Correlation Function of Modified Gaussian-Cosine Rational Asymmetric Potential via Numerical Shooting Technique

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Abstract

We illustrate compare the time-independent correlation function the theoretical\textsuperscript{[1],[7]} to figure (5)) 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 modify Gaussian-Cosine rational asymmetric potential by numerical shooting method(see figure (6)).

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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 modify Gaussian-Cosine rational asymmetric potential.](image)

2 Basic Theory

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

\[
V(x) = \frac{1}{2} \mu \omega^2 x^2 + cx \cos(bx) + \frac{ae^{-t(x \cosh(x))^2} \cos^2(bx)}{1 + g x^2}.
\] (1)

The potential energy \( V(x) \) is called the harmonics oscillator modify Gaussian-Cosine rational asymmetric potential. The hamitonian of the harmonics oscillator modify Gaussian-Cosine rational asymmetric potential is

\[
\hat{H} = \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{1}{2} \mu \omega^2 x^2 \right) + \left( cx \cos(bx) + \frac{ae^{-t(x \cosh(x))^2} \cos^2(bx)}{1 + g x^2} \right). \] (2)
If $\psi_n(x)$ represents the wave-function of the time-independent Schrödinger equation, we obtain

$$
\frac{d^2\phi_n(x)}{dx^2} + \frac{2\mu}{\hbar^2} \left( \mathcal{E}_n - V(x) \right) \phi_n(x) = 0,
$$

where $E_n$ is the total energy eigenvalue. Substituting equation (1) into equation (3) leads to the equation

$$
\frac{d^2\phi_n(x)}{dx^2} + \frac{2\mu}{\hbar^2} \left( \mathcal{E}_n - \frac{1}{2} \mu \omega^2 x^2 - cx \cos(bx) - \frac{ae^{-t(x \cosh(bx))^2} \cos^2(bx)}{1 + gx^2} \right) \phi_n(x) = 0.
$$

Equation (4) can be solved in one way. The one approach we use is the numerical shooting method. To simplify the arithmetic involved in the shooting solution, we define some new dimensionless variables. The position variable $x$ is replaced with dimensionless variable $\xi$.

$$
\xi \equiv \sqrt{\frac{\mu \omega}{\hbar} x}, \quad \xi^2 = \frac{\mu \omega}{\hbar} x^2, \quad \frac{d^2}{d\xi^2} = \frac{\hbar}{\mu \omega} \frac{d^2}{dx^2}, \quad \varepsilon = \frac{2\mathcal{E}}{\hbar \omega}.
$$

Substituting equation (5) into equation (4), we can rewrite the Schrödinger equation completely in terms of $\xi$ as

$$
\frac{d^2\phi_n(\xi)}{d\xi^2} + \left( \varepsilon - \xi^2 - 2c \xi \cos(b\xi) - \frac{2ae^{-t(\xi \cosh(\xi))^2} \cos^2(b\xi)}{1 + g\xi^2} \right) \phi_n(\xi) = 0.
$$
The second-derivative for the first term of equation (6) can be approximated in finite difference form as follows

\[
\frac{d^2\phi_n(\xi)}{d\xi^2} \approx \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{(\Delta\xi)^2}. \tag{7}
\]

We can obtain the form of the Schrödinger equation in terms of finite difference by substituting equation (7) into equation (6), we obtain

\[
\phi_{i+1} = 2\phi_i - \phi_{i-1} - (\Delta\xi)^2\left(\varepsilon - \xi^2 - 2c\xi \cos(b\xi) - \frac{2ae^{t(\xi \cosh(b\xi))} \cos^2(b\xi)}{1 + g\xi^2}\right)\phi_i; \quad i = 2, 3, \ldots, \tag{8}
\]

where \(\xi_{i+1} = \Delta\xi + \xi_i\). The special potential given by harmonics oscillator modify Gaussian-Cosine rational asymmetric potential has been used in evaluate equation (8) in the section(3)

3 Numerical Shooting Method and Results

We construe the new variable for using in calculating the ground-state and excited-state energy eigenvalue(\(E_n\)), wave-function and the time-independent correlation function of the harmonics oscillator modify Gaussian-Cosine rational asymmetric potential.
Correlation function of modified Gaussian-cosine asymmetric potential

Figure 4: Schematic representation for behavior of correlation function for the ground-state energy (n=0).

1. $\xi_{\text{min}}$ is the begin position in the analysis range.
2. $\xi_{\text{max}}$ is the innermost 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 modify Gaussian-Cosine rational asymmetric potential.

- Input values $\xi_{\text{min}}$ and $\xi_{\text{max}}$ in mathematica program for the harmonics oscillator modify Gaussian-Cosine rational asymmetric potential and Input equation (8) into mathematica program.

- Plot the probability the average atomic density $\tilde{\eta}(x) = |\phi(x)|^2$ for the harmonics oscillator modify Gaussian-Cosine rational asymmetric potential.

- Input values $\xi_{\text{min}}$ and $\xi_{\text{max}}$ in the mathematica program for the harmonics oscillator potential.
• Input equation $\phi_{i+1} = 2\phi_i - \phi_{i-1} - (\Delta \xi)^2(\varepsilon - \xi^2)\phi_i$ into the mathematica program for the harmonics oscillator potential.

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

• Plot the probability the average atomic density $\tilde{\vartheta}(x) = |\phi(x)|^2$ 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 $C(s) = \frac{\delta \eta(x)\delta \eta(x')}{\tilde{\eta}(x)\tilde{\eta}(x')}$ when $s = |x - x'|$ is a distance between point $x$ and $x'$ [2].

4 Conclusion

On another, we compare the effect of width size ($t$) on the shape of wave function for setting parameters of modify Gaussian-Cosine rational asymmetric potential to be $t = 3$ and $t = 12$ and $t = 70$, in figure (2)(d-f). Finally we show the calculation results of the time-independent correlation function for the ground-state and excited-state wave function in figure (4) to figure (5) and the result of the time-independent atomic density fluctuation $\delta \eta(x)$ obtained.
Figure 6: Schematic representation for shapes of the time-independent atomic density fluctuation.

is illustrated in figure (6), respectively. From figure (6)(a-f) if the values of the \(a\) and \(t\) parameter has increase, the atomic density fluctuation \(\delta \eta(x)\) has decrease.

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References


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