Correlation Function of Gaussian-Sine Asymmetric Potential by Shooting Method

Artit Hutem\textsuperscript{1,*}, Surachest Iamsamang\textsuperscript{2}

1. Physics Division, Faculty of Science and Technology Phetchabun Rajabhat University, Phetchabun, Thailand 67000 *Corresponding author

2. Biology Program, Faculty of Science and Technology Phetchabun Rajabhat University, Phetchabun, Thailand 67000

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Abstract

We show that the idea of program of evaluate correlation function of atomic density for the harmonics oscillator Gaussian-Sine asymmetric potential from the numerical shooting method of this problem. Compare the correlation function the theoretical (NSM\textsuperscript{[1]} see figure (3)) for particle into harmonics oscillator Gaussian-Sine asymmetric potential and the intensity correlation experiment by reference\textsuperscript{[3]}. We show that the intensity of atomic density fluctuation (\(\delta \eta(x) = \tilde{\eta}(x) - \tilde{\vartheta}(x)\)) in harmonics oscillator Gaussian-Sine asymmetric potential by NSM (see figure (4)).

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1 Introduction

More often than not, it is impossible to find exact solution to the eigenvalue problem of the Hamiltonian. To solve general problems, one must resort
to approximation methods. A variety of such methods have been developed, and each has its own area of applicability. There exist several means to study them, e.g. Wentzel-Kramers-Brillouin, perturbation, the variational method, the analytical transfer matrix method and numerical shooting method (NSM).


![Figure 1: The harmonics oscillator potential is perturbed by Gaussian-Sine asymmetric potential.](image)

2 The Schrödinger Equation in Finite Difference Formula

The potential energy for the harmonics oscillator Gaussian-Sine asymmetric is of the form show in figure(1) and is given by

\[
V_{GSA}(x) = \frac{1}{2} \mu \omega^2 x^2 + cx \cos(dx) + ae^{-bx^2} \sin^2(dx). 
\] (1)

The hamitonian of the harmonics oscillator Gaussian-Sine asymmetric potential is

\[
\hat{H}_{GSA} = \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{1}{2} \mu \omega^2 x^2 \right) + \left( cx \cos(dx) + ae^{-bx^2} \sin^2(dx) \right). 
\] (2)

If \( \varphi_n(x) \) represents the wave-function of the time-independent Schrödinger equation, we obtain

\[
\frac{d^2 \varphi_n(x)}{dx^2} + \frac{2\mu}{\hbar^2} \left( E_n - V_{GSA}(x) \right) \varphi_n(x) = 0, 
\] (3)
Substituting the harmonics oscillator Gaussian-Sine asymmetric potential from equation (1) and \( \xi \equiv \sqrt{\frac{\mu}{\hbar}} x \), \( \xi^2 = \frac{\mu \omega}{\hbar} x^2 \), \( \frac{d^2}{d\xi^2} = \frac{\mu \omega}{\hbar} \frac{d^2}{dx^2} \), \( \varepsilon = \frac{2\mu}{\hbar} \) and \( \hbar = \mu = \omega = 1 \) into equation (3) leads to the equation

\[
\frac{d^2 \varphi_n(\xi)}{d\xi^2} + \left( \varepsilon - \xi^2 - 2c\xi \cos(d\xi) - 2ae^{-bk^2} \sin^2(d\xi) \right) \varphi_n(\xi) = 0. \tag{4}
\]

We can find the numerical solution equation (4) by dividing \( \xi \) into many small segments, each of \( \Delta \xi \) in length. The second-derivative for the first term of equation (4) can be approximated in finite difference form as follows

\[
\frac{d^2 \varphi_n(\xi)}{d\xi^2} \approx \frac{\varphi_{i+1} + \varphi_{i-1} - 2\varphi_i}{(\Delta \xi)^2}. \tag{5}
\]

We can obtain the form of the time-independent Schrödinger equation in terms of finite difference by substituting equation (5) into equation (4), we obtain

\[
\varphi_{i+1} = 2\varphi_i - \varphi_{i-1} - (\Delta \xi)^2 \left( \varepsilon - \xi^2 - 2c\xi \cos(d\xi) - 2ae^{-bk^2} \sin^2(d\xi) \right) \varphi_i; \tag{6}
\]

where \( \xi_{i+1} = \Delta \xi + \xi_i \). The special potential given by harmonics oscillator Gaussian-Sine asymmetric potential has been used in evaluate equation (6) in the section(3)
3 Numerical Shooting Method and Results

We construe the new variable for using in calculating the ground-state energy eigenvalue, wave-function and the time-independent correlation function of the harmonics oscillator Gaussian-Sine asymmetric potential.

1. $\xi_{\text{min}}$ is the start position in the analysis range.

2. $\xi_{\text{max}}$ is the ultimate position in the analysis range.

3. $\xi$ is any position in the analysis range.

4. $nn$ is a number of very small bars in the analysis range.

5. $\Delta\xi = \frac{\xi_{\text{max}} - \xi_{\text{min}}}{nn}$ is the length of very small bars so that

Logic of the numerical shooting method evaluation of energy eigenvalue, eigenfunction and time-independent correlation function for the harmonics oscillator Gaussian-Sine asymmetric potential.

- Input values $\xi_{\text{min}}$ and $\xi_{\text{max}}$ in mathematica program for the harmonics oscillator Gaussian-Sine asymmetric potential and input equation (6) into mathematica program.
Figure 4: Schematic representation for behavior of atomic density fluctuation \( \delta \eta(x) = \bar{\eta}(x) - \bar{\vartheta}(x) \).

- Input the period amount.

- Plot the wave-function is normalized by the graph related to \( i \).

- Plot the probability the average atomic density \( \bar{\eta}(x) = |\varphi(x)|^2 \) for the harmonics oscillator Gaussian-Sine asymmetric potential.

- Input values \( \xi_{\text{min}} \) and \( \xi_{\text{max}} \) in the mathematica program for the harmonics oscillator potential.

- Input equation \( \varphi_{i+1} = 2\varphi_i - \varphi_{i-1} - (\Delta \xi)^2 (\varepsilon - \xi^2) \varphi_i \) into the mathematica program for the harmonics oscillator potential.

- For example, if \( |\varphi(x)| \leq 10^{-6} \), we stop the evaluation and accept the final energy as the numerical solution.

- Plot the wave-function is normalized for the harmonics oscillator potential by the graph related to \( i \).

- Plot the probability the average atomic density \( \bar{\vartheta}(x) = |\varphi(x)|^2 \) for the harmonics oscillator potential.
• Plot the density fluctuation $\delta \eta(x) = \tilde{\eta}(x) - \tilde{\vartheta}(x)$ [2] by the graph related to $i$.

• Plot the time-independent correlation function $C(s) = \frac{\delta \eta(x) \delta \eta(x')}{\eta(x) \eta(x')}$ when $s = |x - x'|$ is a distance between point $x$ and $x'$ [2].

4 Conclusion

Figure (2)(a-f) if the values of the $b = \frac{1}{\text{width}}$ and $c$ parameter has increase, the energy eigenvalues($E_n$) for the ground-state has lessen and figure (3)(a-c) the values of the correlation function($C(S)$)(part of positive) has lessen but figure (3)(d-f) the values of the correlation function($C(S)$)(part of positive) has supplement. From figure (4)(a-f) if the values of the $d$ and $c$ parameter has increase, the atomic density fluctuation $\delta \eta(x)$ has lessen.

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References


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