Correlation Function of Gaussian Rational Asymmetric Potential by Shooting Method

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Abstract

A detailed procedure based on numerical shooting method (NSM) is presented to solve bound state problems. This work aims at computing excited-state correlation function of a particle under the harmonics oscillator Gaussian rational asymmetric potential use shooting method.

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1 Introduction

Bound state problems in foundation quantum mechanics have long been of interest in various branches of physics since the advent of the famous Schrödinger equation. Hutem A. and Boonchui S. 2014[1] show that calculate correlation function of the Gaussian random potential by NSM. Hutem A. 2014[2] illustrates the calculated the atomic density fluctuation for harmonic oscillator Sine asymmetric potential in the mathematica program. To study problem of stationary states, we focus on one approximation method: numerical shooting method useful evaluate correlation function of a particle around of attraction by the harmonics oscillator Gaussian rational asymmetric potential.
2 The time-independent Schrödinger equation in finite difference formula

The stationary state energies $E_n$ and wave-functions $\psi_n(x)$ are solutions of the eigenvalue equation, $\mathcal{H}\psi_n(x) = E_n\psi_n(x)$, which is the time-independent Schrödinger equation. In the case of the harmonics oscillator Gaussian rational asymmetric potential, the Hamiltonian is of the form

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2 + cx + ae^{-bx^2} + \frac{gx^2}{(1 + qx^4)}, \quad (1)$$

where $cx + ae^{-bx^2} + \frac{gx^2}{(1 + qx^4)}$ is the Gaussian rational asymmetric potential. Then the eigenvalue equation for energy is given by

$$-\frac{2mE_n}{\hbar^2}\psi_n(x) = \frac{d^2\psi_n(x)}{dx^2} - \frac{m\omega^2x^2}{\hbar^2}\psi_n(x) - \frac{2mcx}{\hbar^2}\psi_n(x) - \frac{2mae^{-bx^2}}{\hbar^2}\psi_n(x) - \frac{2mgx^2}{\hbar^2(1 + qx^4)}\psi_n(x). \quad (2)$$

To simplify the writing in what follows, we introduce the dimensionless variables (setting $\hbar = m = \omega = 1$)

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}x}, \quad x^2 = \frac{\hbar}{m\omega}\xi^2, \quad \varepsilon = \frac{2E}{\hbar\omega}. \quad (3)$$

Thus, the time-independent Schrödinger equation given by equation 3 may be rewritten as

$$\frac{d^2\psi_n(\xi)}{d\xi^2} + \left(\varepsilon - \xi^2 - \eta\xi - ae^{-b\xi^2} - \frac{\lambda\xi^2}{(1 + \beta\xi^4)}\right)\psi_n(\xi) = 0. \quad (4)$$

In short, the second-derivative for the first term of equation (4) is approximated given by

$$\frac{d^2\psi(\xi)}{d\xi^2} \approx \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{(\Delta\xi)^2} \quad (5)$$

Equation (5) can be transformed into

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta\xi)^2\left(\varepsilon - \xi^2 - \eta\xi - ae^{-b\xi^2} - \frac{\lambda\xi^2}{(1 + \beta\xi^4)}\right)\psi_i, \quad (6)$$

where $\xi_{i+1} = \Delta\xi + \xi_i$. The special potential given by harmonics oscillator Gaussian rational asymmetric potential has been used in evaluate equation (6) into the mathematica program (see Sect.3).
Figure 1: Diagram showing of the correlation function in case of the amplitude of barrier equal $a = 10$ and vary $\beta = 0.1, 0.3, 0.5$.

3 Numerical shooting method and result

Logic of the numerical shooting method evaluation of correlation function for the harmonics oscillator Gaussian rational asymmetric potential.

- Input values $\xi_{\text{min}}$ and $\xi_{\text{max}}$ in mathematica program for the harmonics oscillator Gaussian rational asymmetric potential.
- Input the period amount.
- Input eq.(6) into mathematica program.

By input $\psi_1$ and $\psi_2$ as two initial values for calculation, we can find $\psi_3$ from eq.(6). In the same way, we can find $\psi_4$ by substituting $\psi_2$ and $\psi_3$ in the equation. Keep doing this, we can find $\psi_n$.

- The next task is to calculate wave-function in eq.(6)($\psi_{i+1}$) so that it approaches zero as closely as desired. Normally, we assign a small value as the standard to make sure wave-function in eq.(6) get close enough to zero. For example, if $|\psi_{i+1}| \leq 10^{-6}$, we stop the calculation and accept the final energy as the numerical solution.
Figure 2: Schematic representation of the correlation function in case of the amplitude of barrier equal $a = 15$ and vary $\eta = 0.05, 0.17, 0.35$.

- Plot the probability the average atomic density $\tilde{n}(x) = |\psi(x)|^2$ for the harmonics oscillator Gaussian rational asymmetric potential.
- Input equation $\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2(\varepsilon - \xi^2)\psi_i$ into the mathematica program for the harmonics oscillator potential.
- For example, if $|\psi(x)| \leq 10^{-6}$, 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 $\tilde{m}(x) = |\psi(x)|^2$ for the harmonics oscillator potential.
- Plot the density fluctuation $\delta n(x) = \tilde{n}(x) - \tilde{m}(x)$ by the graph related to $i$.
- Plot the time-independent correlation function $C(x, \dot{x}) = \frac{\delta n(x)\delta n(\dot{x})}{\tilde{n}(x)\tilde{n}(\dot{x})}$. 

- Plot the probability the average atomic density $\tilde{n}(x) = |\psi(x)|^2$ for the harmonics oscillator Gaussian rational asymmetric potential.
4 Conclusion

This paper interested in finding the correlation function by numerical shooting method. The results from show that the magnitude of the correlation function \( C(S) \) vary according to the parameters \( a, \eta, \lambda, b, \beta \), respectively. The correlation function oscillates with the amplitude gradually decreasing to zero. It is called one-half of critical damping case. Negative correlations were obtained in our calculations. They were predicted to exist in reflection of waves from a thick disordered slab.

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References


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