Evaluate Correlation Function of the Harmonics Oscillator Gaussian Cosine Angle Two Degree Rational Asymmetric Potential via NSM

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Abstract

We use the numerical shooting method(NSM) for solving the Schrödinger’s equation of quantum mechanics system for evaluating the correlation function under the harmonics oscillator Gaussian Cosine angle two degree rational asymmetric potential. We show that the idea of program of evaluate correlation function of atomic density for the potential in figure(1) from the NSM of this problem. Compare the correlation function the theoretical(NSM[5],[8]) and the intensity correlation experiment by reference[7].

Keywords: correlation function, energy-eigenvalue, wave-function

1 Introduction

An exact solution of the time-independent Schrödinger equation exists only for a few idealized problems; normally it has to be solved using an approximation method. Example, Perturbation theory is applied to those cases in which the real system can be described by a small change in an easily solvable, idealized system. The Hamiltonian of the system is then of the form $\hat{H} =$...
$H_0 + \varepsilon \hat{H}$, where $\hat{H}$ and $H_0$ do not differ very much from each other. $\hat{H}_0$ is called Hamiltonian of the unperturbed system; the perturbation $\hat{H}$ has to be very small. The parameter $\varepsilon$ is also called the smallness parameter. There exist several means to study them, e.g. function analysis[1, 2], the analytical transfer matrix method[3][4] and NSM[5][8].

N.Cherroret and S.E.Skipetrov 2008 [6] show that the average atomic density as a function of time. In this paper we consider approximation methods that deal with stationary states corresponding to time-independent Hamiltonian. To study problem of stationary states, we focus on one approximation method: NSM useful evaluate wave-function and correlation function of a particle around of attraction by the harmonics oscillator with Gaussian Cosine angle two degree rational asymmetric potential.

![Figure 1: Plot of the harmonics oscillator Gaussian Cosine angle two degree rational asymmetric potential.](image)

Figure 1: Plot of the harmonics oscillator Gaussian Cosine angle two degree rational asymmetric potential.

## 2 Schrödinger Equation in Finite Difference

The potential energy ($V(x)$) for the harmonics oscillator Gaussian Cosine angle two degree rational asymmetric is of the form show in figure(1) and is given by

$$V(x) = \frac{1}{2} m \omega^2 x^2 + b x \cos(10x) + \frac{ae^{-\mu x^2} \left( \cos(10x^2) \right)^2}{1 + gx^2}.$$  

(1)

The Hamiltonian of the harmonics oscillator Gaussian Cosine angle two degree rational asymmetric potential is

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

$$\hat{H}' = \left( - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) + \left( b x \cos(10x) + \frac{ae^{-\mu x^2} \left( \cos(10x^2) \right)^2}{1 + gx^2} \right),$$

(2)

where $k = m \omega^2$ is the force constant describing the attractive force. If $\psi(x)$ represents the wave-function of the time-independent Schrödinger equation, we obtain

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left( E - V(x) \right) \psi(x) = 0,$$

(3)
where $E$ is the energy eigenvalue, $m$ is the effective mass. Substituting the potential $V(x)$ from equation (1) into equation (3) leads to the equation

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 x^2 - bx \cos(10x) - \frac{ae^{-\mu x^2} \left( \cos(10x^2) \right)^2}{1 + gx^2} \right) \psi(x) = 0. \quad (4)$$

Equation (4) can be solved in one ways. To simplify the arithmetic involved in the shooting solution. The position variable $x$ is replaced with dimensionless variable $\xi$.

$$\xi \equiv \sqrt{\frac{m \omega}{\hbar}} x, \quad \xi^2 = \frac{m \omega}{\hbar} x^2, \quad \frac{d^2}{d\xi^2} = \frac{\hbar}{m \omega} \frac{d^2}{dx^2}. \quad (5)$$

Substituting in for $x$ in terms of $\xi$ and setting $\varepsilon = \frac{2E}{\hbar \omega}$, $2b = \beta$, $2a = \lambda$ and $\hbar = m = \omega = 1$ into equation (4), we can rewrite the Schrödinger equation completely in terms of $\xi$ as

$$\frac{d^2 \psi(\xi)}{d\xi^2} + \left( \varepsilon - \xi^2 - \beta \xi \cos(10\xi) - \frac{\lambda e^{-\mu \xi^2} \left( \cos(10\xi^2) \right)^2}{1 + g\xi^2} \right) \psi(\xi) = 0. \quad (6)$$

The second-derivative for the first term of equation (6) can be approximated in finite difference form as follows

Figure 2: Sketch of the wave function for the potential shown in figure(1) $\lambda = 5, 7$. 

\[\text{Evaluate correlation function}\]
Figure 3: Plot of the wave function for the potential shown in figure(1) $\lambda = 10, 13, 16$.

\[ \frac{d^2 \psi(\xi)}{d\xi^2} \approx \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{(\Delta \xi)^2}. \]  

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

\[ \psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2 \left( \varepsilon - \xi^2 - \beta \xi \cos(10\xi) - \frac{\lambda e^{-\mu \xi^2} \left( \cos(10\xi^2) \right)^2}{(1 + g\xi^2)} \right) \psi_i; \ i = 2, 3, \ldots, \] (8)

where $\xi_{i+1} = \Delta \xi + \xi_i$. The special potential given by the potential in figure(1) 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 correlation function for the potential in figure(1). $\xi_{\text{min}}$ is the start position in the analysis range. $\xi_{\text{max}}$ is the ultimate position in the analysis range. $\xi$ is any position in the analysis range. $\Delta \xi$ is the length of very small bars so that $\Delta \xi = \frac{\xi_{\text{max}} - \xi_{\text{min}}}{n}$. 
Logic of the NSM evaluation of correlation function for the potential in figure(1).

- Input values $\xi_{\text{min}}$ and $\xi_{\text{max}}$ in mathematica program for the potential shown in figure(1) and input eq.(8) into mathematica program.

- The next task is to calculate wave-function in eq.(8)($\psi_{i+1}$) so that it approaches zero as closely as desired. Normally, we assign a small value as the standard to make sure wave-function in $\Delta \xi$ 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.

- Plot the average atomic density $\tilde{n}(x)$ for the potential shown in figure(1).

- 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.

- Plot the average atomic density $\tilde{m}(x)$ for the harmonics oscillator potential.

- Plot the density fluctuation $\delta n(x) = \tilde{n}(x) - \tilde{m}(x)$[6] by the graph related to $i$. 

Figure 4: Sketch of the correlation function for the potential shown in figure(1) $\lambda = 5, 7$. 
Plot the correlation function $C(s)$ when $s = |x - x'|$ is a distance between point $x$ and $x'$ [6].

4 Conclusion

However the NSM[5],[8] does not use complicated formulas, it requires much less computational effort when compared to the Green functions techniques[6]. Generally regarded as one of the most efficient methods, the NSM give very accurate results because it integrates the Schrödinger equation directly, though in the numerical sense. From figure (2)(a-f) if the values of $g$ and $\mu$ has incline, the ground-state energy eigenvalues $(E_n)$ has lessen and figure (4)(a-f) the values of the correlation function (part of positive) has little. From figure (3)(a-c) if the values of $\beta$ has increase, the ground-state energy eigenvalues has lessen but figure (5)(a-c) the values of the correlation function has supplement. From figure (3)(d-f) if the values of $\lambda$ has increase, the ground-state energy eigenvalues has incline and the amplitude of wave-function has split up asymmetric has increase and figure (5)(d-f) the values of the correlation function has supplement.
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References


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