Barrier penetration with a finite mesh method

K. Hagino
Department of Physics, Kyoto University, Kyoto 606-8502, Japan

(Received 1 November 2023; accepted 20 February 2024; published 14 March 2024)

A standard way to solve the Schrödinger equation is to discretize the radial coordinates and apply a numerical method for a differential equation, such as the Runge-Kutta method or the Numerov method. Here I employ a discrete basis formalism based on a finite mesh method as a simpler alternative, with which the numerical computation can be easily implemented by ordinary linear algebra operations. I compare the numerical convergence of the Numerov integration method to the finite mesh method for calculating penetrabilities of a one-dimensional potential barrier and show that the latter approach has better convergence properties.

DOI: 10.1103/PhysRevC.109.034611

I. INTRODUCTION

In most physics problems, the Schrödinger equation cannot be solved analytically but has to be solved numerically. For a bound-state problem, one may expand wave functions on some finite basis and diagonalize the resultant Hamiltonian matrix. Alternatively, one may discretize the radial coordinates and successively obtain a wave function at the mesh points with, e.g., the Runge-Kutta method or the Numerov method [1].

A yet different method, referred to as a discrete-basis formalism,[1] has been proposed in Ref. [2]. In this method, one first forms a Hamiltonian matrix based on discretized radial meshes and solve it with a linear algebra with appropriate boundary conditions. An advantage of this method is that the method is well compatible with a many-body Hamiltonian, in particular in a configuration-interaction formulation [6–8]. Notice that the discrete-basis formalism is referred to as a three-dimensional (3D) mesh method in the context of nuclear density-functional theory [9–14].

Even though the discrete-basis formalism has been applied to an induced fission problem [2–5,7], its applicability has not yet been clarified, at least for a scattering problem. In this paper, I therefore apply the discrete-basis formalism to a simple one-dimensional barrier penetration problem and carry out a comparative study of the numerical accuracy. To this end, I consider a Gaussian barrier and compare the penetrabilities obtained with the discrete-basis formalism to those with the standard Numerov method.

The paper is organized as follows: In Sec. II, I detail the discrete-basis formalism for a one-dimensional problem. In Sec. III, I apply it to a barrier penetration of a one-dimensional Gaussian barrier and discuss the applicability of the discrete-basis formalism. I then summarize the paper in Sec. IV.

[1]Even though the term "discrete-basis formalism" was not introduced in Ref. [2], the method given in Ref. [2] is equivalent to the discrete-basis formalism shown in later publications [3–5].

II. DISCRETE-BASIS FORMALISM FOR BARRIER PENETRATION

Consider a one-dimensional system for a particle with mass m under a potential $V(x)$. The Hamiltonian for this system reads

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{1}$$

I discretize the radial coordinate as $x_i = x_{\rm min} + (i-1)\Delta x$ and consider the model space from $x_1 = x_{\rm min}$ to $x_N \equiv x_{\rm max}$. Using the three-point formula for the kinetic energy in H, the Hamiltonian (1) is transformed to a matrix form of

$$H_{ij} = -t\delta_{i,j+1} + (2t + V_i)\delta_{i,j} - t\delta_{i,j-1}, \tag{2}$$

where t is defined as $t = \hbar^2/2m(\Delta x)^2$ and $V_i \equiv V(x_i)$. The wave function $\phi_i \equiv \phi(x_i)$ then obeys

$$-t\phi_0\delta_{i,1} + \sum_{j=1}^{N} H_{ij}\phi_j - t\phi_{N+1}\delta_{i,N} = E\phi_i. \tag{3}$$

In the absence of the potential V, the wave function $\phi_n^{(0)}$ obeys the equation

$$-t\left(\phi_{n+1}^{(0)} - 2\phi_n^{(0)} + \phi_{n-1}^{(0)}\right) = E\phi_n^{(0)}. \tag{4}$$

I consider a free-particle solution given by

$$\phi_n^{(0)} \propto e^{-ikn\Delta x} - e^{ikn\Delta x}. \tag{5}$$

Substituting this into Eq. (4), one finds

$$\cos(k\Delta x) = 1 - \frac{E}{2t}. \tag{6}$$

In the presence of the potential V, I consider the case where the particle is incident from the left-hand side of the potential. Assuming that the potential V almost vanishes at $x_{\rm max}$, the wave function ϕ_{N+1} is given by $\phi_{N+1} = e^{ik\Delta x}\phi_N$. Substituting this into Eq. (3), one finds

$$\phi_i = [(\tilde{H} - E)^{-1}]_{i1}t\phi_0 \equiv G_{i1}t\phi_0, \tag{7}$$

 ©2024 American Physical Society

where $\tilde{H}$ is defined as $\tilde{H}_{ij} = H_{ij} - te^{ik\Delta x}\delta_{i,N}\delta_{j,N}$, and the Green's function G is defined as $G = (\tilde{H} - E)^{-1}$.

Assuming that the potential $V(x)$ is negligible at $x = x_1$ and x_2, the wave functions at these points are given as linear superpositions of $e^{\pm ikn\Delta x}$ with $n = 1$ and 2, respectively. I parametrize the coefficients of the linear superpositions in terms of t and the wave function ϕ_0 as

$$\phi_1 = (Ae^{ik\Delta x} + Be^{-ik\Delta x})t\phi_0, \tag{8}$$

$$\phi_2 = (Ae^{2ik\Delta x} + Be^{-2ik\Delta x})t\phi_0. \tag{9}$$

This is equivalent to assuming

$$G_{11} = Ae^{ik\Delta x} + Be^{-ik\Delta x}. \tag{10}$$

Substituting Eqs. (8) and (9) into Eq. (3) and using Eq. (6), one finds

$$Ae^{2ik\Delta x} + Be^{-2ik\Delta x} = 2\cos(k\Delta x)G_{11} - \frac{1}{t}. \tag{11}$$

Combining this with Eq. (10), one finds

$$A = \frac{e^{-ik\Delta x}}{e^{ik\Delta x} - e^{-ik\Delta x}}(e^{ik\Delta x}G_{11} - 1/t), \tag{12}$$

$$B = -\frac{e^{ik\Delta x}}{e^{ik\Delta x} - e^{-ik\Delta x}}(e^{-ik\Delta x}G_{11} - 1/t). \tag{13}$$

Writing the wave function ϕ_N as $\phi_N = G_{N1}t\phi_0 \equiv Te^{ik\Delta x}t\phi_0$, the penetrability $P(E)$ reads

$$P(E) = \left|\frac{T}{A}\right|^2 = \left|\frac{2\sin(k\Delta x)G_{N1}}{e^{ik\Delta x}G_{11} - 1/t}\right|^2. \tag{14}$$

III. PENETRABILITY OF A GAUSSIAN BARRIER

Let us now numerically evaluate the penetrability for a given potential. For this purpose, I consider a Gaussian potential,

$$V(x) = V_0\, e^{-x^2/2s^2}. \tag{15}$$

Following Refs. [15–17], the parameters are chosen to be $V_0 = 100$ MeV and $s = 2$ fm together with $m = 29m_N$, where m_N is the nucleon mass, to mimic the fusion reaction of ^{58}Ni + ^{58}Ni. I set $x_{\rm min} = -10$ fm and $x_{\rm max} = 10$ fm.

The upper panel of Fig. 1 shows the penetrabilities of the Gaussian barrier obtained with $\Delta x = 0.05$ fm. The dashed line and the solid circles denote the results with the standard Numerov method and the discrete-basis formalism, respectively. The value of Δx is small enough in this case, and both the methods lead to accurate results. The lower panel shows the results with a larger value of Δx, that is, $\Delta x = 0.15$ fm. In this case, the numerical error is significantly large with the Numerov method: the penetrabilities do not reach unity even at energies well above the barrier (see the dashed line). This is the case also with the modified Numerov method [18], with which the penetrability even exceeds unity at high energies with a nonmonotonic behavior (see the dotted line). In marked contrast, the results with the discrete-basis formalism is rather robust and the penetrabilities are almost the same as the one with $\Delta x = 0.05$ fm shown in the upper panel. Notice that the discrete-basis formalism employs the simple three-point

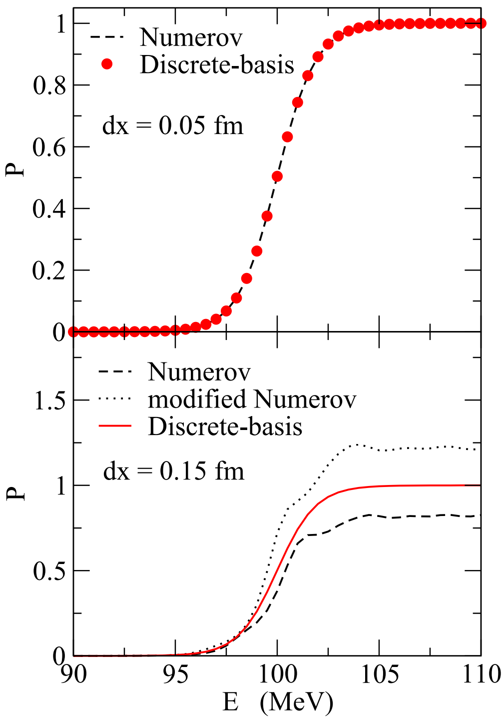

FIG. 1. The penetrabilities of a Gaussian barrier given by Eq. (15) with $V_0 = 100$ MeV and $s = 2$ fm. The mass is set to be $m = 29m_N$, where m_N is the nucleon mass. The upper panel is obtained with the Numerov method (the dashed line) and the discrete-basis formalism (the filled circles) with the mesh size of $\Delta x = 0.05$ fm. On the other hand, the lower panel shows the results of the Numerov method (the dashed line), the modified Numerov method (the dotted line), and the discrete-basis formalism (the solid line) with a mesh size of $\Delta x = 0.15$ fm.

formula for the kinetic energy, while a more sophisticated formula is used in the Numerov and the modified Numerov methods. Yet, it is interesting to notice that the discrete-basis method is numerically more stable than the Numerov and the modified Numerov methods. I point out that Δx cannot be taken larger than $(2\hbar^2/Em)^{1/2}$, though. If Δx exceeds this value, the right-hand side of Eq. (6) exceeds unity and the wave number k cannot be defined unless it is extended to a complex number.

IV. SUMMARY

I examined the applicability of the discrete-basis method for a reaction theory. To this end, I considered barrier penetration of a one-dimensional Gaussian barrier. It was demonstrated that the discrete-basis method provides a more accurate and stable method than the standard Numerov method. This property may be helpful in obtaining numerically stable solutions of coupled-channels equations [19,20].

The discrete-basis formalism has a good connection to a many-body Hamiltonian. As a matter of fact, there have been several applications of this method to microscopic descriptions of induced fission. In such applications, absorbing potentials, or imaginary energies, are introduced to a model Hamiltonian, and the absorbing probability is computed with the so-called Datta formula [2]. Even though the model setup is somewhat different from a barrier problem in one-dimension, in which there is no absorbing part in the Hamiltonian, the conclusion in this paper would remain the same in the fission problem as well.

ACKNOWLEDGMENTS

The author thanks G.F. Bertsch for helpful discussions and for a careful reading of the paper. This work was supported in part by JSPS KAKENHI Grants No. JP19K03861 and No. JP23K03414.

[1] S. E. Koonin and D. C. Meredith, *Computational Physics* (Addison-Wesley, Reading, 1990).
[2] P. Fanto, G. F. Bertsch, and Y. Alhassid, Phys. Rev. C **98**, 014604 (2018).
[3] G. F. Bertsch and W. Younes, Ann. Phys. (NY) **403**, 68 (2019).
[4] Y. Alhassid, G. F. Bertsch, and P. Fanto, Ann. Phys. (NY) **419**, 168233 (2020).
[5] Y. Alhassid, G. F. Bertsch, and P. Fanto, Ann. Phys. (NY) **424**, 168381 (2021).
[6] G. F. Bertsch and K. Hagino, Phys. Rev. C **105**, 034618 (2022).
[7] G. F. Bertsch and K. Hagino, Phys. Rev. C **107**, 044615 (2023).
[8] K. Uzawa and K. Hagino, Phys. Rev. C **108**, 024319 (2023).
[9] K. T. R. Davies, H. Flocard, S. Krieger, and M. S. Weiss, Nucl. Phys. A **342**, 111 (1980).
[10] P. Bonche, H. Flocard, and P.-H. Heenen, Comput. Phys. Commun. **171**, 49 (2005).
[11] W. Ryssens, V. Hellemans, M. Bender, and P.-H. Heenen, Comput. Phys. Commun. **187**, 175 (2015).
[12] Y. Tanimura, K. Hagino, and H. Z. Liang, Prog. Theor. Exp. Phys. **2015**, 073D01 (2015).
[13] Z. X. Ren, S. Q. Zhang, and J. Meng, Phys. Rev. C **95**, 024313 (2017).
[14] B. Li, Z. X. Ren, and P. W. Zhao, Phys. Rev. C **102**, 044307 (2020).
[15] C. H. Dasso, S. Landowne, and A. Winther, Nucl. Phys. A **405**, 381 (1983).
[16] C. H. Dasso, S. Landowne, and A. Winther, Nucl. Phys. A **407**, 221 (1983).
[17] K. Hagino and A. B. Balantekin, Phys. Rev. A **70**, 032106 (2004).
[18] K. Hagino, N. Rowley, and A. T. Kruppa, Comput. Phys. Commun. **123**, 143 (1999).
[19] K. Hagino, K. Ogata, and A. M. Moro, Prog. Part. Nucl. Phys. **125**, 103951 (2022).
[20] K. Hagino and N. Takigawa, Prog. Theor. Phys. **128**, 1061 (2012).