Temporal Auto-Correlation Function Pushed to One Pixel Limit

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Abstract Quantum transport in a neutral atom guide provides intriguing quantum effects that are important aspects in designing atom mechatronic structures such as quantum interferometer, pump, valve, and amplifier structures. We investigate applicability of spatial reduction in temporal auto-correlation function to reduce computational resources in finding eigen-energy inside the guide. We find that we can reduce the size of the correlation function to an area 65,536 times smaller than the entire simulation space (0.0015%), which corresponds to an area of one pixel. The maximum error of all energies is 8.18% for a ground state and the trend of errors reduces exponentially as the principle quantum number increases. The setting of the investigation involves initial Gaussian wave packet evolving in a 2D harmonic potential and the correlation space is concentric to the center of the initial wave packet.

1. Introduction

Transport phenomenon concerns flow of physical quantities, e.g. particle number, energy and momentum, in and out of an observed system [1]. Interaction of the flow with the system gives rise to characteristic transport coefficients that specifies a range of applications a system can have. For example, diffusion from Brownian motion of a particle only restricts to the displacement of a particle being proportional to the square root of the elapsed time [2]. At fundamental level, quantum mechanics plays an important role in exchanges of number, energy and momentum, and therefore a quantum transport can have intriguing properties not realizable by its classical counterparts. Quantum engine, for instant, can exploit a “shortcut-to-adiabaticity” to increase both engine efficiency and output power simultaneously [3]. Based on a neutral-atom based platform, strange quantum transport behaviors can be observed [4-10]. A single atom can be used to demonstrate quantum heat engine [10] while a flow of a toroidal Bose-Einstein condensate (BEC) can be controlled via a tunable weak link [7]. Atomtronics based on neutral atoms transport in an atom circuit can be used to build “atom mechatronic” devices. The devices can have unique mechanical properties based purely on atom-light interaction, e.g., flow of atoms in atomtronic dumbbell capacitor [11] can be used to drive quantum motor to rotate clockwise and counter-clockwise at the same time. The mechanism can depend precisely on a selected quantum state or atomic species that pass by or through the motor.

One essence in designing atomtronic or atom mechatronic structures is the knowledge of spectral distribution and its variation depending on parameters that described the atom-circuit structures [4]. For
numerical calculation, temporal auto-correlation (TAC) allows convenient extraction of spectral distribution (ESD) of the system. However, the calculation of TAC normally requires multiplication between two matrices, which cover the whole simulation space and thus either takes large computational resources or not convenient for using TAC to probe quasi-bound states in narrow structures in the system. In this preliminary work, the calculation assumes non-interacting atoms residing in a two dimensional static harmonic potential. The calculation errors depending on the size of matrices used for computing TAC is investigated.

2. Background

2.1. Temporal Auto-Correlation (TAC) and Extracted Spectral Distribution (ESD)

The TAC of a particle localized in an area of interest can be calculated by keeping a temporal record of the time evolution of a single-particle wave function $\psi(x, y, t)$. For the Hamiltonian $\hat{H}$ and an initial wave function $\psi(x, y, t = 0)$ the evolution gives

$$\psi(x, y, t) = \exp\left(-i \int_0^t \hat{H} \, dt' / \hbar\right) \psi(x, y, 0).$$  \hspace{1cm} (1)

The temporal auto-correlation function is defined as

$$\xi(t) = \langle \psi(x, y, 0) | \psi(x, y, t) \rangle. $$  \hspace{1cm} (2)

Assuming that the eigen-functions are non-degenerate and writing $\psi(x, y, 0)$ in terms of a linear combination of eigen-functions, $\psi(x, y, 0) = \sum_{j=1}^{\infty} c_j \psi_j(x, y)$, Eq.1 gives

$$\psi(x, y, t) = \sum_{j=1}^{\infty} c_j \psi_j(x, y) \exp\left(-\frac{iE_j t}{\hbar}\right),$$  \hspace{1cm} (3)

and Eq.2 becomes

$$\xi(t) = \sum_{j=1}^{\infty} |c_j|^2 \exp\left(-\frac{iE_j t}{\hbar}\right).$$  \hspace{1cm} (4)

The correlation function $\xi(t)$ oscillate with multiple frequencies according to the corresponding eigen-energies, $E_j$. To get the ESD, $\xi(t)$ is Fourier transformed to complementary energy space, i.e.

$$q(E) = \mathcal{F}[w(t) \xi(t)] = \sum_{j} |c_j|^2 \delta(E - E_j),$$  \hspace{1cm} (5)

which gives the energy spectrum of the system with a correct relative proportionality constant $|c_j|^2$ for each eigen-function, the Fourier transformation is denoted as $\mathcal{F}[\xi(t)]$, $w(t)$ is the normalized Hanning window function introduced to force the resulting spectrum to have a specific lineshape $\delta(E - E_j)$, which is the Fourier transform of $w(t) \exp\left(-iE_j t / \hbar\right)$. The lineshape function comprises of several peaks located at $E_j$.

2.2. Split-Operator Approximation

In general, evaluating Eq.1 is difficult because the kinetic and potential operator do not commute. The wave function normally does not have a closed form for an arbitrary potential $V(x, y)$. A second-order approximation of Eq.1 evaluated from $t$ to $t + \Delta t$ can be made by splitting the Hamiltonian into the following form  \[12\]
\[
\psi(x, y, t + \Delta t) = G(\hat{R}) \psi(x, y, t) = G(\hat{K} + \hat{V}) \psi(x, y, t)
\]

\[
= G \left( \frac{\hat{V}}{2} \right) G(\hat{K}) G \left( \frac{\hat{V}}{2} \right) \psi(x, y, t)
\]

where \( G(\hat{\delta}) = \exp \left( -i \frac{\Delta t}{\hbar} \hat{\delta} \right) \). In this regard, Eq.6 allows Eq.1 to be evaluated explicitly by operating kinetic and potential propagator on \( \psi(x, y, t) \) in succession.

3. Method
The TAC function in Eq.2 is an overlapped function of \( \psi(x, y, 0) \) and \( \psi(x, y, t) \), which can be represented as \( N \times N \) square matrices when \( x \) and \( y \) are discretized into vectors of length \( N \). The TAC in the discrete form is essentially the total summation of element-by-element multiplication of the two matrices. In this work, \( N = 256 \) and the configuration space covers the range from \(-5 \, \mu m \) to \(5 \, \mu m \) in both \( x \) and \( y \) axes. The initial wave packet is a Gaussian function and it evolves from \( t = 0 \) to \( t = 0.5 \, s \) with \( \Delta t = 10^{-6} \, s \). The calculation errors in eigen-energies are investigated upon the variation of the size of the overlapped matrices. In the simulation, the size restriction is simplified to a multiplication between discrete TAC matrices and a square \( N \times N \) aperture matrix, \( A \), where

\[
A = \begin{cases} 
1, & r \leq R \\
0, & \text{elsewhere.}
\end{cases}
\]

The aperture’s radius is \( R = 2.5 \, \mu m \) and \( r = \sqrt{x^2 + y^2} \) is the radial coordinate. The calculation of TAC is repeated until \( \xi(t) \) is obtained for each discrete time step. After the Fourier transform, \( q(E) \), is matched against the theoretical values and the spectral errors (or errors in calculated eigen-energies) are computed for all eigen-states. Figure 1.c shows a stem plot of the spectral errors along with an inset that compares the size of an aperture with \( R = 2.5 \, \mu m \) (black circle) to the entire simulation space.

![Figure 1](image1.png)

**Figure 1.** (a) and (b) show the ESD from the aperture radius \( R = 2.5 \, \mu m \) and \( R = 0.028 \, \mu m \) respectively against even energy level (principle quantum number). Figure (c) shows the stem plot of the spectral error. The inset in (c) compares the boundary of an aperture with \( R = 2.5 \, \mu m \) to the entire simulation space. The width of the simulation space is \( 10 \, \mu m \), which corresponds to 256 pixels.

4. Results and Discussion
The spectral distributions \( q(E) \) and its spectral error for each of the even eigen-state are shown in Figure 1 for the aperture radii \( 2.5 \) and \( 0.028 \, \mu m \) respectively. For \( R \geq 2.5 \, \mu m \) the shape of the ESD and the linewidth of its lineshape function are essentially the same as when \( R = 5 \, \mu m \), which is almost the entire
simulation space. The shape of the ESDs implies that the decomposition of the initial wave packet into eigen-states are the same in both cases, even though the proportionality constant or the peak’s height from \( R = 2.5 \mu m \) is roughly three times less than that of \( R = 5 \mu m \). The shape of the ESD changes when \( R \) is reduced further to 1 \( \mu m \). This means that at this radius, the calculation of the decomposition is not accurate. The contribution from the high energy eigen-states is neglected. The reason is because the spatial profiles of the high energy states have peaks at larger radius compared to the one with low energy. Thus reducing the size of the aperture obviously partially excludes significant amount of the high energy states from the TAC. Despite the distorted shape, the ESD gives the same spectral error distribution across all eigen-states when \( n < 78 \). An interesting result occurs when the aperture radius is pushed further to 0.028 \( \mu m \), which corresponds to 1 pixels (floor value) in the actual simulation. At this radius, \( n > 70 \) begins to wash out. The surprising result is that spectral errors for all aperture radii remain the same for quantum number \( n < 70 \). This implies that only one pixel aperture is required to acquire accurate eigen-energies out of a \( 256 \times 256 \) matrix or 65,536 pixels. Even more surprising result occurs when the one pixel aperture is move away from the center of the wave packet. At a particular radius, even though contribution from a certain eigen-state is greatly suppressed due to that one pixel being placed at the zero crossing point with zero probability amplitude, as long as there are eigen-states that can find their ways through that one active pixel, the ESD prevails with accuracy. The trend from all spectral errors indicates that the error reduces exponentially as quantum number \( n \) increases. Note that the low lying states have large errors due to the Heisenberg uncertainty principle. The low energy states fluctuate slowly. Therefore, the TAC captures smaller number of oscillations as compared to that captures from a high energy one.

5. Conclusion

Only one pixel is required to obtain accurate TAC function from the evolution of a Gaussian wave packet, represented by a square matrix of size \( 256 \times 256 \), inside a harmonic oscillator potential. Emphasis is placed on robustness of eigen-energy oscillations regardless of the strength of the non-zero probability amplitude that reaches the TAC region of interest.

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