# Students' difficulties with solving bound and scattering state problems in quantum mechanics

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In quantum mechanics courses, students are often asked to solve bound and scattering state problems. The use of an ordinary differential equation is a standard technique to solve these questions. Here, we investigated students' problem-solving processes for two typical problems of a single particle in one spatial dimension: a bound state problem and a scattering state problem. We analyzed students' solutions to written exams and utilized think-aloud interviews using a framework that includes four stages: activation, construction, execution, and reflection. We found that the students encountered various difficulties when they solved the ordinary differential equations to obtain the properties of bound or scattering states. Common difficulties included recognizing when the time-dependent Schrödinger equation is the appropriate model; selecting a range of the energy constants that satisfies the bound or scattering state; justifying when to use a superposition form of the wave functions; grasping the physical definition of scattering coefficients; and using an effective checking method for their solutions. In addition, we observed qualitatively different difficulties in students' solutions to the two problems and discussed possible explanations for the underlying reasoning mechanisms that cause these difficulties. Finally, we discussed the potential implications of our findings for instruction.

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## I. INTRODUCTION

Bound and scattering states are two fundamental concepts in quantum mechanics. When the energy of a particle is less than the potential energy at infinity, the particle is in a bound state. Otherwise, it is in a scattering state. Different shapes between the bound and scattering state wave functions give rise to measurable differences in the experimental results. One canonical example is the quantum tunneling effect. When a particle scatters on a barrier, its wave function can be described as incident, reflected, and transmitted waves, resulting in measurable reflection and transmission probabilities. As a case where quantum mechanics is very different from classical mechanics and has a wide range of applications, the quantum tunneling effect and associated scattering states are an important part of any quantum mechanics course. Therefore, a solid understanding of the bound and scattering states is a key element in mastering the fundamental content of quantum mechanics.

The study of students' difficulties in learning quantum mechanics is an active area of upper-division physics education research [1–32]. Most of the literature has focused on students' difficulties in understanding the basic concepts and formulas of quantum mechanics. Some of these efforts examined how students conceptually understand bound and scattering states. Zhu and Singh [5] investigated students' ability to understand the basic concepts of quantum mechanics for a particle in a one-dimensional potential. In particular, they examined student ability to distinguish the properties of bound and scattering states when given the potential. The results showed that many students confuse the bound and scattering states and have difficulty reasoning about the corresponding physical properties. McKagan *et al.* [3] identified student difficulties with scattering states for particle tunneling through a barrier. Some of the tasks they used prompted students to predict experimental outcomes for the quantum tunneling effect under various conditions. They found that many students have difficulty relating the models of wave functions and energy to real-world quantum phenomena.

In the context of quantum mechanics, students are often asked to combine abstract concepts and sophisticated mathematical calculations to solve problems. For example, how to solve the problems of a particle in a one-dimensional potential is an important topic in quantum mechanics curricula. Students need to combine the physical concepts of bound and scattering states with the mathematical technique of ordinary differential equations (ODEs) to solve these problems. There are several investigations on students' difficulties in understanding the concepts of bound and scattering states [3,5]. However, we are not

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aware of any studies that specifically probed students' difficulties in relating the concepts of bound and scattering states to the ODE tools to solve problems.

In the present work, we investigate students' problem-solving skills when using the ODE tools in the context of bound and scattering states. Students in the School of Physics at the University of Science and Technology of China (USTC) have used the ODE tools several times in their physics courses, for example, for solving the motion equation of a particle in the context of classical mechanics. Despite previous experience, some students still encounter difficulties when using the ODE tools to solve problems in the context of quantum mechanics. Although a certain mathematical tool such as the ODE technique is general, how this tool is used when solving physics problems is highly dependent on the specific physics context [32–36]. Therefore, when students apply a certain mathematical tool to solve a physics problem, they encounter various difficulties in the problem-solving process, especially in how to integrate the physics content with the mathematical tool. For these reasons, more work is needed to investigate the students' difficulties in using the ODE tools in the context of quantum mechanics. These investigations have the potential to provide more insights into how students understand quantum physics concepts and use the corresponding mathematical tools.

Here, we focus on two typical cases of a particle interacting with a one-dimensional potential: a bound state problem, and a scattering state problem. They offer important context regarding the wave mechanics part of the quantum mechanics course. The two types of problems ask for the energy eigenvalues or the scattering coefficients of a particle. Students need to distinguish between bound and scattering states and manipulate the corresponding ODEs. The study presented here can provide a sampling of students' difficulties when they understand quantum physics concepts and use the ODE tools for problem solving.

In this paper, we analyze investigation data through the activation, construction, execution, reflection (ACER) framework. This analytical framework was originally developed in the analysis of students' use of mathematical tools in physics problem solving [33]. In Sec. II, we provide an overview of the related literature on students' difficulties with bound and scattering states. In Sec. III, we describe the ACER framework and its operationalization structure for our investigations. In Sec. IV, we describe the data sources and offer details regarding the design of the interviews conducted in our study. Then, in Secs. V and VI, we present our findings and analysis of students' difficulties when solving a bound state problem and a scattering state problem, respectively. Finally, in Sec. VII, we discuss the similarities and differences between our findings and those of previous studies on bound and scattering states in detail. We also briefly discuss the implications of the present work for instruction, as well as future work.

## II. REVIEW OF THE LITERATURE AND RESEARCH QUESTIONS

### A. Student difficulties regarding bound and scattering states

Most studies have focused on students' difficulties in understanding the basic quantum concepts. For example, physics education research in this area has found that students have various difficulties in explaining quantum interference phenomena [17–19], in determining the time development of a wave function [9,12,21,26], in obtaining the measurement outcomes of various physical observables [6,7,11], in using different quantum notations (e.g., Dirac notation, algebraic wave-function notation, and matrix notation) and in translating between them [13,22,25,30].

Zhu and Singh explored students' difficulties with the quantum mechanics of a particle in one spatial dimension [5]. They developed a conceptual survey and administered it to students. This survey consisted of a series of multiple-choice questions to probe students' understanding and mastery of various concepts, including wave functions, Hamiltonians, quantum measurements, and bound and scattering states. For a particle in the energy eigenstate, there are two cases: a bound state has an energy less than the potential energy at infinity, and its wave function can always be normalized; a scattering state has an energy larger than the potential energy at infinity, and its wave function cannot be normalized. Research has identified several sets of conceptual difficulties with bound and scattering states [5]: (i) Students had difficulties with understanding the aspects of the bound and scattering state wave functions. For example, many students did not recognize that the scattering states have a continuous energy spectrum and mistakenly claimed that the scattering state wave functions are normalizable. (ii) Students had great difficulties judging whether a given potential energy allows for bound states or scattering states. For example, many students thought that any potential energy that has a well shape would allow for bound states. (iii) Students had a common difficulty claiming that a particle may be in a bound or a scattering state depending on its location. For example, some students incorrectly claimed that when a particle is in the classically allowed region, it is in a bound state, while when it is in the classically forbidden region, it is in a scattering state.

McKagan *et al.* studied student learning of quantum tunneling in modern physics courses [3]. The quantum tunneling effect is a special case of scattering states. The researchers collected data that consisted of student responses and interviews related to the quantum mechanics conceptual survey (QMCS) [4]. Research has identified many difficulties in student understanding of quantum tunneling [3]. These issues include (1) difficulties with drawing wave functions for particle tunneling through a barrier; (2) difficulties with energy loss in tunneling; (3) difficulties with understanding the physical meaning of potential energy; (4) difficulties with the physical meaning of plane waves; and (5) difficulties with representations of complex wave functions. Research also unraveled several reasons why students may think that energy is lost in tunneling: regarding the energy and wave function as interchangeable, invoking dissipation, treating the total energy as a local characteristic of a wave function, etc.

There have been several investigations on the difficulties students have in solving ordinary differential equations (ODEs) in undergraduate mathematics courses. For example, the Refs. [37–39] investigated how students use graphical techniques to solve first-order ODEs. These articles investigated how students come to reason conceptually about a rate of change equation. They also investigated students' abilities converting symbolic information into graphical ones. Reference [40] investigated how students use numerical methods to solve ODEs that cannot be solved analytically.

### B. Research questions

These previous studies focused on students' difficulties when dealing with nonalgorithmic problems in bound and scattering states. However, there is little research on students' problem-solving skills in the context of quantum mechanics [32,41–43]. Learning quantum mechanics is challenging, not only because the concepts of quantum physics are very different from those of classical physics, but also because students struggle with how to build models and how to relate these models to mathematical calculations. An important context of bound and scattering states is solving algorithmic problems, such as solving the time-independent Schrödinger equation for a particle within a one-dimensional complicated potential energy (i.e., solving a typical ODE). We are not aware of any studies that target students' skills to relate the understanding of bound and scattering states to the use of the ODE tools to solve problems.

Students at the University of Science and Technology of China (USTC) were first exposed to the ODE in their mathematics courses. They had much experience with using the ODE tools in the context of classical mechanics before they took a quantum mechanics course. Although the ODE technique is general, the way students use the ODE tools to solve a physics problem is highly dependent on the specific content of the problem [32–36]. To solve a long and complex problem, students need to go back and forth between physics and mathematics many times: representing physical situations as mathematical equations, performing sophisticated mathematical calculations, and understanding the physical meaning of the mathematical results. Thus, it can be expected that students will encounter various difficulties when using the ODE tools in quantum physics content, especially when determining how to map abstract quantum concepts to the ODE procedure step by step.

For these reasons, additional work is valuable to study students' difficulties when using the ODE tools in the context of quantum mechanics, such as in the context of bound and scattering states. Given the previous work that has been done [3,5] and our focus on student problem-solving skills, we are interested in three research questions:

(1) To what extent can students integrate the concepts of bound and scattering states with the ODE tools? That is, to what extent can students correctly relate the elements of the problem-solving procedure in the context of bound and scattering states?

(2) What are the common difficulties students have when solving ODEs in the context of bound and scattering states? Can we classify these difficulties? What are the possible reasons for these difficulties?

(3) What difficulties are similar and what difficulties are different compared to previous studies?

## III. THEORETICAL FRAMEWORK

### A. Context for research

Two of the research tasks used to probe student ability to calculate the analytical solutions of the bound and scattering states are shown in Figs. 1 and 2. In problem 1, students are given a particle interacting with a one-dimensional well potential. Students are asked to determine the possible energies of the bound states. In problem 2, students are given a particle approaching a one-dimensional barrier potential. Students are asked to determine the scattering coefficients of the particle.

**Problem 1**: Consider a particle with mass $m$ interacting with the potential:
$V(x) = \infty$, if $x \leq 0$;
$V(x) = 0$, if $0 < x \leq a$;
$V(x) = V_0$, if $x > a$.
Derive the transcendental equation for the allowed energies of the bound states.

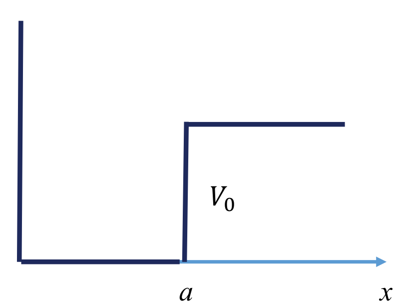


FIG. 1. An example of the exam problem about the bound state.

**Problem 2:** Consider a particle with mass $m$ and energy $E$ approaching the step potential:
$V(x) = 0$, if $x \leq 0$;
$V(x) = V_0$, if $x > 0$.
Calculate the reflection coefficient and transmission coefficient.

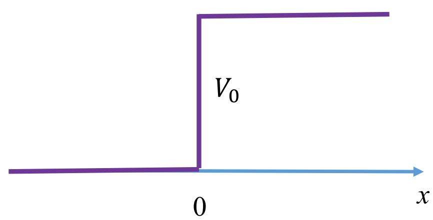


FIG. 2. An example of the exam problem about the scattering state.

## B. Analytical framework and its operationalization

In an upper-division physics course, the problem-solving procedure is long and complex. Students encounter various difficulties and make various errors at different steps of the problem-solving process. To address this complexity, we use an analytical framework known as the activation, construction, execution, reflection framework to guide our investigations of students' work [33]. The ACER framework organizes the problem-solving process into four general components:

(i) Activation stage: recognize the related mathematical tools.
(ii) Construction stage: set up the corresponding equations and conditions for the physics problem.
(iii) Execution stage: calculate the solutions to the equations and conditions.
(iv) Reflection stage: check the final answers.

The ACER framework was initially developed for the analysis of experts' problem-solving processes and was explicitly based on the resources theory of the nature of learning [33]. Then, this framework was applied to study student difficulties in solving various physics problems [32,34–36].

The use of mathematical tools is highly context dependent; thus, the ACER framework is designed to be operationalized for a specific physics topic. The operationalization of the ACER framework for the bound and scattering state problems (Figs. 1 and 2) is discussed in the following. One of us worked through these problems, documented the complete steps of solving the problems, and carefully classified these steps into the four stages of the ACER framework. All of us discussed and refined the outline until we agreed that the key elements of solving the problems had been accounted for according to the ACER framework. Then, this expert-designed outline was used as a coding scheme to analyze students' work. A summary of the operationalized framework is listed below. A detailed description can be found in the Appendix.

**(i) Activation of the relevant tools:** The activation stage identifies appropriate tools to solve the bound and scattering state problems. Activation is influenced by the prompt text for a given problem. Considering a particle interacting with a one-dimensional potential, one needs to solve the one-dimensional time-independent Schrödinger equation, which is an ODE, to obtain the wave function of the particle. We found that this kind of prompt A1 in the question text can motivate students to use relevant tools, i.e., to solve the ODE to obtain the results.

- A1: The question provides a potential $V(x)$ in one spatial dimension and asks for the wave functions or related quantities (e.g., energy eigenvalues for the bound state problem and reflection and transmission coefficients for the scattering state problem).

**(ii) Construction of the physical equations:** The construction stage maps the specific physical situations to the corresponding ODEs and boundary conditions. We operationalized the construction stage into four elements. The numbering of these elements indicates the order of the problem-solving process.

- C1: Set up the relevant ODEs in different regions for the problem (i.e., time-independent Schrödinger equations in different regions).
- C2: Determine the ranges of energy constants in the ODEs that are appropriate for the bound state or the scattering state.
- C3: Build up the boundary conditions to determine all unknown constants in the general solutions to the ODEs.
- C4: Give the expression for the final answer (e.g., using the wave function to give the reflection coefficient for the scattering state problem).

**(iii) Execution of the mathematical calculations:** This stage performs the corresponding mathematical calculations to solve the equations built in the construction stage. We operationalized the execution stage into two elements. The numbering of these elements also indicates the order of the problem-solving process.

- E1: Look up the general solutions to the ODEs in different regions.
- E2: Calculate the values for the unknown constants in the general solutions and organize the expression for the final answer.

**(iv) Reflection on the solutions:** The final stage reflects on the results to ensure consistency. We found that there are several ways for an expert to check whether his or her solution to the present problem is correct. The numbering of these elements is for labeling purposes only and indicates that there are multiple options.

- R1: Check whether the wave functions satisfy the ODEs in different regions.

- R2: Check whether the wave functions match the boundary conditions.
- R3: Check whether the units of the final answers are consistent.
- R4: Check whether the reflection coefficient $R$ and transmission coefficient $T$ satisfy the conditions of $0 \leq R, T \leq 1$ and $R + T = 1$.

In the following sections, we apply this coding scheme to study the students' efforts related to the bound state problem and to the scattering state problem.

## IV. RESEARCH METHOD

### A. Data sources

The research on student difficulties in this study uses both quantitative and qualitative methodologies. We collected data from the senior-level quantum mechanics course at USTC. This course is a one-semester course that covers Chaps. 1–12 of Zeng's book [44] or Chaps. 1–10 of Griffiths's book [45]. The student population is composed of upper-division students in the school of physics, with a typical class size of 60–100 students. There are two distinct data sources for this study: students' solutions to questions on traditional midterm exams and "think-aloud" interviews for problem-solving. For the quantitative data, we analyzed students' written solutions on exams to identify their common difficulties. Then, for the qualitative data, we investigated students' responses in the individual interviews to gain deeper insight into the nature of these difficulties.

### B. Written exams

We all taught the quantum mechanics course at USTC. We collected exam data from different semesters over six years for this study. All of us codesigned the questions on these exams through several discussions. For each exam, the students were asked to solve a bound state question or a scattering state question, and we collected six sets of exam data. One question in our data provided the students with a well potential and asked them to find the possible energies (i.e., problem 1 in Fig. 1). We collected $N_t = 388$ solutions from three sets of exam data. The other question provided students with a barrier potential and asked them to find the reflection and transmission coefficients (i.e., problem 2 in Fig. 2). We collected $N_t = 406$ solutions from another three sets of exam data.

The students' written solutions were then analyzed. Student ideas and difficulties were identified by coding their written responses that appeared in each element of the operationalized ACER framework. Finally, we formulated the results to characterize the patterns of student problem solving that emerged from the data.

### C. Design the interviews

To gain insight into students' difficulties with problem solving and to unravel the possible underlying reasoning mechanisms, we relied further on qualitative data from interviews. For this study, we conducted think-aloud interviews [46] in six sets, each performed after the mid-exam. Three sets of interviews included one question on calculating the bound state energies for a particle in a well (i.e., problem 1 in Fig. 1), and we collected $N = 24$ responses. The other three sets of interviews included one question on calculating the scattering coefficients for a particle approaching a barrier (i.e., problem 2 in Fig. 2), and we collected $N = 30$ responses.

Interviewees were volunteers who responded to a request for research participants. The total number of interviews was smaller than the total number of students who attended the classroom written exams. The exam grades of the interviewed students mostly ranged from 50 to 80, who made various errors in solving the exam questions. We chose these students because we wanted to investigate the mistakes they made on the exams in more depth.

Usually the interviews were scheduled within a week of the exams. Because of the short interval, students who participated in the interviews could still remember how they solved the same problem when they took the exams. We noticed that the solutions they gave in the interviews were very similar to the ones they gave in the exams. In other words, if they made an error on the exams, they still made the same error in the interviews. This allowed us to investigate the possible reasons why they made this mistake.

Interviews were conducted individually outside of the classroom. Each interview lasted approximately 1 h. If the interviews took too long, the students would become tired. At the beginning of each interview, we told the students that "This is only a think-aloud interview. You can explain your thinking aloud while you work through the question. Don't be nervous since it will not be counted for one test grade. It is simply because we are interested in your problem-solving process." None of the interviewed students agreed to a video or audio recording because that would make them nervous. Thus, all interviews for this study were transcribed verbatim. For consistency, all interviews were conducted by one author, T. T.

The interviews were designed using the semistructured, think-aloud protocol. The interviewed students were given problems similar to those on the written exams because we wanted to probe certain aspects of their problem-solving strategies and difficulties that were not assessed by the written exams. Analysis of students' written solutions can offer information on the pattern and frequency of student difficulties. However, it provides little insight into the thinking mechanism underlying students' problem-solving processes. Therefore, we had a list of questions to ask; hence, these interviews were semistructured. In the interviews, we first asked students to formulate and articulate their thought processes by themselves. After the students articulated their thoughts as clearly as possible, we asked them the questions on our list.

Many questions were designed to target the elements of the ACER framework. To probe the activation elements, we asked the students what prompted them to use the related resources to solve the problems. Then, to probe the construction elements, we asked questions to understand how students modeled the relevant equations. The students were asked to explain what each expression represented and/or how they made sense of these expressions. For example, "what does this equation represent?", "can you give an interpretation of this expression?", and "what would you call this quantity in the expression?". To probe the execution elements, we asked the students how they performed the corresponding mathematical calculations. For example, from the written exams, we found that students had difficulties calculating the general solutions to the ODEs. We wanted to know if these errors were caused by simple calculation errors or by other mechanisms. Last, when students solved the problem in the allotted time, we asked whether and how they checked their solutions. Note that from written solutions, it is difficult to determine whether students perform the reflection task. Thus, we designed the questions to target the reflection elements in the interviews. These interview questions clearly addressed all aspects of the ACER framework.

After the students verbalized their thoughts, if they had not mentioned them, we asked them several questions for clarification. Based on a particular student's response, we designed additional questions or provided new information on the spot to explore his or her thought process more deeply. In some interviews, we asked students about broader issues, such as what are the main difficulties in learning quantum mechanics in their opinion. We did not interrupt students while they talked about their thoughts and answered questions because we wanted them to do their best when talking. If students were quiet for a long time, we would remind them to continue to talk. For a detailed description of the interview protocol, please see the Supplemental Material [47].

## V. FINDINGS ON STUDENTS' DIFFICULTIES WHEN ADDRESSING A BOUND STATE PROBLEM

In this section, we use the stages of the ACER framework to classify and identify common student difficulties in solving a bound state problem with a one-dimensional potential (problem 1 in Fig. 1).

### A. Activation of the tools

The boundary state problem in exams explicitly provides an expression of the one-dimensional potential $V(x)$, which could prompt students to activate tools to solve the corresponding ordinary differential equations. There were $N = 388$ students who took the exams for the bound state problem. Among them, $N = 378$ students presented a differential equation form of the Schrödinger equation [e.g., $[-(\hbar^2/2m)d^2/dx^2 + V(x)]\varphi(x) = E\varphi(x)$]. The remaining $N = 10$ students wrote the Hamiltonian operator $\hat{H}$ and attempted to make some transformations while not mentioning the differential equation. These students had difficulty utilizing resources related to the differential equation form of the Schrödinger equation in the position representation.

In the interviews, one student wrote a Hamiltonian operator in the Dirac notation and tried to perform some transformations. For example, he wrote down the expression $\langle\psi|\hat{H}|\psi\rangle = E$. When he was asked why he used this method, he explained, "I remembered that in the quantum mechanics course, I learned two types of formulas, one with wave functions and one with Dirac notation. The teacher emphasized that they are equivalent, and it is more convenient to use the latter one. So I used the Dirac notation to solve the problem. I believe this problem can be solved with some operator transformations in Dirac notation representation." This result suggests that some students overfocused on the operator method in the abstract formulas of quantum mechanics, which may have discouraged them from activating resources to solve a differential equation in the position representation.

### B. Construction of the equations

**Step C1:** In this stage, the students mapped the physical quantities onto a series of mathematical equations. Step C1 constructs a basic equation that the quantities can satisfy. For the present bound state problem, this step provides the ODEs or the time-independent Schrödinger equations in different regions [i.e., $-(\hbar^2/2m)d^2\varphi(x)/dx^2 = E\varphi(x)$ for $0 < x < a$; $[-(\hbar^2/2m)d^2/dx^2 + V_0]\varphi(x) = E\varphi(x)$ for $x > a$]. There were $N = 378$ solutions that included a differential equation, and among them, $N = 364$ solutions provided the correct expression. In the remaining $N = 14$ solutions, the students set up a time-dependent Schrödinger equation but could not reduce it to the time-independent Schrödinger equation or made other errors (e.g., adding an inappropriate $i$ factor; adding or omitting a constant factor).

The most common difficulty with this step is an overfocus on the time-dependent Schrödinger equation. For instance, in the interviews, one student wrote down a time-dependent Schrödinger equation $i\hbar\partial\psi(x,t)/\partial t = [-(\hbar^2/2m)\partial^2/\partial x^2 + V(x)]\psi(x,t)$ and tried to reduce it to the time-independent Schrödinger equation $[-(\hbar^2/2m)d^2/dx^2 + V(x)]\varphi(x) = E\varphi(x)$. He spent much time because he needed to use the separation of variables method to complete the process, but he ultimately failed. When he was asked why he made so much effort to solve the time-dependent Schrödinger equation, he explained, "The time-dependent Schrödinger equation is the fundamental equation of quantum mechanics, so we should start from this fundamental equation to solve any problem." While this is true, for a stationary state problem, it is more convenient to begin with the time-independent Schrödinger equation. Distinguishing between the different application scenarios of the time-dependent and time-independent Schrödinger equations is therefore a difficulty for some students.

**Step C2:** In step C2, the students determined the range of values for the energy constant or compared the energy constant with the potential energy in different regions. Using this strategy, they determined the corresponding signs of the ODEs in different regions. There were $N = 364$ solutions that started from the exact time-independent Schrödinger equation, and among them, $N = 278$ solutions commented that $0 < E < V_0$ such that the resulting two ODEs have different signs in different regions [i.e., $d^2\varphi/dx^2 = -k^2\varphi$ with $k = \sqrt{2mE/\hbar^2}$ in the region $0 < x < a$; $d^2\varphi/dx^2 = \lambda^2\varphi$ with $\lambda = \sqrt{2m(V_0 - E)/\hbar^2}$ in the region $x > a$]. The common errors in the remaining $N = 86$ solutions included inappropriate consideration of two cases $E > V_0$ and $E < V_0$ or an incorrect discussion of $E < 0$.

The interviews provided additional insight into students' difficulties in determining the energy constant. In the interviews, fifteen students commented on the value of the energy constant and obtained the correct expression of the ODEs as $0 < E < V_0$. Then, they were asked why they determined such values of the energy constant. The full answer is as follows: (i) In quantum mechanics, when the energy of a particle is less than the potential energy at infinity (i.e., $E < V_0$ in the present problem), the particle is in a bound state. Otherwise, it is in a scattering state. (ii) In addition, the energy $E$ must exceed the minimum value of the potential energy (i.e., $E > 0$ in the present problem) for every physically acceptable solution to the time-independent Schrödinger equation. Approximately half of the students correctly answered the first point about how to judge whether a given potential energy allows for bound states or scattering states. Only four students successfully interpreted the second point that when the energy is less than the minimum value of the potential energy $E < 0$, there is no acceptable solution to the time-independent Schrödinger equation for the present potential; thus, this fact requires that $E > 0$. Other students could not explain these points at all. This result suggests that many students have difficulties truly understanding the physical properties of bound states in quantum mechanics.

Three interviewed students explicitly considered two situations: $E > V_0$ and $E < V_0$. When they were asked why they studied these two cases, one of the three students stated, "We have encountered similar problems in the course and in homework. When we solved these problems, we always needed to consider two cases since the energy constant can be greater or less than the potential energy." The other two students gave similar responses. Then, they were asked what states these two situations correspond to. For the present problem, the correct answer is $E < V_0 \Rightarrow$ bound states and $E > V_0 \Rightarrow$ scattering states. However, they appeared confused and were unable to answer. Therefore, the interviews indicate that some students remembered only similar problems for the exams, but they did not understand when and how to distinguish between bound and scattering states.

Two interviewed students selected an energy constant smaller than zero. Then, they found that these ODEs have no acceptable solutions to meet the boundary conditions. They were confused and did not know how to continue. When they were asked why they made this choice, one of them answered, "There is a similar problem in the textbook, where a particle interacts with a square potential. I remember the criteria: when the particle has an energy less than zero, the particle is in a bound state. Otherwise, if the particle's energy is larger than zero, it is in a scattering state. So I determined that $E < 0$." The other student gave a similar response. Actually, the correct criteria are: $E < V(\infty) \Rightarrow$ bound states and $E > V(\infty) \Rightarrow$ scattering states. In some situations, such as the example in the textbook, the potential goes to zero at infinity, and the criteria simplify to $E < 0 \Rightarrow$ bound states and $E > 0 \Rightarrow$ scattering states. We speculate that some students simply remembered the criteria only for the special case and directly applied this formula to the exam and were not able to make corresponding modifications to the new case. It is obvious that they ignored the fact that in the present problem, the potential energy at infinity is $V_0$ instead of zero.

**Step C3:** When the students worked through step E1 to obtain the general solutions, they applied boundary conditions to construct equations to determine the unknown constants in the general solutions. There were $N = 262$ solutions that included the general solutions of the ODEs in different regions, and among them, $N = 236$ solutions built accurate equations to match the boundary conditions. The common mistakes in the remaining $N = 26$ solutions included inappropriately setting up an expression for the superposition states or other errors (e.g., not using the boundary condition at infinity; not using the continuity of derivatives of the wave functions; missing or adding a factor or sign).

The most common difficulty identified in this step is inappropriately using an expression for the superposition state. In the interviews, two students included a superposition of the energy eigenstates, e.g., $\Psi = \sum_n c_n \varphi_n$. Then, they tried to determine the values of the coefficients $c_n$; however, they failed. When they were asked why they used the expression for the superposition state, one of the participants stated, "In quantum mechanics, an arbitrary state can be expressed as a superposition of energy eigenstates. Thus, the general solutions of the ODEs should be a superposition of the energy eigenfunctions." In general, for a time-independent Schrödinger equation $H\varphi = E\varphi$, we have a series of energy eigenstates $\varphi_n$. A possible state of the particle can be expressed as $\Psi = \sum_n c_n \varphi_n$, which results in $H\Psi = \sum_n c_n E_n \varphi_n \neq E\Psi$. Therefore, it is incorrect to introduce a superposition state to match the time-independent Schrödinger equation. Researchers pointed out that $H\Psi = E\Psi$ is not true for a linear superposition of the energy eigenstates and asked the students to explicitly write down and derive these equations. They were shocked by this fact. One student excitedly stated, "I believed that the time-independent Schrödinger equation $H\Psi = E\Psi$ holds for any wave function. This notion is actually wrong! I never recognized this before!" Thus, some students did not understand the fact that a linear superposition state does not satisfy the time-independent Schrödinger equation, which may lead to their difficulties in determining possible wave functions for a given system.

### C. Execution of the calculations

**Step E1:** In the execution stage, the students worked through the mathematical procedure of the equations set up in the construction stage. Step E1 attempts to solve the ODEs in different regions built in step C2 (i.e., $d^2\varphi/dx^2 = -k^2\varphi$ in the region $0 < x < a$; $d^2\varphi/dx^2 = \lambda^2\varphi$ in the region $x > a$). There were $N = 278$ solutions that included the proper ODEs, and among them, $N = 262$ solutions provided the correct general solutions of the two ODEs. The remaining $N = 16$ solutions included the incorrect exponential functional form of the general solutions (e.g., obtaining $e^{\pm kx}$ instead of $e^{\pm ikx}$ for $d^2\varphi/dx^2 = -k^2\varphi$; obtaining $e^{\pm i\lambda x}$ instead of $e^{\pm\lambda x}$ for $d^2\varphi/dx^2 = \lambda^2\varphi$) or other errors (e.g., dropping or adding a factor to the expressions).

In the interviews, most participants directly wrote down the solutions. We observed that these students did not write out a detailed mathematical derivation, nor did they substitute these solutions into the ODEs to check whether their solutions satisfy the ODEs. When these students were asked how they provided their solutions, they all claimed that they remembered the solutions to these ODEs. These ODEs are usually taught in mathematical courses, but in upper-division physics courses, the solutions of these ODEs are typically introduced directly and their derivation is rarely shown. Thus, we assume that many students solved these ODEs by remembering the solutions rather than by executing the mathematical procedure. If their memories were wrong, their answers were wrong too.

**Step E2:** This step determines the values of the unknown constants in the general solutions through mathematical calculations. There were $N = 236$ solutions that contained the correct equations for unknown constants, and among them, $N = 233$ solutions yielded the correct results. In addition, there were a few mathematical mistakes ($N = 3$ solutions): losing or adding a constant factor or sign or not compiling a final expression.

In the interviews, the participants who progressed to this step could manipulate the unknown constants to match the boundary conditions without any difficulty. Since the mathematical procedure in this step was mainly algebraic, solving these unknown constants was not a barrier to the students' success.

### D. Reflection on the solutions

The reflection stage checks the final expressions. However, we cannot know whether the students conducted the reflection since they did not write down the reflection process explicitly in their exam solutions. To target this stage, in the interviews, we directly asked participants whether and how they reflected on their solutions. For example, one of them answered, "I carefully checked my calculation process step by step and found no errors." Other participants gave similar responses.

Another interviewed student obtained the wrong answer and only corrected it after he checked the solution steps from beginning to end. We pointed out that he could have found the error in his final answer rather straightforwardly because the units on the left and right sides of the expression did not agree. He answered, "I have rarely applied this check method: to check if the units of the final expression are consistent. When doing homework and taking exams, I used to check the problem-solving process step by step." In summary, our students often attempted to check their solutions from the first expression to the last expression.

### E. Overview of students' performance

There were $N_t = 388$ students who took the exams and were required to solve the bound state problem. For clarity, in Fig. 3, we show a Sankey diagram of students' performance as they progressed through this problem. In the Sankey diagram, the flow is shown as the proceeding from a set of sources (in the left column) to a set of destinations (in the right column). The left column represents the total number of students who took the exams, and the right column indicates the pathways of students' solutions that they had difficulties or made errors at a certain step. The width of the arrows are proportional to the number of solutions in each pathway. Ultimately, approximately 60% ($N = 233$ of 388) successfully worked through the six steps of the problem and obtained the correct final results. As shown in Fig. 3, the number of incorrect solutions are considerably large in steps C1, C2, and C3, indicating that the students experienced many difficulties in the construction stage. The number of incorrect solutions is very noticeably in step C2, which means that determining the range of the energy constant was a significant barrier to our students' success.

## VI. FINDINGS ON STUDENTS' DIFFICULTIES WHEN ADDRESSING A SCATTERING STATE PROBLEM

In this section, we provide our investigations of students' difficulties when dealing with a scattering state problem

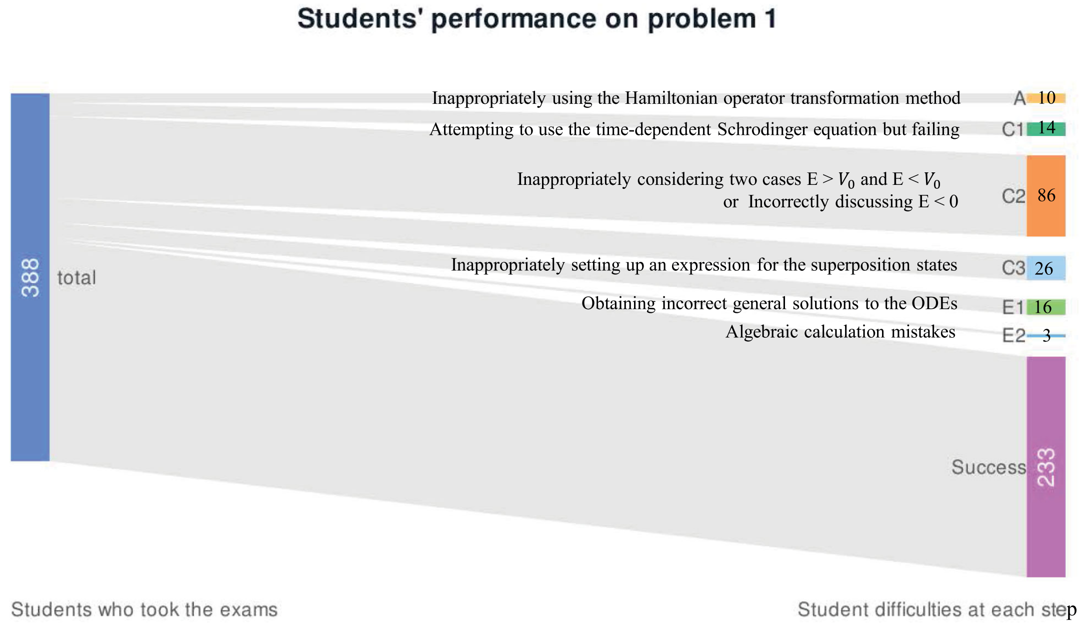


FIG. 3. Sankey diagram depicting the pathways of students' solutions as they progressed through the bound state problem. The diagram shows the flow from the beginning to the different types of solutions that have difficulties at a particular step, where the width of the arrows are proportional to the number of solutions in each flow.

(problem 2 in Fig. 2). The data and analysis are organized according to the ACER framework utilized in Sec. III.

### A. Activation of the tools

There were $N = 406$ students who took the exams for the scattering state problem. Among them, $N = 396$ students utilized the differential equation method. The remaining $N = 10$ students directly used a transmission coefficient formula without showing their work.

The interviews provided additional insight into how the students activated related resources for the scattering state problem. One student provided a transmission coefficient formula in the form $T = \exp[-\sqrt{m(V_0 - E)}a]$. Then, he commented, "This is a quantum tunneling problem. I remember there is a formula in the textbook about the probability of quantum tunneling. But I can't remember the full expression, so I have to write it as this." We pointed out that in the particular case of a square potential barrier between $0 < x < a$, one can solve the scattering state problem to obtain an approximate formula for the quantum tunneling effect, i.e., $T = \exp[-\sqrt{2m(V_0 - E)}a/\hbar]$. He responded, "That's the formula I'm talking about. I remember this formula for the exam. But I really can't remember how to derive this formula." This result suggests that some students remembered only the simple expression of the quantum tunneling effect for a specific case, which may have discouraged them from solving the Schrödinger equation for the scattering state questions.

### B. Construction of the equations

**Step C1:** The construction stage maps a physics problem to a mathematical model. Step C1 establishes the basic equation (i.e., a time-independent Schrödinger equation) in different regions. There were $N = 396$ students that used the ODE method, and among them, $N = 376$ students provided the correct expressions for a time-independent Schrödinger equation. The remaining $N = 20$ students directly wrote down the time-dependent Schrödinger equation but failed to obtain a time-independent Schrödinger equation or committed other errors (e.g., missing or adding a constant factor or sign).

In the interviews, one participant wrote down a time-dependent Schrödinger equation instead of a time-independent Schrödinger equation. He explained, "We are solving the problem of a particle scattered by a potential barrier, which is a dynamical problem. It is obvious that we should use the time-dependent Schrödinger equation to solve the dynamical problem." Then, we asked him why the scattering state problem is a dynamical problem. He drew a diagram on paper: "A small dot represents a particle, and a rectangle represents a potential barrier; the particle moves forward and hits this potential barrier." We then pointed out that this is an image of particle motion in classical mechanics. He argued, "The scattering state problem is a dynamical process both in classical mechanics and in quantum mechanics. In classical mechanics, the scattering dynamics of a particle are described by the Newton equation; whereas in quantum mechanics, the scattering dynamics of a particle are described by the time-dependent Schrödinger equation." We hypothesize that some students used the picture of classical motion to guide their problem-solving for the scattering state problem in quantum mechanics.

**Step C2:** This step determines the possible values for the energy constant. There were $N = 376$ solutions that included the exact ODEs, and among them, $N = 278$ solutions explicitly treated two cases: $E > V_0$ and $E < V_0$. Common errors in the remaining $N = 98$ solutions included discussing only one case: either $E > V_0$ or $E < V_0$.

The interview results provide insights into these findings. In the interviews, two students commented only on the case of $E > V_0$. When they were asked why they considered only this case, one of them claimed, "For one-dimensional potential problems, it is often necessary to distinguish between two cases, the bound states and the scattering states. Specifically, in this problem, when the energy of a particle is greater than the height of the potential, it is in the scattering state. Therefore, we can determine $E > V_0$." Actually, the criteria are $E < V(\infty) \Rightarrow$ bound states and $E > V(\infty) \Rightarrow$ scattering states. Therefore, the correct criteria should be to compare the energy of the particle with the potential energy at infinity, not with the potential energy at the highest point. When we pointed out the correct criteria, they admitted that they had misremembered. This result suggests that some students did not develop a functional understanding of the criteria to distinguish between bound and scattering states.

Another two students considered only the case of $E < V_0$. When they were asked why they discussed only this case, one of them stated, "This is a quantum tunneling process. The quantum tunneling effect means that when the energy of a particle is less than the height of the barrier, it can still tunnel through the barrier. This is a typical quantum mechanical effect, which is not possible in classical mechanics. We are now solving the quantum tunneling problem, so we should choose the case of $E < V_0$." The other student gave a similar response. For the present problem, the correct answer is as follows: $E > 0 \Rightarrow$ scattering states; furthermore, the wave functions of scattering states inside the barrier are different in the two cases $E < V_0$ and $E > V_0$. Therefore, the quantum tunneling process with $E < V_0$ is just one of the two cases. The student's statement about the quantum tunneling effect was correct. However, because they overfocused on the quantum tunneling effect, they could not consider other possibilities for scattering states.

**Step C3:** This step combines a general solution with the boundary conditions to set up the equations to determine the unknown constants. There were $N = 263$ solutions that exploited the correct general solution, and among them, $N = 236$ solutions provided the correct equations to match the boundary conditions. The common mistakes in the remaining $N = 27$ solutions included not using the condition that the transmitted waves come in from one side only, using a superposition state, or other errors (e.g., not including the continuity of derivatives of the wave functions; missing or adding a factor or sign).

In the interviews, two participants tried to utilize a superposition state but failed. Then, they were asked why they chose this superposition state, and their responses were similar to the research findings for the bound state problem (step C3 in Sec. V. B.). Therefore, we hypothesize that whether it is a scattering state or a bound state, some students have the incorrect belief that the equation $H\Psi = E\Psi$ is always true for any possible state of the system. This can lead to difficulties for students in solving energy eigenstate problems.

Another interviewed student wrote down the expression $\varphi(x) = Ce^{ikx} + De^{-ikx}$ for the wave function in the region $x > 0$. Then, he tried to determine the amplitude $D$ and failed. He showed confusion when we told him that the amplitude $D$ was 0. We then explained that the exponential function $e^{ikx}$ represents a traveling wave, with the wave number $k$ and the traveling direction along the $x$ direction. Since the transmitted wave comes in from one side only, the wave amplitude is $D = 0$ in this context. He answered, "This is the first time I recognize the physical meaning of the exponential function form. Previously, I just thought of this exponential function as a solution of the ODE and never considered such an intuitive physical meaning of the exponential function." Thus, the interview findings suggest that some students did not master the mathematical expression and corresponding physical picture of traveling waves.

**Step C4:** This step sets up the expressions for the reflection and transmission coefficients, expressed as the ratios of the probability currents (i.e., $R = J_r/J_i$ and $T = J_t/J_i$, where $J_i$, $J_r$, and $J_t$ are the probability currents of the incident, reflected, and transmitted waves, respectively). There were $N = 236$ students that obtained the expressions of the reflected and transmitted waves, and among them, $N = 191$ students wrote down the correct expressions of $R$ and $T$. The common errors in the remaining $N = 45$ solutions included incorrectly expressing the coefficients as ratios of the amplitudes of the wave functions $R = |B|^2/|A|^2$ and $T = |C|^2/|A|^2$ or other errors (e.g., adding or missing a factor or sign).

In the interviews, two students directly wrote down the expressions $R = |B|^2/|A|^2$ and $T = |C|^2/|A|^2$. They were asked how to define the reflection and transmission coefficients, and one of them replied, "I remember that the reflection and transmission coefficients are associated with the amplitudes of the wave functions, so they should be expressed as such." Actually, for the present question, the correct answer is as follows: (1) the reflection coefficient is given by $R = J_r/J_i = (\hbar k/m|B|^2)/(\hbar k/m|A|^2) = |B|^2/|A|^2$; (2) the transmission coefficient is given by $T = J_t/J_i = (\hbar l/m|C|^2)/(\hbar k/m|A|^2) = l|C|^2/k|A|^2$ for one case and $T = J_t/J_i = 0$ for the other case. Here, the amplitudes of the incident, reflected, and transmitted waves are $A$, $B$, and $C$, respectively; the wave numbers of the incident, reflected, and transmitted waves are $k$, $k$, and $l$, respectively. Thus, the reflection coefficient happens to be the ratio of the amplitudes of the wave functions $R = |B|^2/|A|^2$ since the wave numbers cancel each other out. However, the expression for the transmission coefficient $T = |C|^2/|A|^2$ is wrong because the wave numbers are not accounted for or the probability current of the transmitted wave could be zero for some situations. In general, the expression for the transmission coefficient $T = |C|^2/|A|^2$ is wrong for any other situation in which the potential is different for the incident and transmitted waves. Then, we reminded them that the reflection and transmission coefficients are defined by the ratios of the probability currents. One student responded, "I remember that the concept of the probability current was introduced at the beginning of the textbook, but it was rarely used in the later contents. Thus, I didn't remember that these coefficients are defined by the probability currents." We assume that some students did not know the relationship between the definition of the scattering coefficient and the probability current.

### C. Execution of the calculations

**Step E1:** This step yields general solutions for the ODEs that are established in step C2. There were $N = 278$ solutions that used the correct ODEs, and among them, $N = 263$ solutions obtained the correct solutions to the ODEs. The remaining $N = 15$ solutions included obtaining $e^{\pm i\lambda x}$ instead of $e^{\pm \lambda x}$ for the ODE $d^2\varphi/dx^2 = \lambda^2\varphi$ or other errors (e.g., omitting or adding a constant factor).

The interviews provided similar insight as those for the bound state problem (step E1 in Sec. V.C.). For example, one student provided a solution $e^{\pm i\lambda x}$ for the ODE $d^2\varphi/dx^2 = \lambda^2\varphi$. Then, he thought for a moment, modified this term with his pen, and wrote down a solution $e^{\pm \lambda x}$. When he was asked why he did it, he explained, "I remember that the general solution for the ODE $d^2\varphi/dx^2 = \lambda^2\varphi$ is $e^{\pm \lambda x}$, while the general solution for the ODE $d^2\varphi/dx^2 = -\lambda^2\varphi$ is $e^{\pm i\lambda x}$. The two expressions are so similar that I often confuse them." Therefore, we assume that students usually memorized the general solutions of these ODEs instead of solving them.

**Step E2:** There were $N = 191$ students that built the correct expressions of the reflection and transmission coefficients. The next step E2 uses mathematical calculations to solve these equations to obtain the final answer. Among them, $N = 187$ students successfully completed this step. The remaining $N = 4$ solutions included dropping or gaining constant factors or not giving a final expression. Since the calculations in this step are algebraic, both exam solutions and the interviews suggest that the mathematical manipulations in step E2 did not constitute a main difficulty to student performance in the scattering state problem.

### D. Reflection on the solutions

Students' difficulties in the reflection stage were probed in the interviews. When students were asked how they might check if their solutions were correct, they gave responses similar to those for the bound state problem

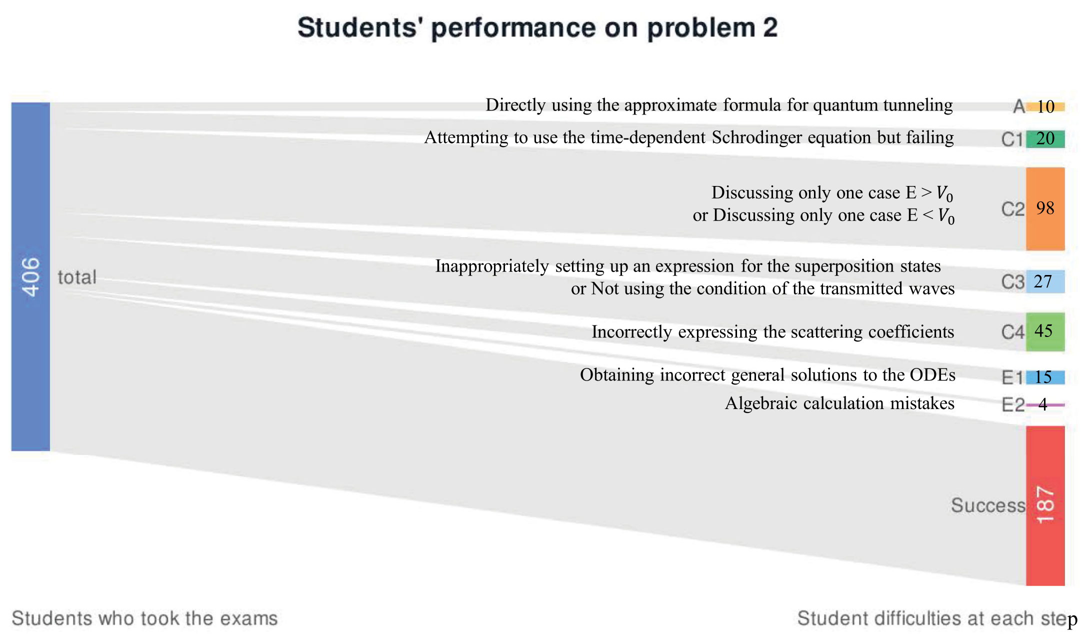


FIG. 4. Sankey diagram depicting the pathways of students' solutions as they progressed through the scattering state problem. The meaning of this Sankey diagram is similar to that of Fig. 3.

shown in Sec. IV. D. In addition, an element of the reflection stage (i.e., checking whether the reflection coefficient $R$ and transmission coefficient $T$ satisfy the condition $R + T = 1$) is specific to scattering state problems. In the interviews, approximately a quarter of the participants, after they calculated the reflection coefficient $R$, directly used $T = 1 - R$ to obtain the transmission coefficient $T$. This means that they knew and utilized this physical relationship $R + T = 1$. On the other hand, one student obtained the results for the reflection and transmission coefficients separately; however, the sum of the two clearly did not satisfy $R + T = 1$. We asked him to examine whether these expressions made sense without going through the calculation. He was surprised and did not know how to proceed. Then, we prompted him to examine whether the results satisfy $R + T = 1$. He responded, "I know that the sum of the reflection and transmission coefficients must be 1, which is required for the conservation of probability. But I didn't spontaneously apply this rule to check my calculations without any prompt." Thus, we may include that our students rarely used effective reflective methods such as checking the physical relationship $R + T = 1$.

### E. Overview of students' performance

There were $N_t = 406$ students who took the exams and were asked to solve the scattering state problem. In Fig. 4, we illustrate the pathways of students' solutions as a Sankey diagram. The Sankey diagram shows the flow of students' solutions that end up with different difficulties at a certain step. The width of the arrows are proportional to the number of solutions in each pathway. In the end, approximately 46% ($N = 187$ of 406) successfully passed seven steps of the problem and provided the correct final answers. As shown in the figure, students had few difficulties in the activation stage and in the execution stage, while they struggled with various difficulties in the construction stage. In particular, step C2, which requires determining the range of energy constants, and step C4, which requires understanding the definition of scattering coefficients, were the main stumbling blocks for our students.

## VII. DISCUSSIONS AND CONCLUSIONS

### A. Findings regarding the bound and scattering state problems

It is often assumed that after students have learned how to solve an example problem in a certain context, they are able to transfer their knowledge and skills from the example problem to solve a new problem. However, this did not happen in our study. To be precise, in the traditional quantum mechanics curriculum at USTC, students are often exposed to a typical example problem: the bound and scattering states in a finite square potential well. Much time is devoted to this topic, with 4 sessions of 50 min each. Despite the effort expended on this example problem, students still did not achieve enough mastery of the relevant physics concepts and mathematical techniques to solve new problems on the exams.

When students used the ordinary differential equation method to solve bound and scattering state problems in the context of quantum mechanics, they made a variety of errors. In this work, we studied students' difficulties by analyzing their solutions to exams and conducting think-aloud interviews. Then, we followed the ACER framework to analyze the data and identified four broad categories of reasoning difficulties within the problem-solving procedure.

We summarize the primary difficulties and possible reasons evident in students' responses to the bound state problem (Table I) and to the scattering state problem (Table II), respectively. Here, primary difficulties refer to the errors made by multiple students (typically >20 students) in each stage of the ACER framework.

### B. Similarities and differences between the bound state and scattering state problems

The previous Secs. IV and V presented our findings on students' difficulties in the context of bound states and scattering states. It is interesting to compare students' difficulties in different contexts to see what the similarities and differences are.

**(i) Activation stage:** In both the bound and scattering state cases, we found that some students were less successful in recognizing the ordinary differential equation as the appropriate mathematical technique to solve these problems. However, the students made different errors in the two cases. In the case of bound states, some students inappropriately activated the resource of the operator method. In contrast, in the case of scattering states, some students used the approximate formula for quantum tunneling, where it is not applicable.

**(ii) Construction stage:** We found that a main issue was that students selected incorrect values for the energy constants in the case of bound states. This difficulty also appeared in the students' work in the case of scattering states. However, the possible explanations of student difficulties in the two cases are largely different (see the summary tables in Sec. VI). These results imply that many students did not develop a functional understanding of the criteria to distinguish between bound and scattering states.

Moreover, in the case of bound states, one issue is not setting up the time-independent Schrödinger equation directly for these eigenfunction problems. This may be due to the students' tendency to use the time-dependent Schrödinger equation as a starting point. This difficulty was also observed in the students' efforts to solve the scattering state problems. In contrast, a potential explanation of this issue is that some students used the classical picture to approach scattering state problems.

TABLE I. Primary difficulties of students in solving bound state problems and the possible reasons for these difficulties.

| Stages | Primary difficulties | Possible reasons | Evidence in previous studies |
|---|---|---|---|
| Activation | Inappropriately using the Hamiltonian operator transformation method | Too much focus on the abstract formalism in quantum mechanics to motivate use of the ODE tools for solving the Schrödinger equation in position representation | Novel |
| Construction | Not setting up the time-independent Schrödinger equation directly for the eigenfunction problem | Overemphasizing the time-dependent Schrödinger equation in the context of quantum mechanics | Partially discussed in Ref. [9] |
| | Selecting energy constants with incorrect values | (1) Remembering an algorithm for similar problems but not understanding the distinction between bound and scattering states | Partially discussed in Ref. [5] |
| | | (2) Remembering the criteria only for the special case but failing to adjust to new cases | Partially discussed in Ref. [5] |
| | Inappropriately setting up a superposition state expression | Incorrect belief that $H\Psi = E\Psi$ holds for any possible wave function $\Psi$ | Novel |
| Execution | Obtaining incorrect general solutions to the ODEs | Remembering only the general solutions to the ODEs instead of actually solving them | Novel |
| Reflection | Rarely using effective check methods to detect errors | Developing a habit of checking the solutions step by step over the years and rarely being taught effective reflection methods | Novel |

TABLE II. Primary difficulties of students in solving scattering state problems and the possible reasons for these difficulties.

| Stages | Primary difficulties | Possible reasons | Evidence in previous studies |
|---|---|---|---|
| Activation | Directly using the approximate formula for quantum tunneling | Remembering the approximate formula for quantum tunneling while not knowing the explicit procedure to derive it | Novel |
| Construction | Not setting up the time-independent Schrödinger equation directly for the scattering state problem | Inappropriately applying the classical physics picture to the scattering state problem and considering the problem as a dynamical process | Novel |
| | Selecting energy constants with incorrect values | (1) Not developing a functional understanding of the criteria for bound and scattering states | Partially discussed in Ref. [5] |
| | | (2) Too much focus on the quantum tunneling effect to consider other possibilities of scattering states | Novel |
| | Inappropriately setting up a superposition state expression | Incorrect belief that $H\Psi = E\Psi$ holds for any possible wave function $\Psi$ | Novel |
| | Not using the condition that the transmitted waves come in from one side only | Not relating the mathematical expressions of traveling waves to their physical meaning | Partially discussed in Ref. [3] |
| | Incorrectly expressing the scattering coefficients as ratios of the amplitudes of the wave functions | Not knowing the definition of scattering coefficients | Partially discussed in Ref. [3] |
| Execution | Obtaining incorrect general solutions to the ODEs | Remembering only the general solutions to the ODEs instead of actually solving them | Novel |
| Reflection | Rarely using effective check methods such as probability conservation properties to detect errors | Developing a habit of checking the solutions step by step over the years and rarely being taught effective reflection methods | Novel |

In particular, a main difficulty related to scattering state problems is that some students incorrectly believed that the scattering coefficients are defined by the ratios of the amplitudes of the wave functions. This difficulty is unique to the context of scattering states.

**(iii) Execution stage:** In this stage, we found that the process of manipulating ODEs was a barrier for some students, which is largely content independent. The interview results suggest that the students memorized the general solutions to the ODEs rather than actually calculating them.

**(iv) Reflection stage:** We found that students usually checked their solutions step by step while rarely using effective checking methods. In particular, in the case of scattering states, although students knew some simple formulas, such as the conservation of probability $R + T = 1$, they did not use them to reflect on their solutions.

In summary, in the construction stage, to solve a bound state or a scattering state problem, the students faced several difficulties. Students struggled with these significant difficulties since in this stage, they were required to convert a physical situation into a mathematical expression (e.g., set up the ODEs in different regions) or explain the physical meaning of a mathematical expression (e.g., select ranges of energy constants). The interview results indicate that the students had not developed a functional understanding of relevant concepts (e.g., the criteria to distinguish between bound and scattering states, the definition of scattering coefficients using probability currents) for solving these quantum mechanics problems. The differences between bound states and scattering states are understandable since the construction stage of the problem-solving process is highly dependent on the specific physical context of what the problem describes.

### C. Comparison with previous studies on bound and scattering states

As mentioned in the literature overview, there are several studies [3,5] on students' difficulties with the concepts of bound and scattering states. It is important to compare our study with previous studies to see which previously existing difficulties are persistent and which difficulties are emerging. We follow the ACER framework to compare these results.

**(i) Activation stage:** We found that students suffered from interference from other concepts, such as Hamiltonian operator transformations, when applying the concepts of bound and scattering states to solve problems. This is a previously unidentified student difficulty. The word "interference" refers to the cognitive process in which the memories and thoughts of one context have a negative influence on comprehending a similar context.

**(ii) Construction stage:** In a previous study [6], the researchers found that some students believed that the time-independent Schröinger equation is the most fundamental equation of quantum mechanics. This belief is conceptually incorrect. This incorrect belief results in students struggling with the time dependence of a wave function. Our findings present an interesting flip on this common misconception. In our study, we found that some students overemphasized that the time-dependent Schröinger equation is the fundamental equation of quantum mechanics. This belief is conceptually correct, but it is inconvenient for problem solving. This correct belief results in students beginning with the time-dependent Schröinger equation to solve the stationary state problems. This requires them to reduce the time-dependent Schröinger equation to the time-independent Schröinger equation using the complicated separation of variables method. They usually failed in this derivation process, leading to a failure of the final solutions.

A previous study [5] found that students had great difficulty in determining whether a particle is in bound states or in scattering states for a given potential energy. For example, one question in the quantum conceptual survey showed four different potential energy wells. Many students thought that a particle is always in the bound states for any potential energy with a well shape. This primary difficulty also appeared in our study, which manifested in the students' errors in determining the range of energy constants. In fact, in our study, we found that this difficulty appeared in more aspects of the students' problem-solving process: students have difficulties not only with how to distinguish between bound and scattering states but also with how to consider the multiple possible cases for scattering states. Thus, our study indicates that the difficulties identified in previous studies not only affect students' conceptual understanding of bound and scattered states but also affect how they translate these concepts into the procedure of ODE calculations.

Another previous study [3] found that students struggled with a common issue: confusion regarding the physical meaning of plane waves. For example, students found plane waves to be less intuitive and preferred the wave packet representation over the plane wave representation. This difficulty also appeared in our study, but from a different perspective: students were not sure how the physical meaning of plane waves relates to its mathematical expression $e^{ikx}$ and were particularly confused regarding the fact that the transmitted waves come in from one side only.

Another issue regarding plane waves in the previous study [3] is that students believed that the probability of a plane wave is related to its amplitude. This difficulty is related to students' difficulty with scattering coefficients in our study. For the case in our study, the incident, reflected, and transmitted waves are expressed as $Ae^{ikx}$, $Be^{-ikx}$, and $Ce^{ilx}$, respectively. Since a plane wave function $e^{ikx}$ is not normalizable, one cannot calculate the reflection and transmission probabilities, as one would naively expect $R = |Be^{-ikx}|^2/|Ae^{ikx}|^2 = |B|^2/|A|^2$ and $T = |Ce^{ilx}|^2/|Ae^{ikx}|^2 = |C|^2/|A|^2$. Therefore, the correct way to obtain the reflection and transmission coefficients for plane waves should be to calculate the probability current. However, we noticed that some students assumed that the scattering coefficients are given by the relative amplitudes as $R = |B|^2/|A|^2$ and $T = |C|^2/|A|^2$. The students' responses in the interviews suggest that they could not explain why it is necessary to introduce the concept of probability current here.

In our study, we found that students tended to build an expression of the superposition state whether they were dealing with bound or scattering states. It is a misconception that all wave functions, especially superposition states, satisfy the time-independent Schrödinger equation. This leads to new difficulties for students in solving the eigenstate problem in quantum mechanics, when the differential equation that students are asked to solve is the time-independent Schrödinger equation.

Previous studies [3,5] found that students often incorrectly assuming that a particle will lose energy when it tunnels through a barrier. This difficulty did not appear in our study. We do not want to say that our students have a solid understanding of the nature of the scattering state, but at least it suggests that the students know that the energy is a constant when the particle is in an energy eigenstate (e.g., a scattering state).

**(iii) Execution stage:** In our study, one issue is to calculate a certain ODE to obtain its general solutions. However, as students were typically not required to perform calculations for multiple-choice questions in the quantum mechanics conceptual survey, this difficulty was not observed in previous studies [3,5].

**(iv) Reflection stage:** In previous studies [3,5], there was no specific research on whether students checked their solutions when dealing with problems. In contrast, we explicitly probed this issue in the interviews. We found that students usually reflected on their solutions step by step despite rarely using effective checking methods.

In summary, the difficulties in distinguishing bound and scattering states and dealing with plane wave functions seem to be persistent in student reasoning for solving both nonalgorithmic problems (as documented in previous studies [3,5]) and algorithmic problems (as documented in the present paper). In addition, some new difficulties in students' problem-solving processes were identified in our study.

### D. General topics on student difficulties

From a general point of view, there has been a great deal of research about students relying on previous example problems in introductory physics courses [9]. In our study, we found such pattern and nature of difficulties which are analogous to those observed in introductory physics courses. Students often do not have functional understanding of the example problems, but only memorize them. Then they use their memorized concepts and algorithms to solve new problems. In this way, they tend to overgeneralize concepts and algorithms learned in one situation to another in which they are not applicable. For example, students just memorize the algorithm for example problems without really understanding the difference between bound and scattering states, leading them to have a difficulty in choosing values of the energy constants for a new potential.

In a previous study [48], researchers have found that students' conceptual difficulties with force and motion can arise from their use and interpretation of the language involved. Students' confusion is a struggle to distinguish between the everyday language and the physical meaning of the terms "force" and "motion."

Interestingly, some similar evidence was found in our study that language may play a role in students' difficulties with quantum concepts. The term "scattering" in everyday language has the meaning of dynamics. When students are exposed to the term scattering, they often have a picture of classical motion, such as a particle hitting a barrier and being bounced off. This can lead students to think of the scattering state in quantum mechanics using a picture of classical motion. This example has been observed in our study (see Sec. VI.B). The term "bound" in everyday language has the meaning of being confined to a region. We speculate that when students are exposed to the term bound, they assume that the energy of the particle is smaller than the value of the external potential. This may be the reason why they choose the wrong values of the energy constants. Of course this is only our hypothesis and needs to be further studied in future work.

### E. Implications for instruction

Our investigation of students' common difficulties can provide several implications for instruction on bound and scattering states in quantum mechanics.

First, students had difficulties determining whether a particle is in a bound state or in a scattering state for a given potential energy. In the traditional quantum mechanics curriculum at USTC, students were often exposed to simple examples, such as bound and scattering states in a square potential well. Students often only remembered these particular examples and then used pattern matching to solve the bound and scattering state problems on the exams. We suggest that several variations of these examples can encourage students to grasp general criteria to distinguish the bound and scattering states. For instance, providing a complex potential instead of a simple square well potential can force students to attempt applying the criteria rather than simply using pattern matching with previous similar questions. It also provides an opportunity for students to realize the fact that the wave function can have different functional forms in different regions (e.g., a complex function $e^{ikx}$ or a real function $e^{kx}$). In this way, they can achieve a more intuitive understanding of the general solutions of the ODEs in different regions.

Second, students had difficulty giving the correct expressions of reflection and transmission coefficients. In a textbook [44] often used in the quantum mechanics course at USTC, these coefficients are calculated directly by the probability current with no explanation of where the formulas come from. In some textbooks, the transmission coefficient is simply given as $T = |C|^2/|A|^2$ with no mention that this formula applies only to the special case in which the transmitted wave and the incident wave have the same wave numbers. We suggest that the teaching of this context should focus on explaining why it is necessary to introduce the concept of the probability current here to define the reflection and transmission coefficients. We can advise students to calculate the reflection and transmission coefficients with the formula of the probability current and ask them further to verify that $R + T = 1$. This approach may lead them to gain a deeper understanding of the conservation of probability. For example, in the interviews, we explained that the probability of finding a particle in a specified range is $P = \int_a^b |\Psi|^2 dx$; thus, the change in the probability is given by $dP/dt = J(a) - J(b)$, where $J(x)$ is the probability current at the point $x$. This equation gives the rate at which probability is flowing past a specified location. One student responded, "I know the principle of the statistical interpretation of wave functions, and I'm used to calculating the probability by integration. I never realized the probability could be represented in such an intuitive form."

Third, students had difficulty determining when to use a linear superposition form of the eigenstates. We suggest asking the students to try the following two approaches: for an energy eigenvalue problem, a single eigenstate state $\varphi_n(x)$ is used to satisfy the time-independent Schrödinger equation; for an evolution problem, a linear superposition of energy eigenstates $\sum_n c_n(t)\varphi_n(x)$ is used to satisfy the time-dependent Schrödinger equation.

In conclusion, we utilized the ACER framework to analyze the student problem-solving process in the context of bound and scattering states in quantum mechanics. We investigated how students' understanding of the concepts of bound and scattering states affected their performance in solving the corresponding time-independent Schrödinger equation. Compared to previous studies in the context of bound and scattering states, our study demonstrated that some students' difficulties can be perpetuated and that new difficulties can occur. The ACER framework can be used to study the student problem-solving process in other contexts of quantum mechanics. Additional studies could provide a broader perspective on students' problem-solving processes, help identify possible patterns in student reasoning, and allow for the development of instructional strategies to address difficulties in student understanding and reasoning.

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## APPENDIX A: OPERATIONALIZATION OF THE ACER FRAMEWORK FOR A BOUND STATE QUESTION

In the following we provide the summary of the process to solve the bound state problem (problem 1 in Fig. 1) according to the ACER framework.

- Step A—The basic equation is the time-independent Schrödinger equation in a one-dimensional potential, which can be solved by the ordinary differential equation (ODE) method.
- Step C1—Express the basic equation (i.e., the time-independent Schrödinger equation) in different regions:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x) \text{ in the region } 0 < x < a,$$
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right]\varphi(x) = E\varphi(x) \text{ in the region } x > a.$$

- Step C2—Choose the range of the energy constant:
  When the energy $E$ is less than the potential energy at both plus and minus infinity, the particle is in a bound state. In addition, the energy $E$ must exceed the minimum value of the potential energy, for every physically admissible solution to the time-independent Schrödinger equation. Thus we have $0 < E < V_0$, and the ODEs read

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \text{ in the region } 0 < x < a,$$
$$\frac{d^2\varphi}{dx^2} = l^2\varphi \text{ in the region } x > a,$$

  where $k = \sqrt{2mE/\hbar^2}$ and $l = \sqrt{2m(V_0 - E)/\hbar^2}$ are real and positive.
- Step E1—Provide the general solutions to the ODEs:
  The above ODEs have the general solutions as

$$\varphi(x) = A\sin kx + B\cos kx \text{ in the region } 0 < x < a,$$
$$\varphi(x) = Ce^{-lx} + De^{lx} \text{ in the region } x > a,$$

  where $A$, $B$, $C$, and $D$ are the unknown constants.
- Step C3—Setup the equations for all unknown constants:
  The second term in the general solution $\varphi(x) = Ce^{-lx} + De^{lx}$ blows up as $x \to \infty$, so we are left with $\varphi(x) = Ce^{-lx}$. Then we impose boundary conditions:

$\varphi$ continuous at $x = 0$, $\varphi$ and $d\varphi/dx$ continuous at $x = a$. We find that

$$B = 0,$$
$$A \sin ka = Ce^{-la},$$
$$kA \cos ka = -lCe^{-la}.$$

- Step E2—Determine the energy eigenvalues:
  Using algebraic calculations, we obtain

$$\cot ka = -\frac{l}{k}.$$

  This is the equation for the allowed energies of the bound states, where $k$ and $l$ are functions of the energy $E$.
- Step R—Use the specific reflection methods to check the solution: checking units; checking the transcendental equation that could be solved only for discrete values of the energy resulting in discrete energy eigenvalues.

## APPENDIX B: OPERATIONALIZATION OF THE ACER FRAMEWORK FOR A SCATTERING STATE QUESTION

Following the ACER framework, a summary of the process to calculate the scattering state problem (problem 2 in Fig. 2) is shown here.

- Step A—The basic equation is the time-independent Schrödinger equation in a one-dimensional potential, which prompts the application of the ordinary differential equation method.
- Step C1—Express the basic equation (i.e., the time-independent Schrödinger equation) in different regions:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x) \text{ in the region } x < 0,$$
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right]\varphi(x) = E\varphi(x) \text{ in the region } x > 0.$$

- Step C2—Choose the range of the energy constant:
  When the energy $E$ is larger than the potential energy at both plus and minus infinity, the particle is in a scattering state. Here we consider two cases and treat them separately.
  Case I: When $E > V_0$, the ODEs read

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \text{ in the region } x < 0,$$
$$\frac{d^2\varphi}{dx^2} = -l^2\varphi \text{ in the region } x > 0,$$

  where $k = \sqrt{2mE/\hbar^2}$ and $l = \sqrt{2m(E - V_0)/\hbar^2}$ are real and positive.
  Case II: When $E < V_0$, the ODEs read

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \text{ in the region } x < 0,$$
$$\frac{d^2\varphi}{dx^2} = \lambda^2\varphi \text{ in the region } x > 0,$$

  where $k = \sqrt{2mE/\hbar^2}$ and $\lambda = \sqrt{2m(V_0 - E)/\hbar^2}$ are real and positive.
- Step E1—Provide the general solutions to the ODEs:
  Case I: When $E > V_0$, the general solutions are

$$\varphi(x) = Ae^{ikx} + Be^{-ikx} \text{ in the region } x < 0,$$
$$\varphi(x) = Ce^{ilx} + De^{-ilx} \text{ in the region } x > 0,$$

  where $A$, $B$, $C$, and $D$ are the unknown constants.
  Case II: When $E < V_0$, the general solutions are

$$\varphi(x) = Ae^{ikx} + Be^{-ikx} \text{ in the region } x < 0,$$
$$\varphi(x) = Ce^{-\lambda x} + De^{\lambda x} \text{ in the region } x > 0,$$

  where $A$, $B$, $C$, and $D$ are the unknown constants.
- Step C3—Setup the equations for all unknown constants:
  Case I: When $E > V_0$, to the right, assuming there is no incoming wave in this region, we have $D = 0$. Continuity of $\varphi$ and $\frac{d\varphi}{dx}$ at $x = a$ gives

$$A + B = C,$$
$$ik(A - B) = ilC.$$

  Case II: When $E < V_0$, the second term in the general solution in the right region blows up as $x \to \infty$, so we have $D = 0$. Continuity of $\varphi$ and $d\varphi/dx$ at $x = a$ yields

$$A + B = C,$$
$$ik(A - B) = -\lambda C.$$

- Step C4—Setup the expressions for the transimission coefficient $T$ and the reflection coefficient $R$:
  For a particle with a wave function $\varphi(x)$, the probability current $J$ is defined as

$$J = \frac{i\hbar}{2m}\left(\varphi\frac{\partial\varphi^*}{\partial x} - \varphi^*\frac{\partial\varphi}{\partial x}\right).$$

  We have the incident probability current $J_i$, the reflected probability current $J_r$, and the transmitted probability current $J_t$. Therefore, the transmission coefficient and the reflection coefficient are defined as

$$T = \frac{J_t}{J_i}, \qquad R = \frac{J_t}{J_i}.$$

- Step E2—Determine the final answer:
  Case I: Using algebraic calculations, we find that $J_i = \frac{\hbar k}{m}|A|^2$, $J_r = \frac{\hbar k}{m}|B|^2$, and $J_t = \frac{\hbar l}{m}|C|^2$. Then we obtain

$$T = \frac{4\sqrt{E(E-V_0)}}{(\sqrt{E}+\sqrt{E-V_0})^2},$$
$$R = 1 - \frac{4\sqrt{E(E-V_0)}}{(\sqrt{E}+\sqrt{E-V_0})^2}.$$

  Case II: Similarly, we find that $J_i = \frac{\hbar k}{m}|A|^2$, $J_r = \frac{\hbar k}{m}|B|^2$, and $J_t = 0$. Then we obtain

$$T = 0, \qquad R = 1.$$

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- Step R—Apply the specific reflection methods to check the solution: checking units; checking limiting cases when energy is very large or is just above the barrier; checking whether the reflection coefficient $R$ and transmission coefficient $T$ satisfy the conditions of $0 \le R, T \le 1$ and $R + T = 1$.

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