



## An introduction to the inverse quantum bound-state problem in one dimension

Thomas D. Gutierrez

Citation: *American Journal of Physics* **82**, 674 (2014); doi: 10.1119/1.4868335

View online: <http://dx.doi.org/10.1119/1.4868335>

View Table of Contents: <http://scitation.aip.org/content/aapt/journal/ajp/82/7?ver=pdfcov>

Published by the [American Association of Physics Teachers](http://www.aapt.org/)

---

### Articles you may be interested in

[Relativistic and nonrelativistic bound states of the isotonic oscillator by Nikiforov-Uvarov method](#)

*J. Math. Phys.* **52**, 122108 (2011); 10.1063/1.3671640

[A novel application of a Fourier integral representation of bound states in quantum mechanics](#)

*Am. J. Phys.* **79**, 201 (2011); 10.1119/1.3531975

[Computational method for the quantum Hamilton-Jacobi equation: Bound states in one dimension](#)

*J. Chem. Phys.* **125**, 174103 (2006); 10.1063/1.2358988

[A class of inverse problems in physics](#)

*Am. J. Phys.* **68**, 698 (2000); 10.1119/1.19530

[Criterion for existence of a bound state in one dimension](#)

*Am. J. Phys.* **68**, 160 (2000); 10.1119/1.19389

---

A screenshot of the APT Career Center website, showing a search interface with fields for keywords, location, and zip code. The website is titled "American Association of Physics Teachers" and "Career Center".

American Association of **Physics Teachers**

Explore the **APT Career Center** –  
access hundreds of physics education and  
other STEM teaching jobs at two-year and  
four-year colleges and universities.

<http://jobs.aapt.org>



# An introduction to the inverse quantum bound-state problem in one dimension

Thomas D. Gutierrez<sup>a)</sup>

Physics Department, California Polytechnic State University, San Luis Obispo, California 93407, USA

(Received 28 August 2013; accepted 28 February 2014)

A technique to reconstruct one-dimensional, reflectionless potentials and the associated quantum wave functions starting from a finite number of known energy spectra is discussed. The method is demonstrated using spectra that scale like the lowest energy states of standard problems encountered in the undergraduate curriculum, such as the infinite square well and the simple harmonic oscillator. © 2014 American Association of Physics Teachers.

[<http://dx.doi.org/10.1119/1.4868335>]

## I. INTRODUCTION

Undergraduate students in an introductory modern physics or quantum mechanics course are exposed to an array of mathematical methods that aid in solving the time-independent Schrödinger equation as an eigenvalue problem.<sup>1,2</sup> The topic is framed in the “direct” or “forward” sense: given some potential function, find the corresponding allowed energy eigenvalues and their associated eigenfunctions. This problem might be set up either in the context of a bound-state problem, where the resultant eigenvalues and functions form a discrete set, or a scattering problem, where the relative reflection and transmission coefficients can be calculated. Advanced quantum mechanics courses at the undergraduate and graduate level often cover the forward scattering problem in some detail, developing the mathematical methods of partial wave analysis, *S*-matrix theory, the Born approximation, and other standard analytical techniques.<sup>2–4</sup>

Advanced quantum mechanics courses sometimes introduce students to the inverse scattering problem:<sup>5</sup> given information about both the asymptotic initial and final states of a system, what information can be gleaned about the interactions that facilitated this transition? Although powerful, these kinds of problems can be nontrivial and often involve laborious analytical or computational efforts. Nevertheless, the inverse quantum scattering problem forms the foundation of many contemporary lines of scientific and applied research. For example, in modern nuclear and particle physics,<sup>5–8</sup> information about the nature of fundamental interactions between colliding systems and their constituents can be gleaned by observing the production and scattering rates of different kinds of final states. In an applied setting, medical diagnostic tools such as PET scans and CT scans are able to reconstruct images based on emission tomography technology, which relies heavily on inverse scattering methods.<sup>9</sup>

However, while the inverse scattering problem is occasionally covered in more advanced courses, the inverse problem for bound states is typically not. The inverse problem for bound systems can be stated as follows.

Given a complete set of negative bound state energies as well as the reflection and transmission coefficients for all positive energies, find the associated potential and wave functions that solve the Schrödinger equation.

Its absence in the introductory curriculum is not entirely surprising because the formal treatment of the problem in the literature<sup>5,10</sup> does not readily lend itself to a first exposure to

the topic. However, some discussion of the inverse bound-state problem in the undergraduate physics curriculum is appropriate—if not in the classroom, perhaps as an independent research project. Exposure to the problem prepares the student for various exciting emerging modern applications. For example, although still experimentally challenging, technologically generating customized potentials to achieve desired energy spectra is becoming a possibility with quantum dots, optical lattices, or nano heterostructures.<sup>11–14</sup> For many applied quantum bound-state problems, it is arguably the energy spectrum, not the shape of the potential, that is of technological or scientific interest. For example, if an application aims to emit or absorb a photon of a particular wavelength or if a certain band structure is desired to affect the conductivity of a material, manipulating the energy levels of the system is of keen interest.

While the formalism is quite general, the treatment below limits itself to a remarkable class of potentials known as *reflectionless potentials*, where the reflection coefficient is zero while the transmission is unity. Reflectionless potentials focus the effort on the inverse bound-state problem and make some of the mathematics more tractable. Because of the curious reflectionless nature of the potentials, there are natural connections with solitons<sup>15</sup> and even supersymmetric quantum mechanics.<sup>16</sup> An accessible analysis of scattering and bound-state characteristics of a particular class of reflectionless potentials can be found in Refs. 17 and 18.

In this work, without excessive formalism, students will be given the necessary tools to explore inverse bound-state problems themselves. After setting up the mathematical algorithms, a few examples to demonstrate the method are outlined. Several exercises, with some hints and solutions, are also provided to generate ideas for instructors and students alike.

## II. THE INVERSE BOUND-STATE PROBLEM

Given the *scattering data* for a system—the bound state negative energies as well as the reflection and transmission coefficients for all positive energies—can a potential function and energy eigenfunctions be found that are consistent with the Schrödinger equation? To address this problem, an approach (among many<sup>5,10,15,19</sup>) is developed to find solutions to the Marchenko integral equation, a special case of the Gel'fand–Levitan equation,<sup>5,15</sup> which is an integral representation of the Schrödinger equation. Following Ref. 20, this will be referred to as the “Marchenko method.” A detailed proof of the Marchenko and associated methods is related to the inverse Sturm–Liouville problem and the

formal procedure for solving the inverse bound-state problem is well established.<sup>5,10,15,19,21</sup> However, it is beyond the scope or intention of this work to derive it from first principles or explain it in detail. The objective is rather to provide a set of distilled mathematical tools and procedures the motivated undergraduate can use. Readers are encouraged to further investigate the underlying formalism as contained in Refs. 5, 10, 15, and 19–21.

The Marchenko method outlined here is appropriate for symmetric one-dimensional potentials and incorporates both scattering and bound-state properties of the system. Armed with this information, the time-independent Schrödinger equation can be inverted for the potential  $V(x)$ , the bound state wave functions  $\psi_n(x)$ , and the scattering wave functions  $\Psi(x, E)$ . Although an abuse of nomenclature, the term “potential” will be used for “potential energy,” a practice not inconsistent with the existing textbooks and literature. It is always understood here that “the potential” is a potential energy.

With the physical constants expressed in convenient units where  $\hbar^2/(2m) = 1$ , the Schrödinger equation for the bound system can be expressed as

$$-\psi_n''(x) + V(x)\psi_n(x) = E_n\psi_n(x), \quad (1)$$

where  $\psi_n(x)$  is the  $n$ th energy eigenstate and  $E_n$  is the associated  $n$ th energy eigenvalue. In this work,  $\psi_n(x)$  refers specifically to the bound state wave functions in contrast to the scattering wave functions  $\Psi(x, E)$  introduced later. The potential is taken to be negative for all  $x$  as are the bound state energies  $E_n$ , and the primes indicate spatial derivatives with respect to position  $x$ . The discrete index  $n$  is included as a reminder that Eq. (1) is representing a set of discrete states.

### III. OBTAINING THE POTENTIAL

Let there be  $N$  negative bound state energy eigenvalues  $E_n = -\kappa_n^2$ , with  $n = 1, 2, \dots, N$  and real  $\kappa_n$ , ordered such that  $\kappa_1 > \kappa_2 > \dots > \kappa_N$  so that  $n=1$  is the ground state (most negative) energy. Also, let the potential be one-dimensional, symmetric about the origin, everywhere negative, and smoothly approaching zero at infinity. As mentioned above, the potential emerging from the following formalism will also be reflectionless; that is, the reflection coefficient is zero so that particles with all energies  $E > 0$  impinging on the potential are completely transmitted. With these assertions, the scattering data for the problem have been completely defined.

Under these conditions, it can be shown<sup>15,21</sup> that the potential solving the Schrödinger equation is of the form

$$V(x) = -2 \frac{d^2}{dx^2} \ln[\det(\mathbf{I} + \mathbf{C})], \quad (2)$$

where  $\mathbf{I}$  is the  $N \times N$  identity matrix. The elements of the matrix  $\mathbf{C}$  are given by

$$C_{ij} = \frac{c_i c_j}{\kappa_i + \kappa_j} e^{-(\kappa_i + \kappa_j)x} \quad (3)$$

and the set of  $N$  normalization constants  $c_n$  are generated by

$$c_n^2 = 2\kappa_n \prod_{m=1, m \neq n}^N \left| \frac{\kappa_m + \kappa_n}{\kappa_m - \kappa_n} \right|. \quad (4)$$

While the origins of these equations are not immediately obvious, they suffice to generate the analytical form for the potential given the energy eigenvalues.

### IV. OBTAINING WAVE FUNCTIONS

A nice extension of the Marchenko method, developed by Kay and Moses,<sup>21</sup> is used to extract the associated bound-state and scattering wave functions from a given finite set of  $N$  known energy eigenvalues. The time-independent Schrödinger equation for the scattering states, with  $E > 0$  and  $V(x) < 0$  for all  $x$ , takes the form

$$-\Psi''(x, E) + V(x)\Psi(x, E) = E\Psi(x, E), \quad (5)$$

which looks similar to the bound-state equation (1) except the scattering wave function  $\Psi(x, E)$  and energy  $E$  are no longer discrete. However, under these conditions,  $\Psi(x, E)$  can be written in terms of the bound state eigenvalues and eigenfunctions,  $\kappa_n$  and  $\psi_n(x)$ , as follows:<sup>21</sup>

$$\Psi(x, E) = \left[ 1 + \sum_{n=1}^N \frac{\psi_n(x)}{\kappa_n + i\sqrt{E}} e^{\kappa_n x} \right] e^{i\sqrt{E}x}, \quad (6)$$

which is taken as a given starting point. The  $N$  energies  $E_n = -\kappa_n^2$  and wave functions  $\psi_n(x)$  separately satisfy the bound-state problem for the potential  $V(x)$  in Eq. (1). Although perhaps not instantly apparent, the form of Eq. (6) can be appreciated by noting that scattering solutions to the Schrödinger equation for reflectionless potentials have the asymptotic form  $\sim e^{i\sqrt{E}x}$  as  $x \rightarrow -\infty$  (incident) and  $\sim e^{i\delta} e^{i\sqrt{E}x}$  as  $x \rightarrow +\infty$  (transmitted) for real  $\delta$ ; the reflection term  $\sim e^{-i\sqrt{E}x}$  is conspicuously absent.

Also, taken here as another given, it can be shown that the  $\psi_n(x)$  satisfy the following  $N$  equations:

$$c_n^2 e^{\kappa_n x} \sum_{\nu=1}^N \left( \frac{e^{\kappa_\nu x}}{\kappa_n + \kappa_\nu} \right) \psi_\nu(x) + \psi_n(x) + c_n^2 e^{\kappa_n x} = 0, \quad (7)$$

where, as before,  $n = 1, 2, \dots, N$ , and the  $c_n$ 's are the normalization constants obtained from Eq. (4). The fully normalized bound state wave functions are  $\psi_n(x)/c_n$  (with the above formalism, the extracted  $\psi_n(x)$  themselves are not normalized).

### V. SUMMARY PROCEDURE

In an effort to help students quickly get started on projects generating potentials and wave functions from their own energy spectra, the previous discussion can be distilled as follows:

1. For a given positive integer  $N$ , select an ordered set of positive numbers  $\kappa_1 > \kappa_2 > \dots > \kappa_N$  related to the energies by  $E_n = -\kappa_n^2$ .
2. Generate the set of  $N$  normalization constants  $c_n$  using Eq. (4).
3. Generate the set of matrix elements of  $\mathbf{C}$  using Eq. (3).
4. Obtain the functional form of the reflectionless potential  $V(x)$  that is consistent with the initial energy eigenstates using Eq. (2).
5. Use standard linear algebra with the set of  $\kappa_n$  and  $c_n$  to solve Eq. (7) for the  $N$  bound-state wave functions  $\psi_n(x)$ ; normalize them by dividing by the corresponding  $c_n$ .

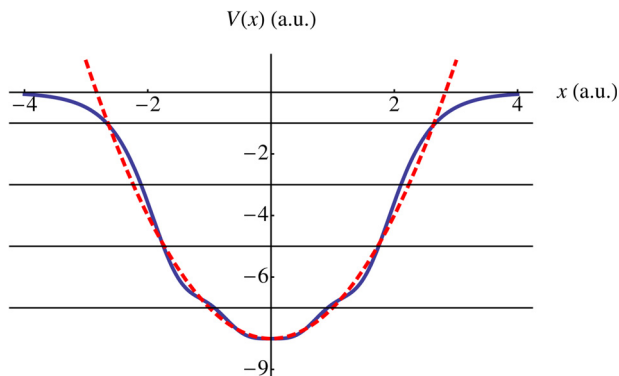


Fig. 1. The solid curve is the reflectionless potential with only four energy levels that are evenly spaced to match the first four levels of a quantum simple harmonic oscillator. The horizontal lines are the associated energy levels. The dashed curve is the exact simple harmonic oscillator potential with a spring constant  $k = 2$ .

6. Use the unnormalized bound-state wave functions  $\psi_n(x)$  to construct the scattering-state wave functions  $\Psi(x, E)$  for this reflectionless potential using Eq. (6).

To obtain analytical solutions for any system with more than a couple of eigenstates, this procedure is best followed using software capable of symbolic manipulation. However, it is worth noting that stability is an intrinsic limitation of inverse problems in general. For example, calculations may become numerically hypersensitive to the precision after just a few iterations and can thus become unstable and noisy. The approaches discussed here are no exception. Also, the algebra, even for a computer, becomes cumbersome and time consuming for six or more states. Thus, for formal research applications constrained by a rich energy spectrum and requiring high precision, considerable computing power (or an entirely different numerical approach) may be necessary. However, precise analytical results can be generated quickly and reliably using straightforward code for roughly four states. The potential shapes tend to be more stable than the wave functions, and potentials that support six or seven states can usually be found. The wave functions tend to become numerically unstable after four or five states. Although not perfect, such problems are sufficient to provide students and instructors alike with interesting pedagogical avenues to explore.

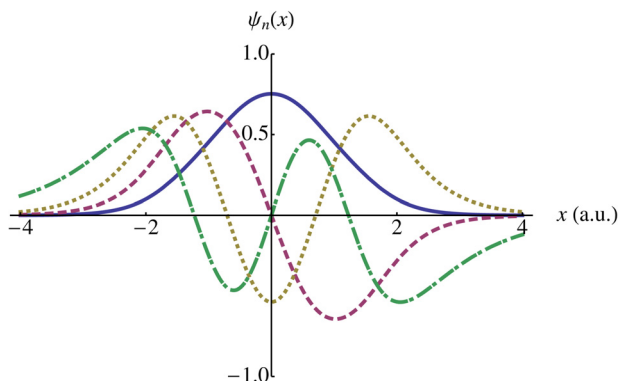


Fig. 2. The first four normalized bound state wave functions for the reflectionless potential in Fig. 1, generated via the Kay and Moses method described in the text. These wave functions should be compared to the corresponding (exact) wave functions for the simple harmonic oscillator in Fig. 3.

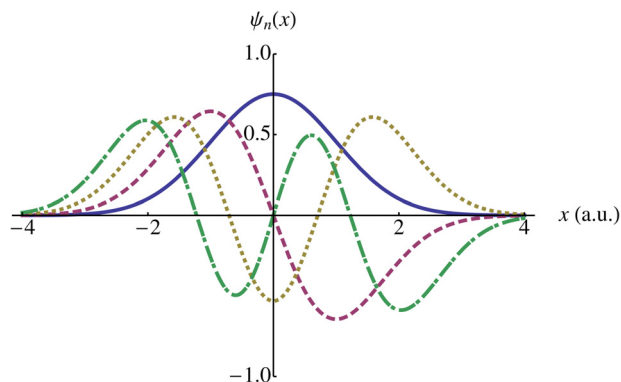


Fig. 3. The first four normalized bound-state wave functions for the exact simple harmonic oscillator with  $k = 2$ . Compare to Fig. 2 and note the differences in the tails of the higher energy wave functions.

## VI. EXAMPLES

Here are some standard systems analyzed using the Marchenko method to obtain the potentials. The Kay and Moses method was used for obtaining the associated normalized wave functions. In all cases, as discussed above, the potentials are reflectionless, but their curious shapes are crafted so their bound states match the first few energy levels of the associated sample system. All potentials and energy levels are negative, consistent with the formalism developed. The simple harmonic oscillator is discussed in Ref. 20, and further clever computationally intensive numerical methods are discussed to greatly extend the number of states that can be explored. The other potentials described below were generated for this paper and have not been treated in the literature using the methods described. The “a.u.” in the plots stands for “arbitrary units” with  $\hbar^2/2m = 1$ .

The simple harmonic oscillator has evenly spaced levels. Figure 1 shows the harmonic oscillator potential (dotted) along with a related reflectionless potential (solid) generated using the Marchenko method. Its four bound states are constructed to match the first four energy levels of the simple harmonic oscillator with spring constant  $k = 2$  in some units. Figure 2 shows the first four normalized wave functions generated using the Kay and Moses method discussed above, and Fig. 3 shows the first four exact wave functions for the

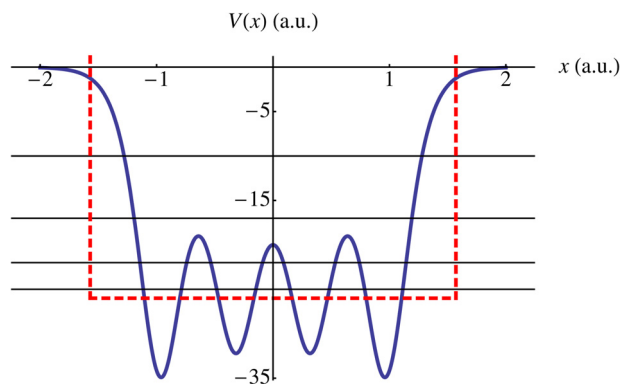


Fig. 4. The solid curve is the reflectionless potential with only four energy levels that match the first four levels of an infinite square well potential, scaling like  $n^2$  relative to the ground state. The horizontal lines are the four energy levels. The dashed lines represent the equivalent infinite square well potential whose walls are at  $\pm\pi/2$  with a base potential of  $V_0 = -26$  in some units.

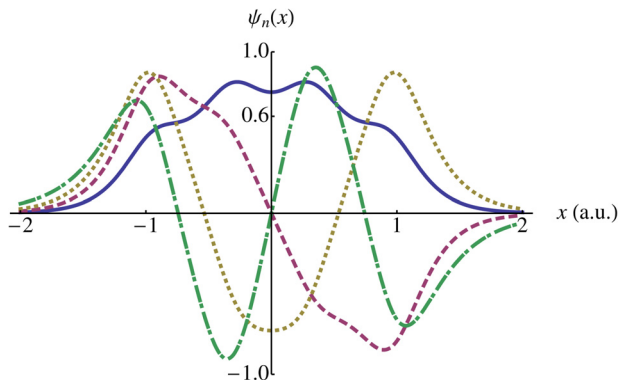


Fig. 5. The first four normalized bound state wave functions for the reflectionless potential in Fig. 4, whose energies match the first four states of the infinite square well potential centered at the origin with width  $L = \pi$  and base potential  $V_0 = -26$  in appropriate units. These functions were generated via the Kay and Moses method described in the text. Notice that the low-lying states only crudely resemble the infinite square well wave functions because they can “feel” the lumpy bottom approximating the potential’s shape. But as we look at higher-energy states, they begin to resemble the expected wave functions. These wave functions should be compared to the corresponding (exact) wave functions for the infinite square well potential in Fig. 6.

corresponding simple harmonic oscillator potential. The shapes of the wave functions for the reflection less potential closely match those for the harmonic oscillator potential. By inspection, the shape of the reflectionless potential appears as only a perturbation on the pure harmonic oscillator system, so this is not entirely unexpected. However, because the potential in Fig. 1 is finite, the tails of its wave functions extend farther than those of the harmonic oscillator wave functions. This effect is more pronounced for excited states, which are more sensitive to the edges of the potential.

The infinite square well has energy levels that scale like  $n^2$  with respect to the ground state. Figure 4 shows the reflectionless potential generated using the Marchenko method for a system with just four bound states that match the first four energies of an infinite square well centered at the origin whose width is  $L = \pi$  (in appropriate units). Figure 5 shows the four normalized wave functions for the reflectionless potential, and Fig. 6 shows the corresponding infinite-square-well solutions. In contrast to the simple harmonic oscillator, this potential only superficially represents the original potential but is a plausible analog given that the potential here is finite. The rapid oscillations at the bottom of the well serve

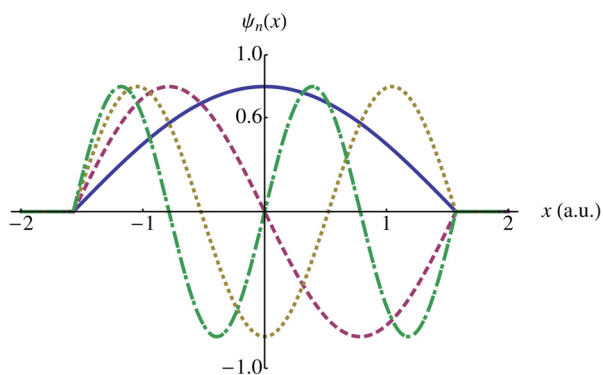


Fig. 6. The first four normalized bound state wave functions for the infinite square well potential centered at the origin with width  $L = \pi$  in appropriate units. Compare to Fig. 5.

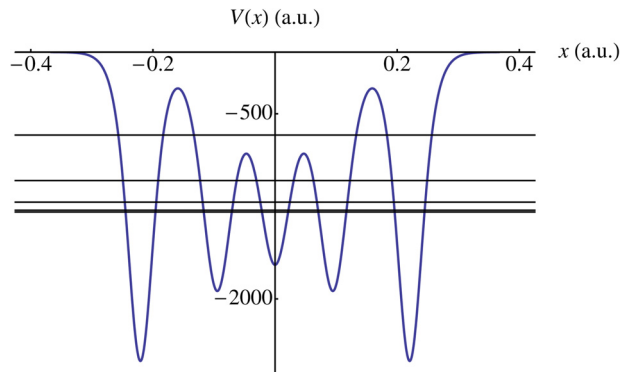


Fig. 7. A reflectionless potential having five energy levels that scale like  $n^4$  relative to the ground state. The horizontal lines are the energy levels. The two lowest energy levels are very closely spaced on this scale.

as a “flat bottom” that conspires with the tapered boundaries to generate the appropriate features of the energy spectra. The associated wave functions suffer distortions compared to the exact solutions; they are sensitive to the lumpy structure and their tails extend beyond the confines of the infinite square well.

An interesting case to consider is when the energy level scaling goes like  $n^p$ , where  $p > 2$ . For an infinite number of states in a confined potential, it can be shown that the energy levels cannot scale faster than  $n^2$ , i.e., at a rate faster than that of an infinite square well. This result can be demonstrated<sup>20,22</sup> using WKB methods.<sup>2</sup> The result has intuitive value: regardless of your potential, you cannot squeeze the quantum energy eigenstate distribution faster than the states generated by the infinite square well, which is, in this context, maximally confining. This limitation applies to bounding potentials that contain an infinite number of energy states. For example, as indicated above, there is no infinitely bound  $V(x)$  in one dimension that can have an energy spectrum scaling like  $n^3$ . However, the Marchenko method can be applied to a finite set of levels that scale faster than  $n^2$  relative to the ground state. For example, Fig. 7 shows the shape of the potential having five energy levels that scale like  $n^4$ .

In the exercises in Appendix A, students are encouraged to explore the forms for reflectionless potentials and associated wave functions for energy spectra of their own choosing. As an example of a custom spectrum, Fig. 8 shows the

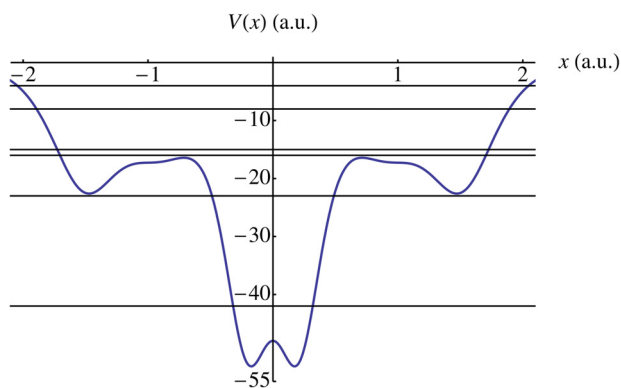


Fig. 8. A reflectionless potential having energy eigenvalues that correspond to the negatives of the six numbers from the television show *Lost*:  $-4$ ,  $-8$ ,  $-15$ ,  $-16$ ,  $-23$ , and  $-42$ . The horizontal lines are the energy levels.

potential having six energy eigenvalues corresponding to the recurring mysterious numbers from the television show *Lost*:<sup>23</sup> {4, 8, 15, 16, 23, 42}. Note that, in keeping with the procedure, the values of the numbers as energies are taken as negative so that  $-42$  is the ground state.

## VII. CONCLUSION

The inverse bound-state problem is a fascinating formal problem in quantum theory. While the nuanced mathematics can be rather involved, the core mathematical technology is accessible to the motivated undergraduate. Here, an algorithm for implementing the Marchenko method was outlined that generates an analytical form for a reflectionless potential from a finite set of energy eigenstates. Another algorithm was discussed, introduced by Kay and Moses, that produces the associated analytical scattering and bound-state wave functions. Instructors and students alike can find pedagogical value in experimenting with these methods.

## ACKNOWLEDGMENTS

Thanks to Matthew Moelter, Thomas Bensky, and Katharina Gillen for their helpful feedback and discussions. This work was performed with the support from NSF Grants PHY-0969852 and PHY-0855524.

## APPENDIX A: EXERCISES

Below are three exercises. The first exercise will help students gain familiarity with the natural units used in this paper. The remaining two exercises are designed to give practice with the procedures outlined above. Solutions to the first two exercises are provided in Appendix B.

- Throughout this paper, units where  $\hbar^2/2m = 1$  are used. Convenient natural unit choices of this kind are common in theoretical physics but can be confusing on first exposure. To gain familiarity with the natural units used in this paper, show that  $L = \pi$  in some natural distance unit for the infinite square well problem investigated above. As in Fig. 4, use  $V_0 = -26$  and  $E_1 = 1$  (with respect to the bottom of the well), expressed in some natural energy unit. Without more information, is it possible to express  $L$  in meters, for example? Express  $L$  in femtometers if it is known that the particle in the infinite well is a pion with mass  $140 \text{ MeV}/c^2$ .
- Work through the procedure as outlined in Sec. V for the case with  $N = 1$ , keeping  $\kappa_1$  as an unspecified parameter. This example represents the simplest reflectionless potential with one bound state. Explore the functional form of the potential  $V(x)$ , the bound state wave function  $\psi_1(x)$ , and the scattering state wave function  $\Psi(x, E)$ . Arrange your exponentials in terms of convenient hyperbolic functions and simplify. Show that the transmission coefficient is unity. Compare  $\Psi(x, E)$  and  $V(x)$  to the reflectionless potential and wave function from problem 2.51 in Griffiths.<sup>2</sup> Do this exercise by hand, but check your work with a computer.
- Using your favorite mathematical software, follow the procedure outlined in Sec. V to produce the associated  $V(x)$  and  $\psi_n(x)$  for your own set of  $N$  values of  $\kappa_n$ . As in the graphs in this paper, plot the wave function, potential, and the energy levels and comment on any interesting

features or structures. Do the solutions seem plausible? By hand, but checking your result with a computer, verify that your ground state wave function  $\psi_1(x)$  satisfies the Schrödinger equation for the bound states, Eq. (1), consistent with your value of  $N$ , your potential  $V(x)$ , and your selected  $\kappa_1$ . Here are some sample suggestions for energy eigenvalues: the first few Fibonacci numbers sans the first 1, so that  $-E_n = \{1, 2, 3, 5, 8, 13\}$ ; the first few notes of the equal-tempered music scale, so that  $-E_n = 2^{(n/12)}$ . Note the minus sign on  $E_n$ . As mentioned in the text, obtaining the potentials for six or seven states should be straightforward, but extracting the wave functions might be numerically unstable beyond four states.

## APPENDIX B: SOLUTIONS AND HINTS FOR EXERCISES

Here are the solutions to exercises 1 and 2 from Appendix A. Exercise 3 involves user-defined spectra, so no solutions are provided.

### 1. Solution to exercise 1

Although language like “units of  $\hbar^2/2m$ ” is commonly used, it should be appreciated that the choice of  $\hbar^2/2m = 1$  fixes one relationship among units but does not by itself uniquely determine the unit system. More information is required to complete the conversion. In the case of the infinite square well, the energy spectra are given by

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2. \quad (\text{B1})$$

In the problem as presented, the ground state energy  $E_1$  has “one energy unit” with respect to the bottom of the well (see Fig. 4). These energy units are not themselves specified. However, if  $E_1 = 1$  and  $\hbar^2/2m = 1$  then, substituting into Eq. (B1), we see that  $L = \pi$  in a still unspecified length unit, which will be called “q” below. This is most that can be said without further information.

However, if the mass of the particle in the well is known, for example, this then fixes an energy scale for the problem and any explicit system of units can be assigned if desired. In this problem, the pion has a rest energy of  $m_\pi c^2 = 140 \text{ MeV}$ , so it is convenient to select MeV as an energy unit. It is helpful to write  $\hbar^2/2m = 1$  by multiplying the top and bottom by  $c^2$ . This gives

$$(\hbar c)^2 = 2mc^2 \quad (\text{B2})$$

or

$$\hbar c = \sqrt{(2)(140)} \text{ MeV} \cdot \text{q} = 16.7 \text{ MeV} \cdot \text{q}. \quad (\text{B3})$$

Notice that the units of  $(\hbar c)^2$  in Eq. (B2) appear to carry units of energy explicitly. However, in Eq. (B3), the units are energy  $\cdot$  distance as always. Equation (B2) is an instruction to configure the units of energy and distance such that the numerical values of  $(\hbar c)^2$  are the same as  $2mc^2$ . This means if the energy units are selected explicitly, then the distance units must shift to accommodate. A conversion of q units to femtometers can be accomplished by noting that  $\hbar c = 197 \text{ MeV} \cdot \text{fm}$ , so q length units are about 11.8 fm. The width of the well is then

$$L = \pi q = (\pi)(11.8) \text{ fm} = 37.1 \text{ fm}. \quad (\text{B4})$$

## 2. Solution to exercise 2

First, set  $N = 1$  and  $E_1 = -\kappa_1^2$ , where  $\kappa_1 > 0$ . There will be one normalization constant, which according to Eq. (4), is

$$c_1^2 = 2\kappa_1. \quad (\text{B5})$$

There will be one matrix element for the “matrix”  $\mathbf{C}$  given by Eq. (3)

$$C_{11} = \frac{c_1^2}{2\kappa_1} e^{-2\kappa_1 x} = e^{-2\kappa_1 x}. \quad (\text{B6})$$

To construct  $V(x)$  from Eq. (2), it will be helpful to first construct the matrix

$$\mathbf{I} + \mathbf{C} = \det(\mathbf{I} + \mathbf{C}) = 1 + e^{-2\kappa_1 x}, \quad (\text{B7})$$

which is equal to its own determinant since it has only one element. Next, it will be helpful to construct the derivative

$$\frac{d}{dx} \ln \det(\mathbf{I} + \mathbf{C}) = \frac{-2\kappa_1 e^{\kappa_1 x}}{1 + e^{-2\kappa_1 x}}, \quad (\text{B8})$$

recalling that

$$\frac{d}{dx} \ln f(x) = \frac{1}{f(x)} \frac{df(x)}{dx}, \quad (\text{B9})$$

with  $f(x) = \det(\mathbf{I} + \mathbf{C})$ . Finally, taking another derivative of Eq. (B8) gives

$$\frac{d^2}{dx^2} \ln \det(\mathbf{I} + \mathbf{C}) = 4\kappa_1^2 \left[ \frac{e^{-4\kappa_1 x}}{(1 + e^{-2\kappa_1 x})^2} - \frac{e^{-2\kappa_1 x}}{1 + e^{-2\kappa_1 x}} \right], \quad (\text{B10})$$

so, plugging into Eq. (2), we find

$$V(x) = -8\kappa_1^2 \left[ \frac{e^{-4\kappa_1 x}}{(1 + e^{-2\kappa_1 x})^2} - \frac{e^{-2\kappa_1 x}}{1 + e^{-2\kappa_1 x}} \right]. \quad (\text{B11})$$

Simplifying, using

$$\text{sech}(\kappa_1 x) = \frac{2}{e^{\kappa_1 x} + e^{-\kappa_1 x}} \quad (\text{B12})$$

gives

$$V(x) = -2\kappa_1^2 \text{sech}^2(\kappa_1 x), \quad (\text{B13})$$

which matches the form of the reflectionless potential in Griffiths problem 2.51 (accounting for our units in which  $\hbar^2/2m = 1$ ). This is a special case of what is sometimes called a modified Pöschl–Teller or “Sech-squared” potential.<sup>17</sup>

To obtain  $\psi_1(x)$ , plug  $c_1^2$  from Eq. (B5) into Eq. (7) and solve for  $\psi_1(x)$ , giving

$$\psi_1(x) = -\frac{2\kappa_1 e^{\kappa_1 x}}{1 + e^{2\kappa_1 x}} = -\kappa_1 \text{sech}(\kappa_1 x), \quad (\text{B14})$$

with the normalized bound state wave function being

$$\frac{\psi_1(x)}{c_1} = -\sqrt{\frac{\kappa_1}{2}} \text{sech}(\kappa_1 x). \quad (\text{B15})$$

The minus sign, an overall phase factor, does not affect the physical picture. Note that Eq. (7) here has only one equation and one unknown,  $\psi_1(x)$ , and the sum over  $\nu$  has only one term.

To obtain the scattering wave function  $\Psi(x, E)$ , plug the result from Eq. (B14) into Eq. (6),

$$\Psi(x, E) = \left[ 1 - \frac{\kappa_1 \text{sech}(\kappa_1 x)}{\kappa_1 + i\sqrt{E}} e^{\kappa_1 x} \right] e^{i\sqrt{E}x}. \quad (\text{B16})$$

This expression can be simplified using

$$\tanh(\kappa_1 x) = \frac{e^{\kappa_1 x} - e^{-\kappa_1 x}}{e^{\kappa_1 x} + e^{-\kappa_1 x}} \quad (\text{B17})$$

and letting  $k = \sqrt{E}$ . After some algebra, we get

$$\Psi(x, E) = \left[ \frac{ik - \kappa_1 \tanh(\kappa_1 x)}{\kappa_1 + ik} \right] e^{ikx}, \quad (\text{B18})$$

which matches the form of the scattering wave function in problem 2.51 from Griffiths. The transmission coefficient is obtained by looking at the asymptotic behavior of  $|\Psi(x, E)|^2$  as  $x \rightarrow \infty$  (assuming an incident beam from the left). In this limit, Eq. (B18) behaves as

$$\lim_{x \rightarrow +\infty} \Psi(x, E) = \left[ \frac{ik - \kappa_1}{\kappa_1 + ik} \right] e^{ikx}, \quad (\text{B19})$$

so the transmission coefficient is

$$\lim_{x \rightarrow +\infty} |\Psi(x, E)|^2 = 1. \quad (\text{B20})$$

This implies (by unitarity) that the reflection coefficient is 0, which can be seen by inspection since there is no  $e^{-ikx}$  term in Eq. (B18). But more to the point, reflectionlessness was a feature by design because of the form of Eq. (6). This problem is treated in Ref. 21 but be mindful of the typographical error in the form of the potential in their Eq. (4.8), where it is written  $V(x) = -2\kappa_1^2 \text{sech}^2(2\kappa_1 x)$  rather than as Eq. (B13) above.

<sup>a)</sup>Electronic mail: tdgutier@calpoly.edu; URL: <http://www.tdgutierrez.com>

<sup>1</sup>Randy Harris, *Modern Physics*, 2nd ed. (Pearson/Addison-Wesley, San Francisco, 2007).

<sup>2</sup>David J. Griffiths, *Introduction to Quantum Mechanics*, 2nd ed. (Pearson/Prentice Hall, Upper Saddle River, NJ, 2005); Chapter 11 introduces partial wave analysis and the Born approximation. Also, Chapter 2 includes an introduction to S-matrix and T-matrix formalism in one dimension. Problem 2.51, which pertains to exercise 2 in Appendix A above, is on p. 89.

<sup>3</sup>R. Shankar, *Principles of Quantum Mechanics*, 2nd ed. (Plenum Press, New York, 1994).

<sup>4</sup>J. J. Sakurai, *Modern Quantum Mechanics*, 2nd ed. (Addison-Wesley, San Francisco, 2011).

<sup>5</sup>K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer-Verlag, Berlin, 1977).

<sup>6</sup>Raymond S. Mackintosh, “Inverse scattering: Applications in nuclear physics,” *Scholarpedia* 7, 12032 (2012).

- <sup>7</sup>Frances Halzen and Alan D. Martin, *Quarks and Leptons: An Introductory Course in Modern Particle Physics* (Wiley, New York, 1984).
- <sup>8</sup>David J. Griffiths, *Introduction to Elementary Particles*, 2nd ed. (Wiley-VCH, Weinheim, 2008).
- <sup>9</sup>*Emission Tomography, The Fundamentals of PET and SPECT*, edited by Miles N. Wernick and John N. Aarsvold (Elsevier, San Diego, 2004).
- <sup>10</sup>L. D. Faddeyev and B. Seckler, "The inverse problem in the quantum theory of scattering," *J. Math. Phys.* **4**, 72–104 (1963).
- <sup>11</sup>D. Bimberg, M. Grundmann, and N. N. Ledentsov, *Quantum Dot Heterostructures* (John Wiley, Chichester, 1999), Vol. 471973882.
- <sup>12</sup>P. S. Jessen and I. H. Deutsch, "Optical lattices," *Adv. At., Mol., Opt. Phys.* **37**, 95–138 (1996).
- <sup>13</sup>I. H. Deutsch, G. K. Brennen, and P. S. Jessen, "Quantum computing with neutral atoms in an optical lattice," *Fortschr. Phys.* **48**, 925–943 (2000).
- <sup>14</sup>D. Nam *et al.*, "Strain-induced pseudoheterostructure nanowires confining carriers at room temperature with nanoscale-tunable band profiles," *Nano Lett.* **13**, 3118–3123 (2013).
- <sup>15</sup>S. Novikov *et al.*, *Theory of Solitons* (Consultants Bureau, New York, 1984). In particular, see Chapter 1, Secs. 1–3 for an overview of inverse scattering theory related to this work.
- <sup>16</sup>F. Cooper, A. Khare, and U. Sukhatme, "Supersymmetry and quantum mechanics," *Phys. Rep.* **251**, 267–385 (1995).
- <sup>17</sup>N. Kiriushcheva and S. Kuzmin, "Scattering of a Gaussian wave packet by a reflectionless potential," *Am. J. Phys.* **66**, 867–872 (1998).
- <sup>18</sup>J. Lekner, "Reflectionless eigenstates of the sech<sup>2</sup> potential," *Am. J. Phys.* **75**, 1151–1157 (2007).
- <sup>19</sup>V. Barcilon, "Iterative solution of the inverse Sturm-Liouville problem," *J. Math. Phys.* **15**, 429–436 (1974).
- <sup>20</sup>D. Schumayer *et al.*, "Quantum mechanical potentials related to the prime numbers and Riemann zeros," *Phys. Rev. E* **78**, 056215 (2008).
- <sup>21</sup>I. Kay and H. E. Moses, "Reflectionless transmission through dielectrics and scattering potentials," *J. App. Phys.* **27**, 1503–1508 (1956).
- <sup>22</sup>G. Mussardo, "The quantum mechanical potential for the prime numbers," e-print [arXiv: cond-mat/9712010](https://arxiv.org/abs/cond-mat/9712010).
- <sup>23</sup>*Lost* was a science fiction television show that ran on ABC from 2001 until 2007. The numbers have no physical significance to the author's knowledge but serve as a symbol of uncanny coincidence, often unpleasant, in the fiction of the show, <<http://ww2.abc.go.com/shows/lost>>.

### ALL BACK ISSUES ARE AVAILABLE ONLINE

The contents of the *American Journal of Physics* are available online. AJP subscribers can search and view full text of AJP issues from the first issue published in 1933 to the present. Browsing abstracts and tables of contents of online issues and the searching of titles, abstracts, etc. is unrestricted. For access to the online version of AJP, please visit <http://aapt.org/ajp>.

Institutional and library ("nonmember") subscribers have access via IP addresses to the full text of articles that are online; to activate access, these subscribers should contact AIP, Circulation & Fulfillment Division, 800–344–6902; outside North American 516–576–2270 or [subs@aip.org](mailto:subs@aip.org).

APPT (individual) members also have access to the American Journal of Physics Online. Not a member yet? Join today <http://www.aapt.org/membership/joining.cfm>. Sign up for your free Table of Contents Alerts at [http://www.ajp.aapt.org/features/toc\\_email\\_alerts](http://www.ajp.aapt.org/features/toc_email_alerts).