Evaluate Correlation Function, Wave Function
and Energy of the Harmonics Oscillator
Hyperbolic Secant-Cosine Rational Asymmetric
Potential via Numerical Shooting Method

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Abstract

In this paper, we develop a simple numerical method for evaluating the correlation function of the atomic density fluctuation under the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential. Instead of using the 6-point kernel, averaged over disorder, we use the numerical shooting method (NSM) for solving the Schrödinger equation of quantum mechanics system with hyperbolic Secant-Cosine rational asymmetric potential. Since our approach does not use complicated formulas, it requires much less computational effort when compared to the Green functions techniques[9].

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Keywords: correlation function, wave-function, 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, e.g. the variational method\[1\], function analysis\[2\], the eigenvalue moment method\[3\], the analytical transfer matrix method\[4\][5][6] and numerical shooting method\[7\][12]. 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 evaluate wave-function and time-independent correlation function of a particle around of attraction by the harmonics oscillator with hyperbolic Secant-Cosine rational asymmetric potential.

Boris Shapiro and Peter Henseler 2008 \[8\] use define the disorder-induced intensity-intensity correlation function, \(C_\omega(\mathbf{r}, \mathbf{r}') = \left| \psi_\omega^*(\mathbf{r})\psi_\omega(\mathbf{r}') \right|^2\) was calculate the normalized density-density correlation function of the Bose-Einstein Condensate for Fermi gas. N.Cherroret and S.E.Skipetrov 2008 \[9\] show that the average atomic density \(n(\mathbf{r}, t) = \left| \psi(\mathbf{r}, t) \right|^2\) as a function of time. The density reaches a maximum at the arrival time \(t_{arrival} \simeq 2z^2/D_\mu\), where \(D_\mu\) is the diffusion coefficient in a random potential.

The scheme of the article is as follows. In Sec. 2 we write the basic time-independent Schrödinger equation in term of finite difference and the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential in terms of the new variable is given by

\[
\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2 (\varepsilon - \xi^2 - \beta |\xi| \sin(10\xi) - \frac{\lambda(\text{sech}(\mu \xi^2))^2 (\cos(30\xi^2))^2}{1 + g\xi^2}) \psi_i
\]

where \(V_h(\xi) = \beta |\xi| \sin(10\xi) + \frac{\lambda(\text{sech}(\mu \xi^2))^2 (\cos(30\xi^2))^2}{1 + g\xi^2}\) is the hyperbolic Secant-Cosine rational asymmetric potential. In Sec. 3 we show that the idea write of program of evaluate energy eigenvalue wave-function and correlation function of atomic density for the hyperbolic Secant-Cosine rational asymmetric potential via the numerical shooting method\[11\][12]. In Sec. 4 contains our conclusions.

2 Schrödinger Equation in Finite Difference

The time-independent Schrödinger equation describing the dynamics of a microscopic particle of mass \(m\) in a one-dimensional the time-independent potential \(V(x)\) is given by

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x),
\]

\[(1)\]

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

Suppose a particle is bound state to around of attraction by the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential (see Fig.1)

$$V(x) = \frac{1}{2}m\omega x^2 + b|x|\sin(10x) + \frac{a(\text{sech}(\mu x^2))^2(\cos(30x^2))^2}{(1 + g x^2)}, \quad (2)$$

where $a, b, \mu, g$ are real and positive constants. When equation (2) is substituted into equation (1) the time-independent Schrödinger equation is obtained

$$-\frac{2m}{\hbar^2}E\psi(x) = \frac{d^2\psi(x)}{dx^2} - \frac{m^2\omega^2x^2}{\hbar^2}\psi(x) - \frac{2mb}{\hbar^2}x|x|\sin(10x)\psi(x)$$

$$-\left(\frac{2ma(\text{sech}(\mu x^2))^2(\cos(30x^2))^2}{\hbar^2(1 + g x^2)}\right)\psi(x). \quad (3)$$

Equation (3) can be solved through a change of variable. When the following substitution are made(setting $\hbar = m = \omega = 1$),

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x, \quad x^2 = \frac{\hbar}{m\omega}\xi^2 \quad (4)$$

Equation (3) can be transformed into

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\varepsilon - \xi^2 - 2b\xi|\sin(10\xi) - \frac{2a(\text{sech}(\mu \xi^2))^2(\cos(30\xi^2))^2}{1 + g \xi^2}\right)\psi(\xi) = 0. \quad (5)$$
We can rewrite the equation (5) by setting $\beta = 2b$, $\lambda = 2a$, $\varepsilon = \frac{E}{\hbar \omega}$ to give

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

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

$$V(\xi) = \xi^2 + \beta|\xi| \sin(10\xi) + \frac{\lambda(\text{sech}(\mu \xi^2))^2}{1 + g \xi^2}. \quad (7)$$

We can find the numerical solution equation (6) by dividing $\xi$ into many small segments, each of $\Delta \xi$ in length. An analogous approximation for the second derivative is actually a bit tricky. There are several methods to calculate it, but a very efficient procedure is called the numerical shooting method. In short, the second-derivative for the first term of equation (6) is approximated given by

$$\frac{d^2 \psi(\xi)}{d\xi^2} \approx \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{(\Delta \xi)^2} \quad (8)$$

Equation (6) can be transformed into

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2(\varepsilon - \xi^2 - \beta|\xi| \sin(10\xi) - \frac{\lambda(\text{sech}(\mu \xi^2))^2}{1 + g \xi^2}) \psi_i. \quad (9)$$

where $\xi_{i+1} = \Delta \xi + \xi_i$. The special potential given by harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential has been used in evaluate equation (9) into the mathematica program (see Sect.3).

**3 Numerical Shooting Method and Results**

We construe the new variable for using in calculating the ground-state energy eigenvalue, wave-function and the time-independent correlation function of the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential.

1. $\xi_{\text{min}}$ is the start position in the analysis range.
2. $\xi_{\text{max}}$ is the ultimate 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. $\Delta \xi$ is the length of very small bars so that
Evaluate correlation function

Figure 2: Figure (a)-(f) plot of the time-independent wave-function in case of ground-state energy in harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential with vary $\mu = 5 = \frac{1}{width}$, $\mu = 10$, $\mu = 15$ and setting $\lambda = 15$ is amplitude of barrier and $\beta = 5$ and $\beta = 7$.

\[
\Delta \xi = \frac{\xi_{max} - \xi_{min}}{nn}. \quad (10)
\]

Logic of the numerical shooting method evaluation of energy eigenvalue, eigenfunction and time-independent correlation function for the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential.

- Input values $\xi_{min}$ and $\xi_{max}$ in mathematica program for the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential.

- Input the period amount.

- Input eq.(9) into mathematica program.

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

\[
\frac{d\psi}{d\xi} \approx \frac{\psi_2 - \psi_1}{\Delta \xi} \Rightarrow \psi_2 \approx \Delta \xi. \quad (11)
\]
Figure 3: Figure (a)-(f) schematic diagram for behavior of the time-independent correlation function in case of ground-state energy in harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential with vary \( \lambda = 5, \lambda = 10, \lambda = 15 \) is amplitude of barrier and setting \( \beta = 3, \beta = 5 \).

By input \( \psi_1 \) and \( \psi_2 \) as two initial values for calculation, we can find \( \psi_3 \) from eq.(9). 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 \( \psi_n \) (see fig.2 in the references[12])

- The next task is to calculate wave-function in eq.(9)\( (\psi_{i+1}) \) 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.(9) 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 wave-function by the graph related to \( i \).

- Plot the wave-function is normalized by the graph related to \( i \).

- Plot the probability the average atomic density \( \tilde{n}(x) = |\psi(x)|^2 \) for the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential.

- Input values \( \xi_{min} \) and \( \xi_{max} \) in the mathematica program for the harmonics oscillator 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 $\delta n(x) = \tilde{n}(x) - \tilde{m}(x)$ for the harmonics oscillator potential.

- Plot the time-independent correlation function $C(x, \dot{x}) = \frac{\delta n(x) \delta n(\dot{x})}{n(x)n(\dot{x})}$.

Figure 4: Figure (a)-(f) plot of the time-independent correlation function in case of ground-state energy in harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential with vary $\mu = 5$, $\mu = 10$, $\mu = 15$ and setting $\lambda = 15$ is amplitude of barrier and $\beta = 5$, $\beta = 7$.

For example, numerical evaluation of energy eigenvalue, eigenfunction and the time-independent correlation function via the numerical shooting method for
the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential.

\[\text{Input}[2]: \xi_{\text{min}} = -5; \xi_{\text{max}} = 5; nn = 100; \Delta \xi = N \left[\frac{\xi_{\text{max}} - \xi_{\text{min}}}{nn}\right]; \psi_1 = 0; N[\psi_2 = \Delta \xi]; \xi_1 = -5; \xi_2 = \xi_1 + \Delta \xi; \lambda = 10; g = 0.1; \beta = 3; \mu = 5; \]

\[\text{Input}[3]: \varepsilon = 2.4419428445; (\text{energy eigenvalue of harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential})\]

\[\text{Input}[4]: N[\text{Table}[\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2 \left(\varepsilon - (\xi_{i+1} = \xi_i + \Delta \xi)^2 - (\beta \text{Abs}[\xi_{i+1} = \xi_i + \Delta \xi]) \sin[10(\xi_{i+1} = \xi_i + \Delta \xi)] - \left(\lambda \text{Sech}[\mu(\xi_{i+1} = \xi_i + \Delta \xi)]^2 \cos[30(\xi_{i+1} = \xi_i + \Delta \xi)^2 \right) \psi_i], \{i, 2, 99\}]; \]

\[\text{Input}[5]: \text{SetPrecision} \left[\frac{1}{2} (4.1695... + 4.1695...), 20\right]; \]

\[\text{Input}[6]: \text{aa1} = \{0, 0.1, 0.22047, ..., 0.000349\}; \]

\[\text{Input}[7]: \text{bb1} = \{0 + 0.1 + 0.22047 + 0.391136 + 0.63894 + ... + 0.000349\} \times (\Delta \xi); \]

\[\text{Input}[8]: \text{ListPlot}[\text{aa1}]; \]

\[\text{Input}[9]: N[\text{Table}[\{\xi = \xi_{\text{min}} + i \Delta \xi, \psi_{i+1}\}, \{i, 0, 100\}]]; \]

\[\text{Input}[10]: \text{ListPlot}[]; \]

\[\text{Input}[11]: \text{kkk1} = \text{Interpolation}[]; \]

\[\text{Input}[12]: \text{Plot}[\text{kkk1}[\xi], \{\xi, -5, 5\}]; (\text{the wave-function is normalized}) \]

\[\text{Input}[13]: \text{Plot}[\left(\text{Abs}[\text{kkk1}][\xi]\right)^2, \{\xi, -5, 5\}, \text{PlotRange} \rightarrow \{0, 0.14\}]; (\text{Probability atomic density for harmonics oscillator Gaussian-Cosine rational symmetric potential}) \]

\[\text{Input}[14]: \text{Clear}[\varepsilon]; \]

\[\text{Input}[15]: \xi_{\text{min}} = -5; \xi_{\text{max}} = 5; nn = 100; \Delta \xi = N \left[\frac{\xi_{\text{max}} - \xi_{\text{min}}}{nn}\right]; \psi_1 = 0; N[\psi_2 = \Delta \xi]; \xi_1 = -5; \xi_2 = \xi_1 + \Delta \xi; (\text{calculation of energy and wave-function for harmonic oscillator potential}) \]

\[\text{Input}[16]: \varepsilon = 0.99937...; (\text{energy eigenvalue of harmonics oscillator potential}) \]

\[\text{Input}[17]: N[\text{Table}[\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta \xi)^2 \left(\varepsilon - (\xi_{i+1} = \xi_i + \Delta \xi)^2 \right) \psi_i], \{i, 2, 99\}]; (\text{harmonics oscillator potential.}) \]

\[\text{Input}[18]: \text{SetPrecision} \left[\frac{1}{2} (0.99937... + 0.9993746...), 20\right]; \]

\[\text{Input}[19]: \text{aa2} = \{0, 0.1, 0.2204, 0.39091, ..., 0.0003316\}; \]

\[\text{Input}[20]: \text{bb2} = \{0 + 0.1 + 0.220406 + 0.39091 + ... + 0.0003316\} \times (\Delta \xi); \]

\[\text{Input}[21]: \text{ListPlot}[\text{aa2}]; \]

\[\text{Input}[22]: N[\text{Table}[\{\xi = \xi_{\text{min}} + i \Delta \xi, \psi_{i+1}\}, \{i, 0, 100\}]]; \]

\[\text{Input}[23]: \text{ListPlot}[]; \]

\[\text{Input}[24]: \text{kkk2} = \text{Interpolation}[]; \]

\[\text{Input}[25]: \text{Plot}[\text{kkk2}[\xi], \{\xi, -5, 5\}]; (\text{the wave-function is normalized}) \]

\[\text{Input}[26]: \text{Plot}[\left(\text{Abs}[\text{kkk2}][\xi]\right)^2, \{\xi, -5, 5\}, \text{PlotRange} \rightarrow \{0, 0.17\}]; (\text{Probability atomic density for harmonic oscillator potential}) \]

\[\text{Input}[27]: \text{Plot} \left(\left(\text{Abs}[\text{kkk2}][\xi]\right)^2 - \left(\text{Abs}[\text{kkk2}][\xi]\right)^2 \right), \{\xi, -5, 5\}, \text{PlotRange} \rightarrow \{-0.095, 0.055\}\];
Evaluate correlation function

Input[28] : \( GF[\xi] := \left( \text{Abs}\left[ \frac{kkk[\xi]}{bb1} \right] \right)^2 - \left( \text{Abs}\left[ \frac{kkk[\xi]}{bb2} \right] \right)^2 \); (the atomic density fluctuation for \( \xi \) position)

Input[29] : \( GF1[\xi] := \left( \text{Abs}\left[ \frac{kkk[\xi]}{bb1} \right] \right)^2 - \left( \text{Abs}\left[ \frac{kkk[\xi]}{bb2} \right] \right)^2 \); (the atomic density fluctuation for \( \xi \) position)

Input[30] : \( CC[\xi] := \left( GF[\xi] \times GF1[\xi] \right) \); (the correlation function)

Input[31] : \( CORR[ss] := \text{NIntegrate}[CC[\xi], \{\xi, -4.5, 4.5\}] \);

Input[32] : \( \text{Plot}[CORR[ss], \{ss, 0, 8\}, \text{PlotRange} \rightarrow \{-0.004, 0.008\}, \text{PlotStyle} \rightarrow \text{RGBColor}[0, 0, 1], \text{Axes} \rightarrow \text{True}, \text{Frame} \rightarrow \text{True}, \text{Ticks} \rightarrow \text{True}] \)

4 Conclusion

In this case, the wave-function of the harmonics oscillator hyperbolic Secant-Cosine rational asymmetric potential similar not to in case of a typical harmonics oscillator (see fig(2)). Figure(2)(a-c) if the values of \( \mu \) has increase, the ground-state energy eigenvalue has lessen and the wave-function has split up asymmetric lessen nodes.

From figure(2)(d-f) if the values of \( g \) has increase, the the ground-state energy eigenvalue has lessen. Figure(3)(a-f) if the values of \( \lambda \) has increase, the time-independent correlation function has incline. Comparison between figure(3)(b) and figure(3)(e) if the values \( \beta \) has increase, the time-independent correlation function has supplement. Figure(4)(a-c) if the values of \( \mu \) has increase, the time-independent correlation function has lessen. From figure(4)(d-f) if the values of \( \mu \) has increase, the time-independent correlation function has little.

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