Solving time-dependent Schrödinger equation using absorbing boundary condition method

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Introduction

In nuclear system dynamics, asymptotic conditions are often applied to simplify the problem into an equivalent stationary one, typically solved using the time-independent Schrödinger equation (TDSE). However, we aim to improve the solution by addressing the TDSE, which has been studied to understand how quantum systems change and behave over time. One of the unitary forms of the quantum mechanical time evolution operator is given by Cayley's approximation [1]. This method, known as Cayley's propagator, effectively describes the dynamics of these systems. However, a common issue with this method is that it treats the boundary as an infinite wall, causing the time-evolving wave to reflect back, which leads to unphysical behavior in certain situations. To avoid this reflection, we can integrate over a larger grid size, which is computationally expensive. To overcome this, we can modify the time evolution method to allow waves to be absorbed at the boundary, resulting in more realistic behavior for specific problems, such as calculating the time-dependent decay rate in nuclear physics. To avoid these reflections, Shibata [2] made an approach to design absorbing boundary conditions for the one-dimensional case. These conditions minimize undesirable reflections at the artificial boundaries of the computation area. In this work, we utilize the absorbing boundary condition (ABC) method to simulate the evolution of the nuclear wave function.

Formalism

From a physical point of view, particles can be absorbed in dissipative media. This type of boundary condition occurs when particles (nucleons) pass through the boundary of a specific area without reflecting. Consider the one-dimensional time-dependent Schrödinger equation, describing the motion of a nucleon with the mass m under the influence of nuclear potential $V(r)$ as,

$$i\hbar\frac{\partial}{\partial t}\psi_p(r,t) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right]\psi_p(r,t). \tag{1}$$

Where nuclear potential is given by [3]

$$V(r) = V_n(r) + V_c(r) + V_{cf} + V_s. \tag{2}$$

$V_n(r)$ is Woods-Saxon part, $V_c(r)$ is Coulomb potential, V_{cf} is centrifugal term and V_s is Thomas spin-orbit term. To eliminate the reflection from the boundaries, we modified the boundary condition so that the wave function at the boundary can be treated as a plane wave,

$$\psi_p(r,t) = \exp[-i(\omega t - kr)]. \tag{3}$$

The dispersion relation imposed at that boundary ensures that the wave will be annihilated [4]. Following the above formalism, we have simulated the time evolution of a Gaussian wave packet in the nuclear potential given by Eq.(2) and presented the results.

Results and discussion

Without modifying the boundary conditions, we see the reflection from the edges of

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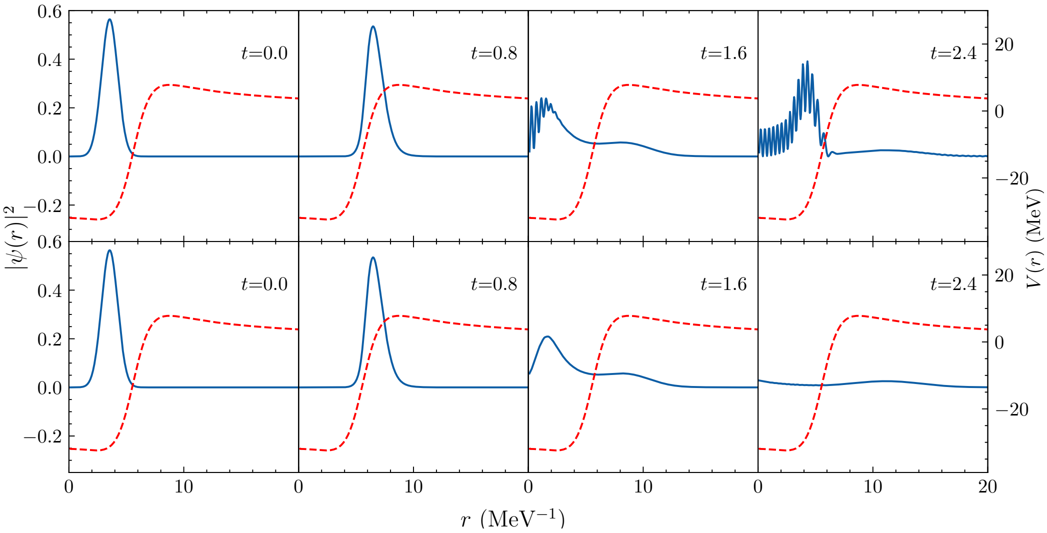

FIG. 1: Snapshots of the time evolution of a Gaussian wave-packet (nucleon) passing through a nuclear potential given by Eq. (2). The top panel is without the absorbing boundary condition (ABC), and the bottom panel is with ABC.

the grid chosen for the simulation. We have simulated and plotted the snapshots of wave functions in Fig. 1. However, after implementing the absorbing boundary conditions, we observe that the outgoing waves are absorbed by the boundary of the grid, as shown in Fig. 1. The time-dependent probability inside the box is plotted for both cases, i.e., with and without absorbing boundary conditions in Fig. 2. From this, it is clear that after implementing ABC, the wave function is absorbed by the boundary of the grid, which correctly represents the outgoing wave function for the nucleon. These adjustments for the nuclear potential can be further applied to calculate additional nuclear properties.

Conclusion

Without ABC, TDSE is not suitable for studying particle emission from the nucleus. This indicates that the ABC method is more effective and requires less memory to simulate nucleon tunneling from the nucleus. The application of this model will help simulate the particle or cluster emission from the nucleus. We will be presenting the calculation regarding the nucleon emission from the nucleus in the future.

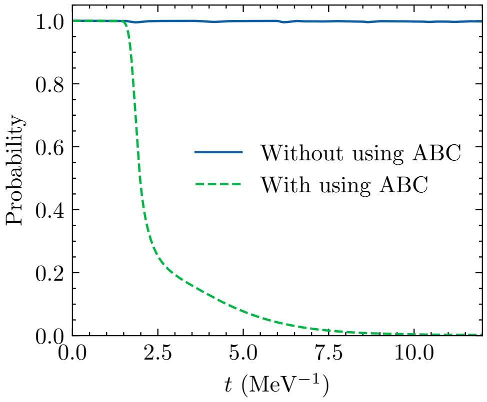

FIG. 2: Time-dependent probability of nucleon inside the boundary of the box with and without the use of ABC.

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