Research Article

Evaluated Excited-State Time-Independent Correlation Function and Eigenfunction of the Harmonics Oscillator Cosine Asymmetric Potential via Numerical Shooting Method

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We aimed to evaluate the ground-state and excited-state energy eigenvalue (E_n), wave function, and the time-independent correlation function of the atomic density fluctuation of a particle under the harmonics oscillator Cosine asymmetric potential (Saad et al. 2013). Instead of using the 6-point kernel of 4 Green's function (Cherroret and Skipetrov, 2008), averaged over disorder, we use the numerical shooting method (NSM) to solve the Schrödinger equation of quantum mechanics system with Cosine asymmetric potential. Since our approach does not use complicated formulas, it requires much less computational effort when compared to the Green functions techniques (Cherroret and Skipetrov, 2008). We show that the idea of the program of evaluating time-independent correlation function of atomic density is underdamped motion for the Cosine asymmetric potential from the numerical shooting method of this problem. Comparison of the time-independent correlation function obtained from numerical shooting method by Boonchui and Hutem (2012) and correlation function experiment by Kasprzak et al. (2008). We show the intensity of atomic density fluctuation ($\delta n(x) = \bar{n}(x) - \bar{m}(x)$) in harmonics oscillator Cosine asymmetric potential by numerical shooting method.

1. Introduction

Most problems encountered in quantum mechanics cannot be solved exactly. Exact solutions of the Schrödinger equation exist only for a few idealized systems. 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, for example, Wentzel-Kramers-Brillouin [1], perturbation [2], the quasilinearization method [3], the variational method [4], function analysis [5, 6], the eigenvalue moment method [7], the analytical transfer matrix method [8–10], and numerical shooting method [11, 12].

Grobe et al. 1994 [13] proposed a criterion to determine the numerical degree of global correlation function of the multiparities quantum system. They applied this method to several situations, including electron-atom scattering and strong-field photoionization. Lye et al. 2005 [14] discussed

the effect of a weak random potential, indicated by stripes in the expanded density profile of the Bose-Einstein Condensate and damped dipole oscillations. Henseler and Shapiro 2008 [15] defined the disorder-induced intensity-intensity correlation function, $C_\omega(\mathbf{r}, \mathbf{r}') = |\psi_\omega^*(\mathbf{r})\psi_\omega(\mathbf{r}')|^2$, for the Bose-Einstein Condensate for Fermi gas. Cherroret and Skipetrov 2008 [16] showed decay of the average atomic density ($\overline{n(\mathbf{r}, t)} = \overline{|\psi(\mathbf{r}, t)|^2}$) as a function of time. The density reaches a maximum at the arrival time $t_{\text{arrival}} \approx 2z^2/D_\mu$, where D_μ is the diffusion coefficient in random potentials. Now, a few works have concerned the expansion of Bose-Einstein Condensate in three-dimensional potentials and evaluate correlation function. Cherroret and Skipetrov 2009 [17] had shown the typical diffusion coefficient of the Bose-Einstein Condensate in a three-dimensional random potential. Beilin et al. 2010 [18] considered diffusion of cold-atomic Fermi gas in the presence of a random optical speckle potential.

Pezze et al. 2011 [19] numerically studied the dynamics regimes of classical transport of cold atoms gases in a two-dimensional anisotropic disorder potential. 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: numerical shooting method useful to evaluate wave function and time-independent correlation function of a particle around attraction by the harmonics oscillator with Cosine asymmetric potential. The scheme of the paper is as follows. In Section 2, we write the basic time-independent Schrödinger equation in terms of finite difference and the harmonics oscillator Cosine asymmetric potential in terms of the new variable is given by

$$\begin{aligned} \psi_{i+1} &= 2\psi_i - \psi_{i-1} \\ &- (\Delta\xi)^2 \left(\varepsilon - \xi^2 - 2c\xi - 2a \cos(b\xi) \right) \psi_i; \quad (1) \\ i &= 2, 3, 4, \dots, \end{aligned}$$

where $2c\xi + 2a \cos(b\xi)$ is the Cosine asymmetric potential. In Section 3, we show the idea of writing a program for evaluating energy eigenvalue wave function and correlation function of atomic density for the Cosine asymmetric potential via the numerical shooting method (Asaithambi, Ledoux and van Daele, Boonchui and Hutem [12, 20, 21]). Section 4 contains our conclusions.

2. Time-Independent Schrödinger Equation in Finite Difference Formula for Harmonics Oscillator Cosine Asymmetric Potential

We consider a particle of mass μ moving on the x -axis in a time-independent potential $\mathcal{V}(x)$. The time-independent Schrödinger equation corresponding to this one-dimensional motion is

$$-\frac{\hbar^2}{2\mu} \frac{d^2\psi_n(x)}{dx^2} + \mathcal{V}(x) \psi_n(x) = \mathcal{E}_n \psi_n(x), \quad (2)$$

where $\mathcal{E}_n$ is the total energy eigenvalues of the particle. The solution of this equation yields the allowed energy eigenvalues $\mathcal{E}_n$ and the corresponding wave function $\psi_n(x)$. To solve this partial differential equation, we need to specify the potential $\mathcal{V}(x)$ as well as the boundary condition; the boundary condition can be obtained from the physical requirement of the system.

Suppose a particle is bound state to around of attraction by the harmonics oscillator Cosine asymmetric potential (see Figure 1):

$$\mathcal{V}(x) = \frac{1}{2}\mu\omega^2 x^2 + cx + a \cos(bx), \quad (3)$$

FIGURE 1: The harmonics oscillator potential is perturbed by Cosine asymmetric potential, with $a = 5$, $b = 10$, and $c = 0.4$.

with $cx + a \cos(bx)$ that is called the Cosine asymmetric potential [22], where c , a , and b are positive constants. Substituting the harmonics oscillator Cosine asymmetric potential from (3) into (2) leads to the following equation:

$$\begin{aligned} \mathcal{E}_n \psi_n(x) &= -\frac{\hbar^2}{2\mu} \frac{d^2\psi_n(x)}{dx^2} \\ &+ \left(\frac{1}{2}\mu\omega^2 x^2 + cx + a \cos(bx) \right) \psi_n(x). \end{aligned} \quad (4)$$

For our approach (4) can be solved in the numerical shooting method. It is convenient to simplify the arithmetic involved in the shooting solution. We define some new dimensionless variables. Then the position variable x is replaced with the dimensionless variable ξ :

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

With this definition, the second-derivative term can be written as

$$\frac{d^2}{d\xi^2} = \frac{\hbar}{\mu\omega} \frac{d^2}{dx^2}. \quad (6)$$

Substituting in for x in terms of ξ and setting $\varepsilon = 2E/\hbar\omega$ and setting $\hbar = \mu = \omega = 1$ into (4), we can rewrite the time-independent Schrödinger equation completely in terms of ξ as follows:

$$\frac{d^2\psi_n(x)}{d\xi^2} + (\varepsilon - \xi^2 - 2c\xi - 2a \cos(b\xi)) \psi_n(x) = 0. \quad (7)$$

Also, the time-independent potential in terms of the new variable is given by

$$\mathcal{V}(\xi) = \xi^2 + 2c\xi + 2a \cos(b\xi). \quad (8)$$

For the finite difference method, (7) is rewritten in the form of many small segment $\Delta\xi$ in the ξ domain length. The second-derivative of the first term in (7) can be approximated in finite difference form as follows:

$$\frac{d^2\psi_n(x)}{d\xi^2} \approx \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{(\Delta\xi)^2}. \quad (9)$$

FIGURE 2: Figures (a)–(c) show plot of the time-independent wave function for the ground-state energy ($n = 0$) in case of varying $a = 8, 10, 12$ (the amplitude of barrier potential) in harmonics oscillator Cosine asymmetric potential. Figures (d)–(f) show the wave function for the ground-state energy with varying $b = 14, 18, 24$ harmonics oscillator Cosine asymmetric potential.

We can obtain the form of the time-independent Schrödinger equation in terms of finite difference by substituting (9) into (7), and we get

$$\begin{aligned} \psi_{i+1} &= 2\psi_i - \psi_{i-1} \\ &- (\Delta\xi)^2 (\varepsilon - \xi^2 - 2c\xi - 2a \cos(b\xi)) \psi_i; \quad (10) \\ i &= 2, 3, 4, \dots, \end{aligned}$$

where $\xi_{i+1} = \Delta\xi + \xi_i$. The special potential given by harmonics oscillator Cosine asymmetric potential has been used in calculating (10) in the mathematica program (see Section 3).

3. Numerical Shooting Method and Results

We construe the new variable to be used in calculating the ground-state energy eigenvalue, wave function, and the time-independent correlation function of the harmonics oscillator Cosine asymmetric potential.

FIGURE 3: Schematic representation for behavior of the wave function for the ground-state energy ($n = 0$) and the second excited-state energy ($n = 2$) in case of the harmonic oscillator Cosine asymmetric potential with varying $c = 0.3, 0.4, 0.5$.

- (1) $\xi_{\min}$ is the start position in the analysis range.
- (2) $\xi_{\max}$ is the ultimate position in the analysis range.
- (3) ξ is any position in the analysis range.
- (4) nm is a number of very small bars in the analysis range.
- (5) $\Delta\xi$ is the length of very small bars so that

$$\Delta\xi = \frac{\xi_{\max} - \xi_{\min}}{nm}. \quad (11)$$

The logic of the numerical shooting method evaluation of energy eigenvalue, eigenfunction, and time-independent correlation function for the harmonic oscillator Cosine asymmetric potential is as follows.

- (i) Input values $\xi_{\min}$ and $\xi_{\max}$ in mathematica program for the harmonic oscillator Cosine asymmetric potential.
- (ii) Input the period amount.
- (iii) Input (10) into mathematica program.

FIGURE 4: Plot of the wave function for the first excited-state energy ($n = 1$) and the third excited-state energy ($n = 3$) in case of the harmonics oscillator Sine asymmetric potential with varying $c = 0.3, 0.4, 0.5$.

Find the initial value for calculation. Input the initial condition by setting $\psi_1 = 0$ for the position imprints and set $d\psi/d\xi = 1$ from the slope of positions 1 and 2, so that

$$\frac{d\psi}{d\xi} \approx \frac{\psi_2 - \psi_1}{\Delta\xi} \Rightarrow \psi_2 \approx \Delta\xi. \quad (12)$$

By inputting ψ_1 and ψ_2 as two initial values for calculation, we can find ψ_3 from (10). In the same way, we can find ψ_4 by substituting ψ_2 and ψ_3 in the equation. As we keep doing this, we can find ψ_n (see Figure 2 in [12]).

- (i) The next task is to calculate wave function in (10) (ψ_{i+1}) so that it approaches zero as closely as desired. Normally, we assign a small value as the standard to make sure that wave function in (10) gets 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.

- (ii) Plot the wave function by the graph related to i .
- (iii) Plot the wave function that is normalized by the graph related to i .
- (iv) Plot the probability of the average atomic density $\bar{n}(x) = |\psi(x)|^2$ for the harmonics oscillator Cosine asymmetric potential.
- (v) Input values $\xi_{\min}$ and $\xi_{\max}$ in the mathematica program for the harmonics oscillator potential.
- (vi) Input equation $\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta\xi)^2(\epsilon - \xi^2)\psi_i$ into the mathematica program for the harmonics oscillator potential.
- (vii) For example, if $|\psi(x)| \leq 10^{-6}$, we stop the evaluation and accept the final energy as the numerical solution.

FIGURE 5: Figures (a)–(c) show plot of the time-independent correlation function for the ground-state energy ($n = 0$) in case of varying $a = 8, 10, 12$ (the amplitude of barrier potential) in harmonics oscillator Cosine asymmetric potential. Figures (d)–(f) show the correlation function for the ground-state energy with varying $b = 14, 18, 24$ harmonics oscillator Cosine asymmetric potential.

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

(ix) Plot the probability of the average atomic density $\bar{m}(x) = |\psi(x)|^2$ for the harmonics oscillator potential.

(x) Plot the time-independent atomic density fluctuation $\delta n(x) = \bar{n}(x) - \bar{m}(x)$ [16] by the graph related to i .

(xi) Plot the time-independent correlation function $C(x, \dot{x}) = \overline{\delta n(x) \delta n(\dot{x})} / \overline{n(x) n(\dot{x})}$ [16].

4. Conclusion

In conclusion, we then represented the method by obtaining numerical solution of the one-dimensional harmonic oscillator, perturbed from a set of the Cosine asymmetric potentials.

FIGURE 6: Schematic representation for behavior of the time-independent correlation function for the ground-state energy ($n = 0$) and the second excited-state energy ($n = 2$) in case of the harmonics oscillator Cosine asymmetric potential with varying $c = 0.3, 0.4, 0.5$.

In our calculation, we can obtain the time-independent correlation function corresponding with the Green functions techniques [16]. Although the numerical shooting method does not use complicated formulas, it requires much less computational effort when compared to the Green functions techniques. Generally, regarded as one of the most efficient methods, the numerical shooting method [12] gives very accurate results because it integrates the Schrödinger equation directly, though in the numerical sense.

In this case, the wave function of the harmonics oscillator Cosine asymmetric potential is different from that in case of a typical harmonics oscillator potential ($\mathcal{V}(x) = (1/2)\mu\omega^2x^2$) (see Figures 2–4). In this case, the time-independent correlation function ($C(S)$) of the harmonics oscillator Cosine asymmetric potential via numerical shooting method and the intensity correlation experiment by reference [23] have the same appearance (see Figures 5–7). From Figures 2(a)–2(c), if the values of the amplitude barrier potential a

FIGURE 7: Plot of the time-independent correlation function for the first excited-state energy ($n = 1$) and the third excited-state energy ($n = 3$) in case of the harmonics oscillator Cosine asymmetric potential with varying $c = 0.3, 0.4, 0.5$.

incline, the ground-state energy eigenvalues (E_n) lessen, but the amplitude of the wave function has supplement and in Figures 5(a)–5(c) the values of the time-independent correlation function ($C(S)$) (part of positive) incline and the time-independent correlation function is underdamped motion. From Figures 2(d)–2(f) if the values of b increase, the ground-state energy eigenvalues (E_n) have supplement, but in Figures 5(d)–5(f) the values of the time-independent correlation function lessen.

From Figures 3(a)–3(f), if the values of the c parameter increase, the ground-state ($n = 0$) and the second excited-state ($n = 2$) energy eigenvalues (E_n) lessen, but in Figures 6(a)–6(f) the values of the time-independent correlation function have supplement. From Figures 4(a)–4(f), if the values of the c parameter increase, the first excited-state ($n = 1$) and the third excited-state ($n = 3$) energy eigenvalues (E_n) lessen, but in Figures 7(a)–7(f) the values of the time-independent correlation function have supplement. From

FIGURE 8: Schematic representation for behavior of the time-independent atomic density fluctuation $\delta n(x) = \bar{n}(x) - \bar{m}(x)$ for the ground-state energy ($n = 0$) in case of the harmonic oscillator Cosine asymmetric potential with varying $c = 0.2, 0.4$ and $a = 6, 8, 10$.

Figures 8(a)–8(c) if the values of the c , a , and b parameters increase, the time-independent atomic density fluctuation ($\delta n(x)$) for the ground-state ($n = 0$) has supplement.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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