wavefunctions of the SAS (dashed) and the SOM (line), for the groundstate and first excited state. Evidently, the wavefunctions are very similar. Figure 2 shows  $\hat{H}\psi(x) - E\psi(x)$ , which for a perfect wavefunction should amount to 0 for all values of  $x$ . There are two segments where the difference is not equal to 0. However, the maximum error is approximately  $-10^{-6}$ , which is relatively small. Lastly, Figure 3 shows the difference between the normalized SAS and SOM wavefunctions. The discrepancy is small, with a maximum magnitude of  $10^{-5}$  close to the center of the well.

## DISCUSSION

As seen in the results section, the SAS gives very accurate energies and also wavefunctions, when compared to the SOM and other methods from the literature. There are, however, some issues with the method or its implementation in Mathematica. For shallow wells the SAS did not give a solution, although there should be an eigenstate according to Nandi [9]. In Table 4 this occurs for  $V_0 = 0.2$ . Furthermore, Table 1 shows how the SAS energy converges to some value as the number of coefficients increases. However, for the last few values, this convergence stops. This effect occurs faster for more shallow wells and it is suspected that it originates from the Mathematica code used, rather than the SAS itself. To be precise, the error is likely to stem from numerical limitations when solving the polynomial equation for the energy. The prior computations are performed analytically, such that there should not be any error coming from these steps. Since

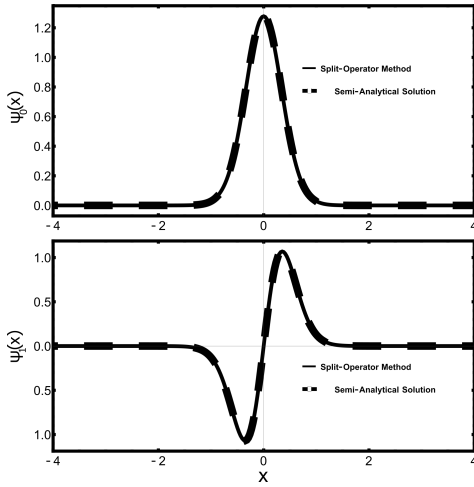


Figure 1: The normalized wavefunction of the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$  from the SAS (dashed) and the SOM (line) for the groundstate  $\psi_0$  and first excited state  $\psi_1$

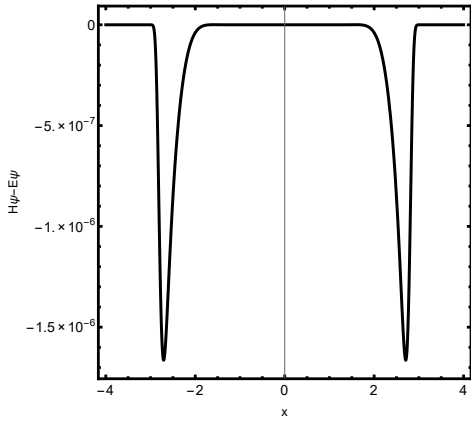


Figure 2:  $H\psi - E\psi$  for the SAS groundstate wavefunction for  $V_0 = 40$  and  $\alpha = 1$ . For a perfect wavefunction, the function is 0 at all values of  $x$

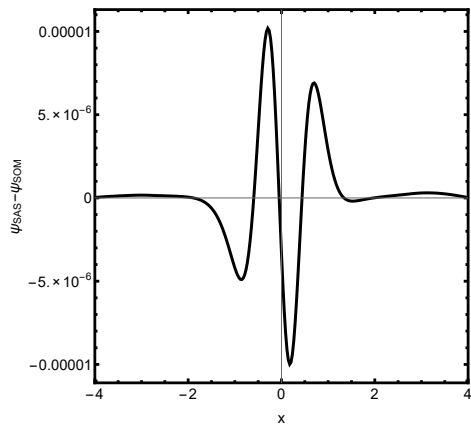


Figure 3: The difference between normalized SAS and SOM groundstate wavefunctions  $\psi_{SAS} - \psi_{SOM}$ , for the Gaussian well with  $V_0 = 40$  and  $\alpha = 1$

the wavefunction is directly dependent on the energy, erroneous energies also cause the wavefunction to be wrong.

Apart from these concerns, the SAS yields very accurate results even for low number of terms used. In Table 1, the final groundstate energy with 6 significant digits is reached already for 5 coefficients, i.e. computing up to  $x^8$ . Thus, the problem of non-convergence at higher terms does not matter for applications that do not require 10 digit accuracy.

## CONCLUSION

The semi-analytical solution proposed in this paper gives accurate energies both for the ground state and for excited states. Furthermore it yields truncated analytical wavefunctions that agree with other numerically obtained wavefunctions. While there are some computational issues that require more research, the method in itself is deemed accurate.

## ROLE OF THE STUDENT

Achim Byl was an undergraduate student under the supervision of Dr. Richard van den Doel when the research in this report was performed. The supervisor proposed the topic and supplied Mathematica code for the Semi-Analytic Solution and Split-Operator Method. The Mathematica code for the other methods comes from the student, who also surveyed the literature, compiled and processed the results, and wrote the report.

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