

Evaluation of correlation functions and wave-functions of the Gaussian random potentials by numerical shooting method

Artit Hutem · Sutee Boonchui

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Abstract In this paper, we apply a simple numerical method for evaluating a correlation function of atomic density fluctuation under Gaussian random potentials. Instead of using the 6-points kernel, averaged over disorders, we use the numerical shooting method for solving the Schrödinger equation of this quantum system and directly calculate the correlation function from these solutions. Since our approach does not use complicated formulas, it requires much less computational effort when compared to Green function techniques. Finally, we show results of calculations for setting each of parameters of Gaussian random potentials.

Keywords Correlation function · Gaussian random potentials · Schrödinger equation · Atomic density fluctuation · Numerical shooting method

1 Introduction

Most problems encountered in quantum mechanics cannot be solved exactly. Exact solutions of Schrödinger equation exist only for a few idealized systems. To solve general problems, one has to approximation methods. A variety of such methods have

A. Hutem

Physics Division, Faculty of Science and Technology, Phetchabun Rajabhat University,
Phetchabun 67000, Thailand

S. Boonchui (✉)

Department of Physics, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand
e-mail: fscistb@ku.ac.th

S. Boonchui

Center of Excellence in Forum for Theoretical Science, Chulalongkorn University,
Bangkok 10330, Thailand

been developed, and each method has its own area of applicability. Examples are, e.g. Wentzel–Kramers–Brillouin [1], perturbation [2], the quasi-linearization 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 [22]. Grobe et al. [12] proposed a criterion to determine the numerical degree of global correlation function of a multipartite quantum system. He had applied this method to several situations, including electron-atom scattering and strong-field photoionization. Lye et al. [13] 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. In 2008 Shapiro and Henseler [14] defined the disorder-induced intensity–intensity correlation function, $C_n(\mathbf{r}, \mathbf{r}') = \overline{|\psi_n^*(\mathbf{r})\psi_n(\mathbf{r}')|^2}$ for the Bose–Einstein Condensate for Fermi gas. Cherroret and Skipetrov [15] 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 $t_{arrival} \simeq 2z^2/D_\mu$, where D_μ is the diffusion coefficient in random potentials. Now, a few works had concerned the expansion of Bose–Einstein Condensate in three-dimensional potentials and evaluate correlation function. Cherroret and Skipetrov [16] had showed the typical diffusion coefficient of the Bose–Einstein Condensate in a three-dimensional random potential. Shapiro et al. [17] considered diffusion of a cold-atomic Fermi gas in the presence of a random optical speckle potential. Pezze et al. [18] numerically studied the dynamics regimes of classical transport of cold atoms gases in a two-dimensional anisotropic disorder potential.

In this paper, we consider a particle moving in the harmonics potential, perturbed by Gaussian random potentials. To study a problem of stationary states, we focus on the numerical shooting method for evaluating wave functions and the time-independent correlation functions. The scheme of the paper is as follows. In Sect. 2 we write the basic time-independent Schrödinger equation in the form,

$$\psi^{(i+1)} = 2\psi^{(i)} - \psi^{(i-1)} - (\Delta\xi)^2(\varepsilon - \xi^2 - U_G(\xi))\psi^{(i)}; \quad i = 2, 3, 4, \dots,$$

where $U_G(\xi)$ is the summation of Gaussian random potentials. In Sect. 3 we show the logical ideas of program for evaluating energy eigenvalues, wave-functions and the correlation function of the atomic density fluctuation via the numerical shooting method (Asaithambi, Ledoux and Van Daele, Boonchui and Hutem [19–22]). Finally we summarize our results in conclusion, Sect. 4.

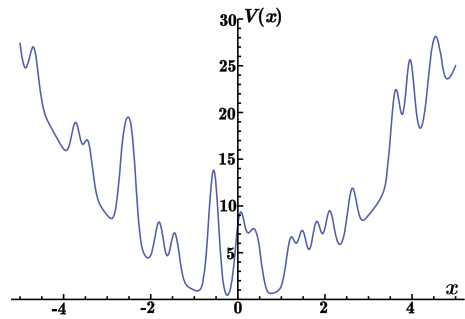
2 Finite difference formula for time-independent Schrödinger equation

We consider a particle of mass μ moving in an one-dimensional harmonic potential $\frac{1}{2}\mu\omega^2x^2$ and the summation of Gaussian random potentials $V_G(x)$,

$$V_G(x) = \sum_{i=1}^{R.D.} A e^{-(x-k_i)^2/\ell^2}, \quad (1)$$

where A is a strength of the scattering potential and 2ℓ is a standard deviation.

Fig. 1 The total potential, $\frac{1}{2}\mu\omega^2x^2 + V_G(x)$ is plotted when parameters of a Gaussian random are determined as $A = 5$, $a = 50$ ($\ell = 1/\sqrt{a}$). $R.D = 20$ is a number of Gaussian random potentials. Now the anti-symmetry harmonics potential is obtained



Gaussian potential represents a noise or disorder, which occurs at the given region of the harmonic oscillator. A random variable k_i is a fixed scattering centre of Gaussian potential. The statistics of random variables k_i is chosen to be the completely random. The time-independent Schrödinger equation of this system is given by

$$-\frac{\hbar^2}{2\mu} \frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2}\mu\omega^2x^2 + V_G(x) \right) \psi(x) = E\psi(x). \quad (2)$$

For an example, the total potential is showed in Fig. 1.

An average of physical quantity $O(x)$ on the present of the random potentials is defined

$$\overline{O(x)} = \int dx O(x) |\psi_m(x; k_1, k_2, \dots, k_N)|^2. \quad (3)$$

The density fluctuation $\delta n(x)$ and the correlation function of density fluctuation $C(s)$ are respectively defined as

$$\delta n(x) = n(x) - n^{(f)}(x) \quad \text{and} \quad C(s) = \int dx \delta n(x) \delta n(x - s), \quad (4)$$

where $s = |x - x'|$ is a distance between two points x and x' , $n(x) = |\psi_m(x)|^2$ is an atomic density of the quantum state m for the harmonics oscillator potential, perturbed by the Gaussian random potentials and $n^{(f)}(x) = |\psi_m^{(f)}(x)|^2$ is that for the free harmonics oscillator potential, respectively.

For starting the calculation, we solve the wave functions, satisfied Eq. (2) by using the numerical shooting method. It is convenient to simplify the arithmetic involved in the shooting solution. We define a 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 position variable x is replaced with the dimensionless variable ξ and the second-derivative term can be written as

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

Multiplying the Schrödinger equation Eq. (2) by $(-2/\omega\hbar)$,

$$\frac{\hbar}{\mu\omega} \frac{d^2\psi(x)}{dx^2} - \frac{\mu\omega}{\hbar} x^2\psi(x) - \frac{2V_G(x)}{\hbar\omega}\psi(x) + \frac{2E}{\hbar\omega}\psi(x) = 0, \tag{7}$$

and substituting x in terms of ξ and setting $\varepsilon = \frac{2E}{\hbar\omega}$, $U_G(\xi) = \frac{2}{\hbar\omega} V_G(x)$, we can obtain the Schrödinger equation in terms of ξ as

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\varepsilon - \xi^2 - U_G(\xi))\psi(\xi) = 0. \tag{8}$$

Also, the total potential in terms of the new variable is given in the form,

$$V(\xi) = \xi^2 + U_G(\xi). \tag{9}$$

For the finite difference method, Eq. (7) is rewritten in the form of many small segments $\Delta\xi$ in the ξ domain length. The second-derivative of the first term in Eq. (7) can be approximated in the finite difference form [20,21] as

$$\frac{d^2\psi(\xi)}{d\xi^2} \approx \frac{\psi^{(i+1)} + \psi^{(i-1)} - 2\psi^{(i)}}{(\Delta\xi)^2}. \tag{10}$$

We can obtain the Schrödinger equation in the form of finite difference by substituting Eq. (10) into Eq. (7). Thus we have

$$\psi^{(i+1)} = 2\psi^{(i)} - \psi^{(i-1)} - (\Delta\xi)^2(\varepsilon - \xi^2 - U_G(\xi))\psi^{(i)}; \quad i = 2, 3, 4, \dots, \tag{11}$$

where $\Delta\xi = \xi_{i+1} - \xi_i$.

3 Numerical shooting method and results

We assign the new variable for calculating the ground-state and the excited-state energy eigenvalues, the wave functions and the time-independent correlation functions of the atomic density fluctuation, respectively. Let us start with initial values,

1. ξ_{min} is the starting position in the analysis range.
2. ξ_{max} is the end position in the analysis range.
3. A set of random variables $\{k_i\}$ is generated in the range ξ_{min} to ξ_{max} .
4. ξ is any position in the analysis range.
5. nn is a number of very small bars in the analysis range.
6. $\Delta\xi$ is the length of very small bars,

$$\Delta\xi = \frac{\xi_{max} - \xi_{min}}{nn}. \tag{12}$$

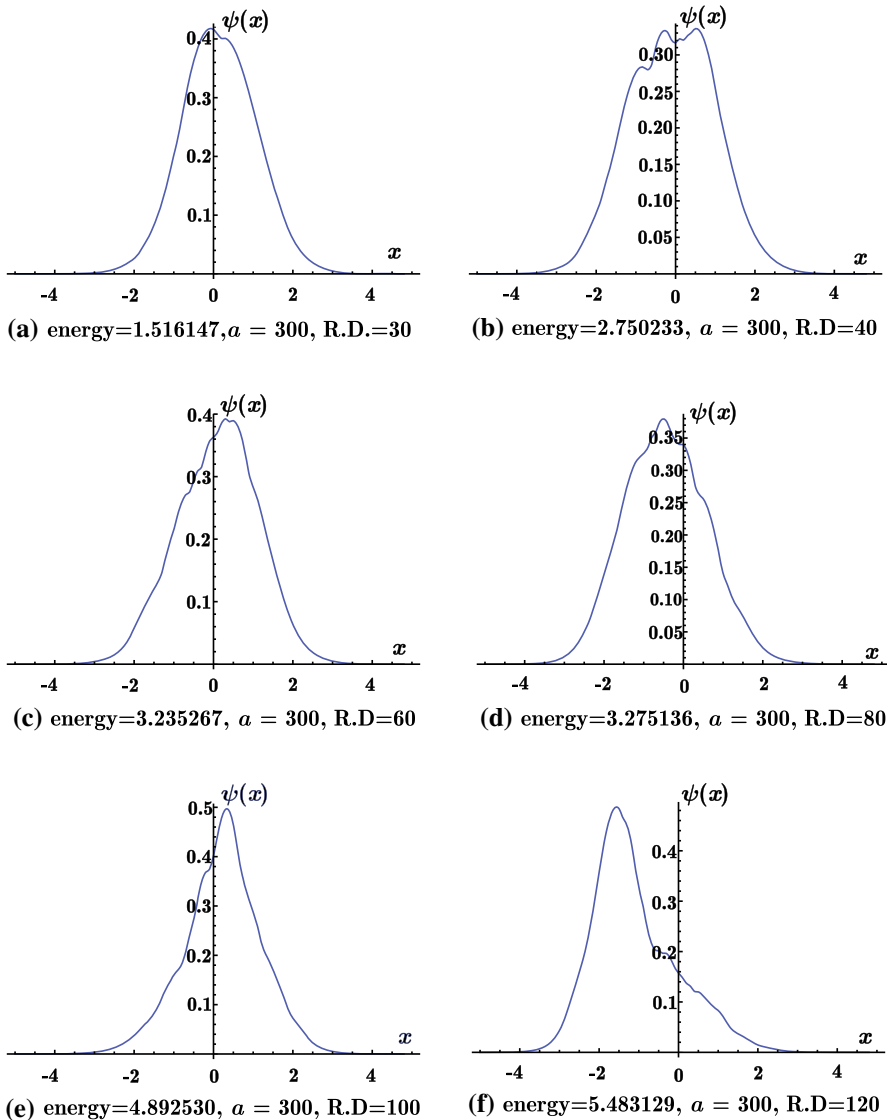


Fig. 2 Plot of wave functions at ground state by varying the random numbers (R.D.) for parameters of the Gaussian random potentials $A = 5$ and $a = 300$ ($\ell = 1/\sqrt{a}$)

For the beginning of the numerical shooting method, we need to input parameters ξ_{min} (ξ_{max}), and Eq. (11) into mathematica program. Next, two initial wave functions are determinate by following two initial conditions as (i) $\psi^{(1)} = 0$ is the fixed position and (ii) $\frac{d\psi}{d\xi} = 1$ is the slope of position ξ_1 and ξ_2 .

So we have

$$\frac{d\psi}{d\xi} \approx \frac{\psi^{(2)} - \psi^{(1)}}{\Delta\xi} \Rightarrow \psi^{(2)} \approx \Delta\xi. \quad (13)$$

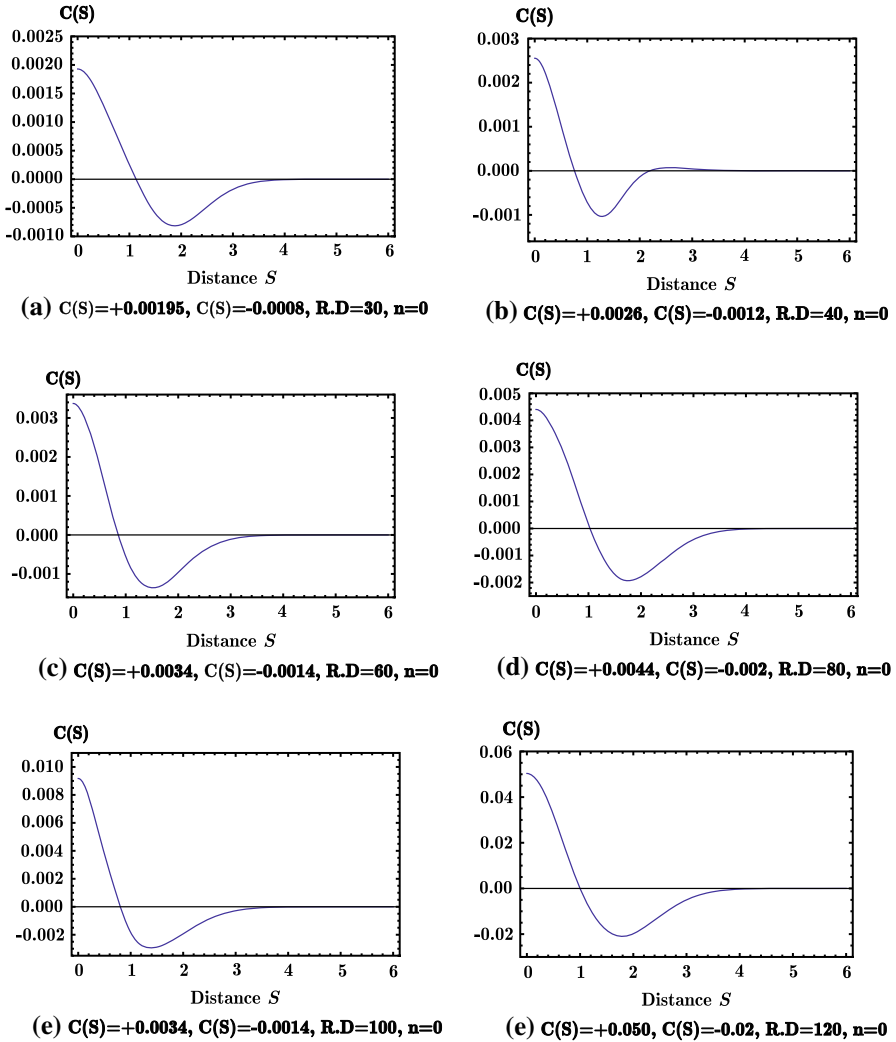


Fig. 3 Schematic diagram for behavior of the time-independent the correlation function of density fluctuations for the ground state energy with vary number of random, 30, 40, 60, 80, 100 and 120

By inputting $\psi^{(1)}$ and $\psi^{(2)}$ as two initial values for calculation, we can find $\psi^{(3)}$ from Eq. (11), which contains the effects of Gaussian random potentials. In the same way, we can find $\psi^{(4)}$ by substituting $\psi^{(2)}$ and $\psi^{(3)}$ in the equation. Keeping this way, we obtain any $\psi^{(n)}$ (see fig. 2 in the references [22]).

- When $|\psi^{(i+1)}|$ approaches to a desired value, accuracy of calculation, the next task of wave function in Eq. (13) is calculated. For example, we would like to stop the calculation and to accept the final energy when $|\psi^{(i+1)}| \leq 10^{-6}$.
- Plot the wave-function by the graph related to i .

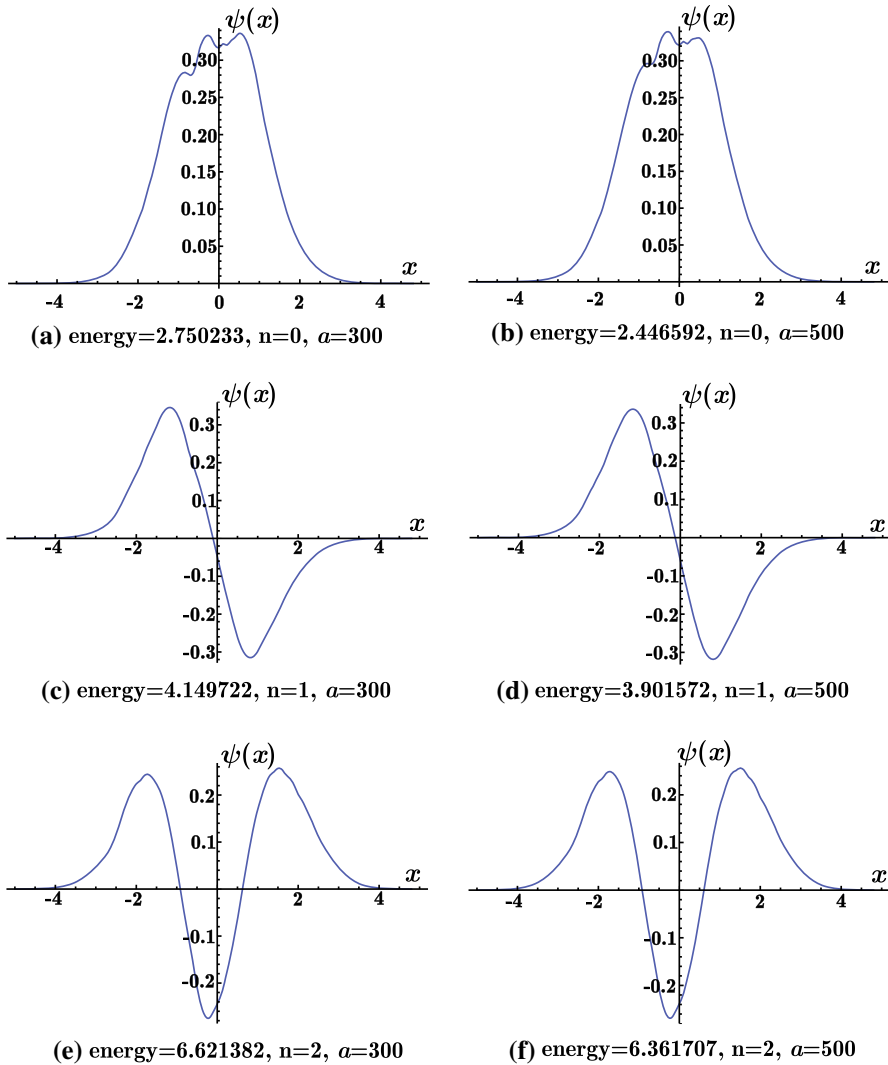


Fig. 4 We show the effect of width size ($\ell = 1/\sqrt{a}$) on the wave-function for setting parameters of Gaussian random potential to be $a = 300$ and $a = 500$. Figure (a) – (b) are plot of the ground-state wave-function. Figure (c) – (d) are plot of the first excite-state wave-function. Figure (e) – (f) are plot of the second excite-state wave-function

- Plot the wave-functions, and the correlation function $C(s)$ by the graph related to i .
- Plot the average of the correlation function $C(s)$ over the random variables k_i by the graph related to i .

In the present of random potentials, we assume that statistics of the random variables k_i is chosen to be the completely random. Following ref. [15], an average correlation function of the atomic density fluctuation $\widehat{C}(s)$ over random variables k_i , is defined as

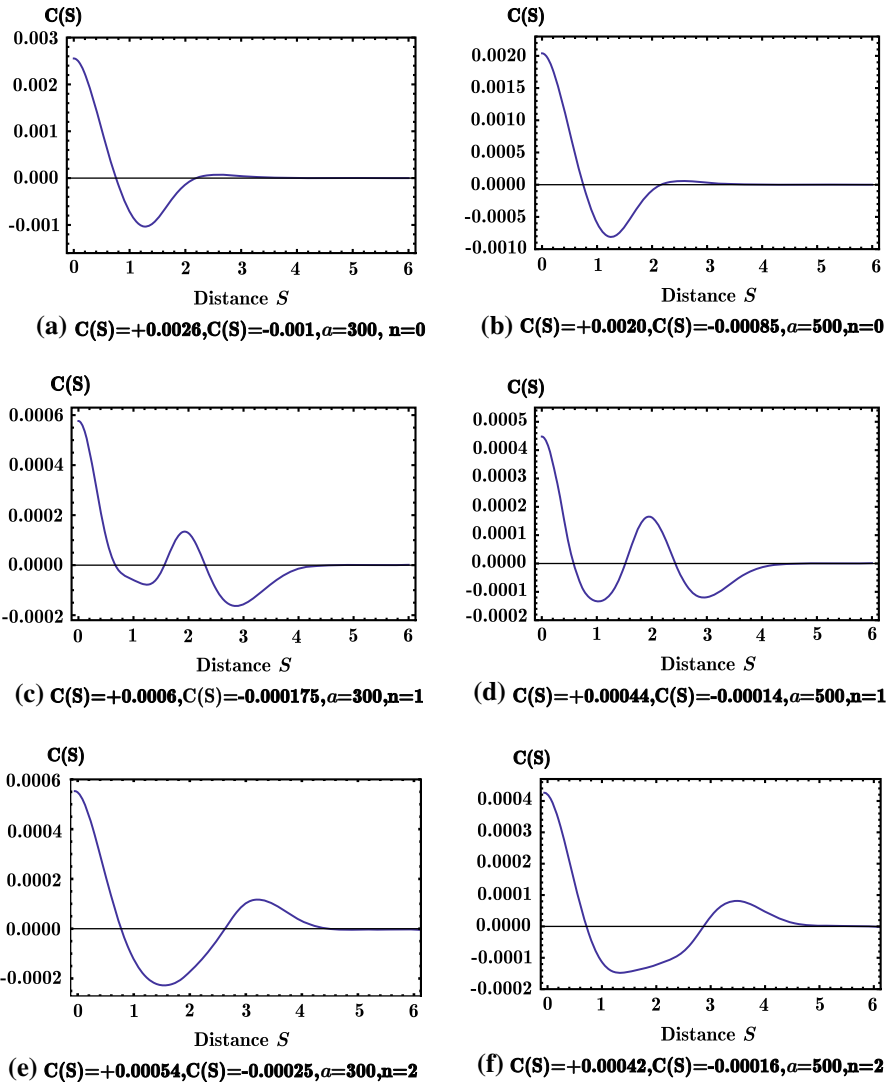
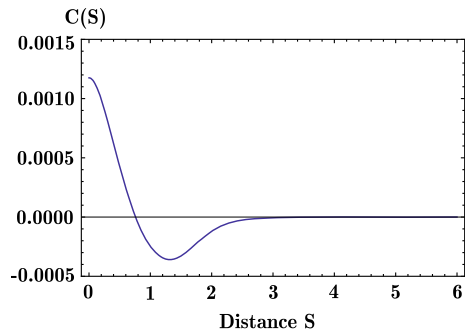


Fig. 5 We show the effect of width size $\ell = 1/\sqrt{a}$ on the time-independent correlation function for setting parameters of Gaussian random potential to be $a = 300$ and $a = 500$. Figure (a) – (b) are plot of the time-independent correlation function for the ground-state wave-function. Figure (c) – (d) and (e) – (f) are plot the time-independent correlation function for the first and the second excite-state wave-function, respectively

$$\widetilde{C}(s) = \frac{1}{NR} \sum_{j=1}^{NR} \int dx \delta n^{(j)}(x) \delta n^{(j)}(x - s) \tag{14}$$

when j and NR are an index and a number of the set of random variables $\{k_i\}$, respectively.

Fig. 6 Plot the average correlation function of the atomic density fluctuation $\widetilde{C}(s)$ for the ground-state wave-function with NR = 20, R.D = 40



For examples, we show the solutions of Schrödinger equation for the one-dimensional harmonic system induced random potentials by using the numerical shooting method. The ground state wave function $n = 0$ and the correlation function for each parameters are showed as Figs. 2 and 3, respectively. The correlation functions for these cases oscillate with the amplitude gradually decreasing to zero. It is called one-half of critical damping case. Negative correlations are obtained in our calculations. These results were predicted to exist in waves reflection from a thick disordered slab [23]. Form Fig. 3, we show that magnitude of correlation functions increase from 0.002 to 0.6 with increasing the number of individual scattering potentials (R.D). In Figs. 4 and 5, we consider an effect of width size of a Gaussian random potential, ℓ on the wave functions and the correlation functions for (i) ground state $n = 0$, (ii) first excitation $n = 1$ and (iii) second excitation $n = 2$, respectively. Results of calculation show that the magnitude of correlation functions depend on the width size of Gaussian random potential.

Finally, we show the average correlation function $\widetilde{C}(s)$ for the ground-state wave-function in Fig. 6. This average has characteristic curve as one-half of critical damping case. Positive and negative correlations occur at short distances (small s) and long distances (large s) between points x and x' , respectively. The positive correlation coefficients mean that the value of the density fluctuation at point x increases, the value of the other at point x' increases; as one decreases the other decreases. Negative correlation coefficients indicate that the density fluctuation increases, the other decreases, and vice-versa. These results are effects of the anti-symmetry harmonics potential, induced by the Gaussian random potentials.

4 Conclusion

We illustrate the numerical method for solving the one-dimensional harmonic oscillator, perturbed from a set of the Gaussian random potentials. Our calculations, we can get the time-independent correlation function corresponding with the Green functions techniques [15]. However 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 numer-

ical shooting method gives very accurate results because it integrates Schrödinger equation directly, though in the numerical sense.

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References

1. G.A. Dobrovolsky, R.S. Tutik, *J. Phys. A Math. Gen.* **33**, 6593 (2000)
2. M.I. Jaghob, *Eur. Phys. J. A* **27**, 99 (2006)
3. E.Z. Liverts, V.B. Mandelzweig, *Ann. Phys.* **322**, 2211 (2007)
4. N. Saad et al., *J. Phys. A Math. Gen.* **39**, 7745 (2006)
5. M.C. Zhang, *Chin. Phys. B* **17**, 3214 (2008)
6. M.C. Zhang, Z.B. Wang, *Chin. Phys.* **16**, 1863 (2007)
7. C.R. Handy et al., *J. Phys. A Math. Gen.* **26**, 2635 (1993)
8. Z. Cao, *Phys. Rev. A* **63**, 054103–054106 (2001)
9. A. Hutem, C. Sricheewin, *Eur. J. Phys.* **29**, 577 (2008)
10. H. Ying et al., *Chin. Phys. B* **19**, 040306 (2010)
11. S. Boonchui, A. Hutem, *J. Math. Chem.* **50**, 2103 (2012)
12. R. Grobe et al., *J. Phys. B At. Mol. Opt. Phys.* **27**, 503 (1994)
13. J.E. Lye et al., *Phys. Rev. Lett.* **95**, 070401 (2005)
14. P. Henseler, B. Shapiro, *Phys. Rev. A* **77**, 033624 (2008)
15. N. Cherroret, S.E. Skipetrov, *Phys. Rev. Lett.* **101**, 190406 (2008)
16. N. Cherroret, S.E. Skipetrov, *Phys. Rev. A* **79**, 063604 (2009)
17. B. Shapiro et al., *Phys. Rev. A* **81**, 033612 (2010)
18. L. Pezze et al., *New J. Phys.* **13**, 095015 (2011)
19. A. Asaithambi, *Appl. Math. Comp.* **215**, 4400 (2010)
20. J. Killingbeck, *J. Phys. A Math. Gen.* **20**, 1411 (1987)
21. V. Ledoux, M. Van Daele, *Comp. Phys. Comm.* **184**, 1287 (2013)
22. S. Boonchui, A. Hutem, *J. Math. Chem.* **50**, 1582 (2012)
23. D.B. Rogozkin, M.Y. Cherkasov, *Phys. Rev. B* **51**, 12256 (1995)