Perturbative and Numerical Approach on The Quantum Harmonic Oscillator with a Negative Gaussian Potential

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Abstract. Modeling a system in a harmonic oscillator approach still beneficial for the researcher to elucidate the physical mechanism in a small system such as a quantum dot. In this paper, we investigated the quantum harmonic oscillator system with the addition of a negative Gaussian potential (QHONGP). The effect of this Gaussian term was calculated analytically using a perturbative approach, and numerically using the Numerov and shooting method. The results showed that both approaches were able to show the unique feature of a pairing formation, i.e the decreasing energy of the system and the localization of particles in all (odd and even) states, at the lower pairing strength. For the higher pairing strength, the perturbative results highly depend on the number of energy levels and the expansion terms included in the calculation. The limited number of energy levels and the expansion terms resulted in the inaccuracy of the perturbative approach in giving the solution of QHONGP system as compared to the shooting method.

Keywords: Gaussian potential, harmonic oscillator, Numerov and shooting method, perturbation, quantum dot

1. Introduction
Quantum harmonic oscillator is the most common approach used by researchers to study the properties of a physical system in nature. The simplicity of the system and the wide range of problems modeled by this approach has made this system as an almost-default system in approaching many problems in nature. It had been used to model diatomic molecules, DNA, nucleons, quarks, economics, sociology and many more [1–5].

Quantum harmonic oscillator has been coupled with a various type of potentials for various purposes. It has been coupled with a positive Gaussian potential (a double-well potential) [6] and had successfully described the NH3 molecule degeneracy in molecular physics [7,8]. In condensed matter, the Gaussian potential had been used as a new confinement potential for spherical quantum dots [9] and also for electron pairs system [10].
The pairing formation is a common phenomenon that occurred in nature as a consequence of many-body interactions. This phenomenon manifest itself in any scale of physics, from superconductivity of electrons in the solid state, Bose-Einstein condensate in dilute atomic gas, or even superfluidity in nuclei and compact stars. The common features of pairing are the decreasing of the total energy of the system and the localization of particles. Those properties usually studied and obtained by solving the pairing problem within the framework of BCS theory which deploys mechanical operators based on the second quantization. The pairing bound state formation alternatively can be solved by using a regular quantum mechanics procedure in the harmonic and anharmonic oscillator basis, as shown by some researchers [11–13].

In this paper, we will demonstrate the ability and limitation of the perturbative and numerical approaches in describing the pairing formation in a quantum harmonic oscillator with a negative Gaussian potential (QHONGP) model. The perturbative approach is limited only up to the first five terms of the expansion and the analysis was done for the ground state up to the fourth excited state. The analysis will be focused on the energetic aspect of pairing and the wavefunction’s profile of each state. Some advantages and limitations of those approaches will also be discussed here.

2. Methods
We start solving the QHONGP by writing the Hamiltonian of the problem as follows

\[ H = \frac{\hat{p}^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 - ge^{-\frac{x^2}{\sigma^2}} \]  \hspace{1cm} (1)

where \( \hat{p} = -i\hbar \partial / \partial x \) is the momentum operator, and \( \mu = m/2 \) is the reduced mass of harmonic oscillator of two identical mass system. For simplicity, we set \( \hbar = \omega = \mu = \sigma = 1 \). The constant \( g \) is the pairing strength and denotes the strength of the external perturbing potential. The parameters \( \omega, \sigma \) represent the angular speed and the deviation’s width of Gaussian potential respectively.

The Hamiltonian of the system due to the introduction of small perturbation around the equilibrium point of the system can be expressed as \( H = H_0 + \lambda H_1 \) with \( H_0 \) the unperturbed Hamiltonian and \( \lambda H_1 \) the perturbing potential term. The first order correction of energy was calculated using the equation below which can be found in many quantum mechanics textbook [14].

\[ E_n^1 = \langle \psi_n^0 | H | \psi_n^0 \rangle \]  \hspace{1cm} (2)

and the corresponding first order correction on the wave function is

\[ \psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H | \psi_n^0 \rangle}{(E_n^0 - E_m^1)} \psi_m^0 \]  \hspace{1cm} (3)

Note that \( m \) and \( n \) denote the two interacting levels. The wave functions of harmonic oscillator are expressed in terms of Hermite polynomial \( H_k \) and take this form,

\[ \psi_k = \frac{1}{\sqrt{\sqrt{\pi} 2^k k!}} H_k e^{-\frac{x^2}{2}} \]  \hspace{1cm} (4)
where \( H_k \) for several terms (\( k \) is the polynomial’s order) are shown below

\[
H_0(y) = 1, \quad H_1(y) = 2y, \quad H_2(y) = 4y^2 - 2, \quad H_3(y) = 8y^3 - 12y, \quad H_4(y) = 16y^4 - 48y^2 + 12
\]  

(5)

The expansion is limited only up to five terms, those five terms \( k = 0, 1, 2, 3, 4 \) were assumed to be adequate enough to represent the dominant terms in the perturbative approach of the system. For the second order correction, the energy correction follows this form

\[
E_n^2 = \sum_{m=n} \left| \left( \frac{\psi_0^m}{E_0^n - E_m^2} \right) \right|^2
\]  

(6)

By solving Equation (6) above, the total energy of each state can be calculated by adding the first and second order correction to the unperturbed energy of each state.

Solving Equation (1) can also be done numerically using the Numerov method combined with shooting method [15]. One needs to rewrite the potential term as

\[
V(x) = \frac{1}{2} \mu \omega^2 x^2 - ge^{-x^2/\sigma^2}
\]  

(7)

and rewriting the problem as a second order differential equation, yields

\[
\frac{d^2\psi}{dx^2} = -\frac{2\mu}{\hbar^2} (E - V(x))\psi
\]  

(8)

Solving the differential equation above with the shooting method were done by connecting the previous \( (\psi_{i-1}) \), present \( (\psi_i) \), and the next \( (\psi_{i+1}) \) wave function (state) following this relation

\[
\psi_{i+1} = 2\psi_i - \psi_{i-1} + \Delta_x^2 f_i \psi_i + O(\Delta_x^6)
\]  

(9)

With \( f_i \) is the second order differential equation of our interest. By replacing \( f_i \) with the right side of Equation (11), yields

\[
\psi_{i+1} = 2\psi_i - \psi_{i-1} - \frac{2\mu}{\hbar^2} (E - V(x))\Delta_x^2 \psi_i
\]  

(10)

The appropriate boundary conditions must be chosen by setting the wave function to be very small in either sides of the potential wall, \( \psi(-\infty)=\psi(\infty)\approx 10^{-20} \), and by setting the stopping criterion \( \psi_{i+1} - \psi_i = 10^{-20} \) and \( E_{i+1} - E_i = 10^{-6} \). The eigenvalues and eigenfunctions of the system then can be calculated numerically as a function of pairing constant.

3. Result and Discussions

The results of numerical method and the perturbative approach (the first and second order correction) on the energy spectrum of QHONGP system are shown in Figure 1, in which the energy is plotted as a
function of pairing strength $g$. In this paper, we assumed that the numerical approach produces a better result (closer to the intended solution) as compared to the perturbative approach which was limited only up to the fourth excited state and the first five terms of the expansion. As the pairing strength grows, the energy of the system in all states is decreased, with the exception at the third excited state (using second order correction approach), indicating a stronger pairing formation. The first order correction of perturbative approach showed a linear decrease of energy, while the solution of the numerical method showed a parabolic-like energy decrease in a similar fashion as reported by others in the quantum harmonic oscillator with a delta-function potential [11,12,16]. Note that by tuning $\sigma$, the width constant in Equation (1), the parabolic profile of this energy decrease can be changed, but for simplicity the parameter $\sigma$ have been set to unity, since in this case, we put more attention to the effect of pairing strength $g$ rather than the potential’s width $\sigma$.

For the ground state and the first excited state, it was found that the second order correction produces a better result as compared to the first order correction in approaching the result from the numerical method. The different result was obtained in the second excited state, where the first order correction produces better results than the second order correction. The inaccuracy of the second order correction comes from the oscillating sign in the perturbative expansion which depend on the number of terms included in the perturbative expansion. The inaccuracy of the second order correction becomes even larger in the third excited state, as a result of a bigger pairing repulsion in the energy expansion. In the fourth excited state, the inaccuracy between perturbative approach and numerical approach is basically vanished, which might come from the negative energy term larger than the positive term and stabilize the energy fluctuation to bring the energy back to the numerical result. We assume that for the higher level ($n>5$) the results from both perturbative and numerical approach will be convergent as shown by the result from the fourth excited state. Note that, there is a small bump in the numerical result of the fourth excited state which might come from the numerical artifact.

The energy of the system as calculated by numerical and perturbation method in a small pairing strength region ($g < 4.0$) are almost identical for all states, while for higher pairing strength ($g > 4.0$), the difference between both methods becomes more obvious, especially in the first, second and third excited state. The discrepancy between perturbative and numerical approach at some lower states ($n=1,2,3$) and high pairing strength likely comes from the limited terms included in the perturbative calculation which resulted in the non-negligible competition between the positive and the negative energy terms in a perturbative approach. Inclusion of more terms in the calculation will probably converge the results of the perturbative approach to the values of the numerical approach.
Figure 1. The energy of QHONGP system calculated by a numerical (Numerov and shooting) method and perturbative approaches (first and second order corrections) as a function of pairing strength for the ground state and the first four excited states (n=0,1,2,3,4). All units are in arbitrary.

The feature of QHONGP’s solution is slightly different than the quantum harmonic oscillator with a delta function potential (QHODP) as discussed by others [11–13] in two ways. Firstly, in QHODP the pairing potential only affecting the even states due to the symmetry of the wavefunction at the equilibrium point, while in QHONGP the pairing potential affecting all (odd and even) states. Secondly, the pairing potential in QHODP reduces the energy of the even states to saturate to the energy of the odd states located at one level below, while in QHONGP no such behavior presents. These differences actually tell us the difference nature of pairing explained by those two models. The QHODP with stronger pairing effect is able to describe the transition from a weak pairing (BCS) to a strong pairing (BEC), while the QHONGP basically only explain the weak pairing formation (BCS or a molecular state) in some lower states due to a shallow pairing potential.

The energetic behavior of the system at extremely large pairing strength approached by the perturbative method even though producing a lower energy (stronger pairing) but it seems irrelevant to discuss since in that situation the perturbing potential is larger than the energy of the unperturbed system and makes the perturbative approach no longer valid. The effect of the negative Gaussian potential to the wavefunction of the quantum harmonic oscillator was calculated via a perturbative approach for the first order correction only. The probability density (|Ψ|^2) of ground state at various pairing strength is shown in Figure 2. As the pairing strength grows, the probability density of the system becomes higher as indicated by the formation of a localized system; a pairing bound state. The probability to find the particles is the highest at the equilibrium position where the two particles were brought closer by Gaussian potential and behave like a single state (a Cooper pair). The use of a stronger pairing strength (g=10, in Figure 2) change the profile of ground state probability density from a single peak into the profile of second excited state with three peaks. This finding is consistent with the occurrence of three negative energies (bound state) in Figure 1 at g=10. It is expected that for extremely large g, more peaks which correspond to the energy less than the ground state energy (E < 0.5 \hbar \omega) will present.

For the excited states, the effect of negative Gaussian potential to the probability density of the system was shown in Figure 3. As the pairing strength gets stronger the probability of particles to be localized at a particular distance is increased, and the stronger pairing strength prefers to enhance the probability density at the distance far from the equilibrium point. An interesting result was found in the third excited state, where the number of the peak which initially four (at g=0) was reduced to two (at g=10.0). In that case, the stronger pairing strength eliminates the localization of particles in the region close to the equilibrium point. Similar features of the probability density (or wavefunction) as shown in Figure 3 were also found by other researchers in the case of Bose–Einstein condensation modeled by a quantum harmonic oscillator with a parabolic trap [17].
Figure 2. The probability density of ground state as a function of distance for various pairing strength $g$. All units are in arbitrary.

Figure 3. The Probability density of some excited states. (a) first excited, (b) second excited, (c) third excited, (d) fourth excited states. All units are in arbitrary.

4. Conclusion
Throughout this paper, we have demonstrated the ability of a simple quantum harmonic oscillator with negative Gaussian potential in describing the formation of pairing in the spatial basis using numerical and perturbative approaches. The results from the perturbative approaches, as we expected, only make sense in the limit of small pairing strength and in the region close to the equilibrium point. In the higher pairing strength region, the perturbative approach becomes inaccurate in describing the pairing formation since the perturbation energy terms are larger than the unperturbed energy of the system which violate the first principle of perturbation approach (i.e small perturbation around the equilibrium
point). In general, the numerical and perturbative approach give similar results in the low pairing constant region, but as the pairing constant grows the discrepancy between both approaches becomes larger and destabilize the system. Despite the differences, both methods were able to show the unique feature of pairing formation, i.e the total energy drop and the localization of particle as the pairing strength grows.

Acknowledgments
Author (TS) expresses gratitude to J. Piekarewicz for fruitful discussions in the early stage of this research. Some parts of this research was funded by The Ministry of Research Technology and Higher Education Of The Republic of Indonesia through a Grant No. 1627/IT3.11/PN/2018

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