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Citation: American Journal of Physics 48, 926 (1980); doi: 10.1119/1.12203

View online: http://dx.doi.org/10.1119/1.12203

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Degeneracy in one-dimensional quantum mechanics

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The degeneracy of quantum-mechanical energy levels is discussed from the novel perspective of the inverse scattering problem. The coalescence of energy levels is illustrated for a class of potentials which are completely characterized by their boundstate spectra. Other applications of this style of analysis are suggested.

I. INTRODUCTION

In most quantum-mechanical systems defined on the infinite one-dimensional line, degenerate bound states can in principle not occur. To show this, let us consider two distinct, normalizable solutions $\phi_1(x)$ and $\phi_2(x)$ to the Schrödinger equation

$$(\hbar^2/2\mu)\phi''(x) + [E - V(x)]\phi(x) = 0$$
 (1.1)

with a common energy eigenvalue $E_1 = E_2 = E$. The Wronskian determinant

$$W(x) \equiv \phi_1'(x)\phi_2(x) - \phi_1(x)\phi_2'(x) \tag{1.2}$$

is a constant, independent of position, because by (1.1):

$$\frac{d}{dx}W(x) = \phi_1''(x)\phi_2(x) - \phi_1(x)\phi_2''(x)$$

$$= \frac{2\mu}{\hbar^2}\phi_1(x)\phi_2(x)(E_2 - E_1), \qquad (1.3)$$

and by assumption $E_2 - E_1 = 0$. It is then convenient to evaluate the Wronskian at infinity, where both $\phi(x)$ and $\phi'(x)$ are exponentially vanishing, so that

$$W(x) = 0. ag{1.4}$$

This implies, in the absence of pathologies, that ϕ_1 and ϕ_2 are linearly dependent, contrary to assumption. Hence the levels cannot be degenerate. To keep this phenomenon in perspective, we note that such a no-degeneracy theorem can be evaded in special circumstances. A pair of infinitely deep square wells of finite width is perhaps the most familiar example.

There the matter normally rests in quantum mechanics courses. If any further discussion is given, it is to show by example that the degeneracy of levels in nearby identical wells is lifted by quantum-mechanical tunneling. Here we wish to provide a different and complementary perspective on degeneracy, by investigating what happens to wave functions and bound-state spectra as energy eigenvalues coalesce. This may be done in the context of the inverse scattering problem, the problem of reconstructing a potential from information about its bound-state spectrum and its scattering phase shifts.²

In classical mechanics, an incident particle cannot be

reflected by a potential well or barrier which lies below the particle's energy. This is not generally so in quantum mechanics, but for a special class of potentials, known as reflectionless potentials, the reflection coefficient vanishes identically for all continuum levels. The simplest example

$$V(x) = -(\hbar^2 \kappa^2 / \mu) \operatorname{sech}^2(\kappa x), \tag{1.5}$$

which supports a single bound state at

$$E_{\rm bs} = -\hbar^2 \kappa^2 / 2\mu \tag{1.6}$$

with the bound-state wave function

$$\phi(x) = \sqrt{(\kappa/2)} \operatorname{sech}(\kappa x), \tag{1.7}$$

and for which the continuum wave functions corresponding to energy eigenvalues

$$E_{\rm cont} = \hbar^2 k^2 / 2\mu \tag{1.8}$$

are

$$\phi_k(x) = e^{ikx}(\tanh(\kappa x) - ik/\kappa). \tag{1.9}$$

For the special case of a symmetric, reflectionless potential in one dimension, the potential and the bound-state wave functions are uniquely determined as algebraic functions of the binding energy.^{3,4} The simplicity of the inverse problem for these potentials makes them especially suitable for illustrating by example the approach to degenerate energy levels.

In Sec. II we shall summarize the inverse scattering formalism for symmetric reflectionless potentials, and employ it to exhibit the evolution of a potential and its bound-state wave functions as two or more energy eigenvalues approach one another. This will show how the Wronskian argument is realized. Details of the formalism are not required for an appreciation of the examples, but in Sec. II A we present complete expressions for the reader who wishes to investigate other cases. Suggested extensions of these studies and brief summary remarks make up Sec. III.

II. COLLIDING LEVELS

What becomes of the bound states supported by a sym-

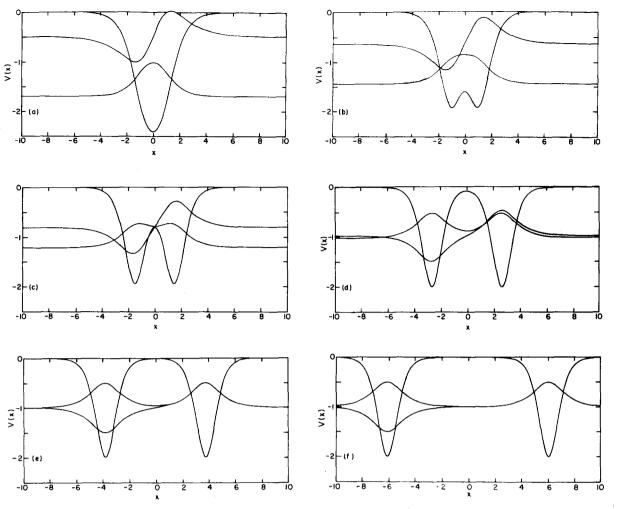


Fig. 1. Evolution of a two-bound-state symmetric, reflectionless potential as the levels become degenerate. In addition to the potential, the normalized wave functions are plotted as $\phi_i(x) + E_i$. The potentials are characterized by (a) $\kappa_1 = 1.3$, $\kappa_2 = 0.7$; (b) $\kappa_1 = 1.2$, $\kappa_2 = 0.8$; (c) $\kappa_1 = 1.1$, $\kappa_2 = 0.9$; (d) $\kappa_1 = 1.01$, $\kappa_2 = 0.99$; (e) $\kappa_1 = 1.001$, $\kappa_2 = 0.999$; (f) $\kappa_1 = 1.00001$, $\kappa_2 = 0.999999$.

metric potential when bound-state energies come together? The inverse scattering technique enables us to construct a potential with a prescribed bound-state spectrum, and to study the changes that take place when the eigenvalue spectrum is varied. To appreciate the examples to be discussed below, it is only required to know that this can be done. For completeness, however, we include a brief resume of the algorithm. Derivations may be found in the original literature. The reader principally concerned with results may pass directly to Sec. II B.

A. Formalism

The symmetric, reflectionless potential that supports N bound states at

$$E_i = V(\infty) - \hbar^2 \kappa_i^2 / 2\mu \qquad i = 1, \dots, N \quad (2.1)$$

is given by⁴

$$V(x) = V(\infty) - \frac{\hbar^2}{\mu} \frac{d^2}{dx^2} \log[D(x)], \qquad (2.2)$$

where the function D(x) is defined by⁵

$$D(x) = \sum_{S} \Pi(S, \overline{S}) \cosh \left[x \left(\sum_{m \in S} \kappa_m - \sum_{n \in \overline{S}} \kappa_n \right) \right]. \quad (2.3)$$

It is convenient to label the bound states so $\kappa_1 > \kappa_2 > \dots > \kappa_N$. Each term in the sum (2.3) is labelled by a subset S of $\{1, \ldots, N\}$; \overline{S} denotes the complement of S. The symbol Π stands for

$$\Pi(S, \overline{S}) = \prod_{i \in S_i} \left| \frac{\kappa_i + \kappa_j}{\kappa_i - \kappa_j} \right|. \tag{2.4}$$

When either S or \overline{S} is empty, $\Pi(S, \overline{S}) \equiv 1$. In the examples considered below we shall choose $V(\infty) = 0$, and $h = 1 = 2\mu$.

One can also derive explicit algebraic formulas for the bound-state wave functions, which make numerical solutions to the Schrödinger equation unnecessary in these exercises. The wave functions may be written most symmetrically as⁵

$$\psi_{p}(x) = \frac{[2\kappa_{p}\Pi(p, \{N\} - p)]^{1/2}}{D(x)}$$

$$\times \sum_{S \neq p} (-1)^{\nu(S,p)}\Pi(S, \overline{S} - p)$$

$$\times \cosh\left[x\left(\sum_{m \in S} \kappa_{m} - \sum_{n \in \overline{S} - p} \kappa_{n}\right)\right] \qquad (p \text{ odd}) \quad (2.5)$$
and

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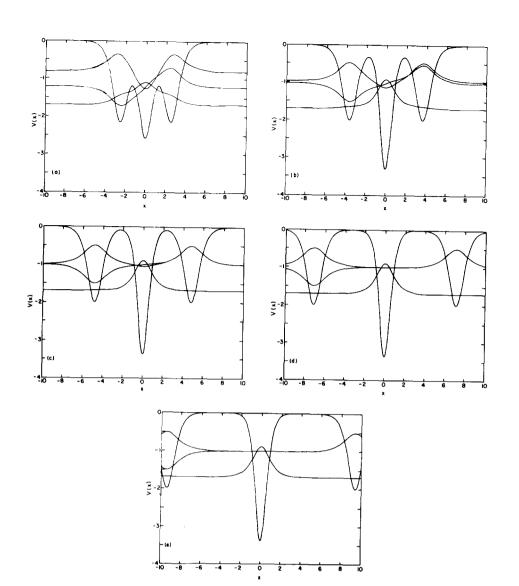


Fig. 2. Evolution of a three-bound-state symmetric, reflectionless potential as two levels become degenerate. In addition to the potential, the normalized wave functions are plotted as $\phi_i(x) + E_i$. The potentials are characterized by $\kappa_1 = 1.3$ and (a) $\kappa_2 = 1.1$, $\kappa_3 = 0.9$; (b) $\kappa_2 = 1.01$, $\kappa_3 = 0.99$; (c) $\kappa_2 = 1.001$, $\kappa_3 = 0.999$; (d) $\kappa_2 = 1.00001$, $\kappa_3 = 0.99999$; (e) $\kappa_2 = 1.0000001$, $\kappa_3 = 0.99999999$ 9.

$$\psi_{p}(x) = -\frac{\left[2\kappa_{p}\Pi\left(p, \{N\} - p\right)\right]^{1/2}}{D(x)}$$

$$\times \sum_{S \neq p} (-1)^{\nu(S,p)}\Pi(S, \overline{S} - p)$$

$$\times \sinh\left[x\left(\sum_{m \in S} \kappa_{m} \sum_{n \in \overline{S}p} \kappa_{n}\right)\right] \qquad (p \text{ even}), \quad (2.6)$$

where $\nu(S; p)$ denotes the number of elements of S with indices less than p, and $\{N\} - p$ is the set $1, 2, \ldots, p - 1, p + 1, \ldots, N$. The forms (2.2)–(2.6) are quite suitable for computer evaluation and are rather compact for small values of N. In them the reflection symmetry properties of the potential and wave function are manifest.⁶

B. Applications

As a first application of these relations, let us consider a potential which supports two initially nondegenerate bound states characterized by $\kappa_1 = 1.3$, $\kappa_2 = 0.7$. The resulting potential and the normalized wave functions $\phi_1(x)$ and $\phi_2(x)$ are shown in Fig. 1(a). The potential is a smooth single well, and the bound-state wave functions have the form of typical textbook idealizations. Now let κ_1 and κ_2 both approach the common limit $\kappa_1 = 1 = \kappa_2$. As the levels approach degeneracy, the potential divides into two buckets,

which retreat toward $x = \pm \infty$, carrying with them the quantum-mechanical bound-state probability [Figs. 1(b) -1(f)]. In this special case of a symmetric, reflectionless potential, it can be seen from Eq. (2.3) that for

$$\left|\frac{\kappa_1 - \kappa_2}{\kappa_1 + \kappa_2}\right| \ll 1$$

the individual wells are centered about

$$x_0 = \pm \frac{1}{2\kappa_1} \log \left| \frac{4\kappa_1}{\kappa_1 - \kappa_2} \right|. \tag{2.7}$$

As Fig. 1 suggests, $|x_0|$ becomes infinite as $\kappa_1 \rightarrow \kappa_2$.

The bound-state wave functions become increasingly similar as the eigenvalues approach one another, so that for x > 0, $\phi_1(x) \approx \phi_2(x)$ and for x < 0, $\phi_1(x) \approx -\phi_2(x)$. Over an increasing (and ultimately infinite) range in x, the wave functions vanish. Because for this case of a symmetric potential the linearly dependent eigenstates have opposite parity, neither level can exist in the $\kappa_1 \rightarrow \kappa_2$ limit. All of this is of course entirely in accord with the familiar Wronskian argument. From the inverse scattering exercise we see how this argument is realized for potentials which are constructed from prescribed bound-state energies. A complementary view of the same phenomenon is obtained by considering a potential consisting of two identical buckets of the form (1.5). When the buckets are widely spaced, the

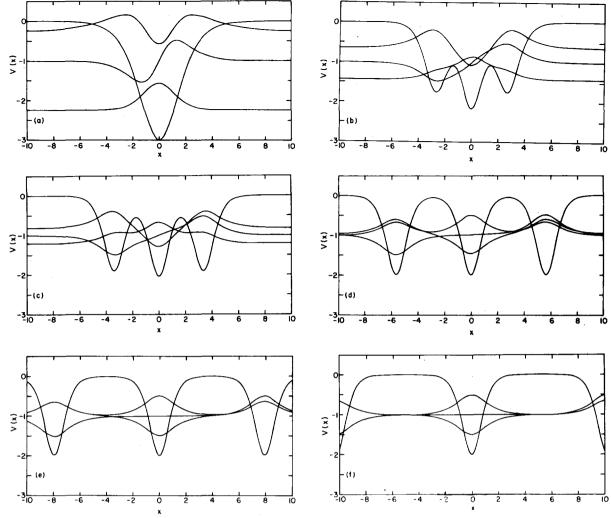


Fig. 3. Evolution of a three-bound-state symmetric, reflectionless potential as the levels become degenerate. In addition to the potential, the normalized wave functions are plotted as $\phi_i(x) + E_i$. The potentials are characterized by $\kappa_2 = 1$ and (a) $\kappa_1 = 1.5$, $\kappa_3 = 0.5$; (b) $\kappa_1 = 1.2$, $\kappa_3 = 0.8$; (c) $\kappa_1 = 1.1$, $\kappa_3 = 0.9$; (d) $\kappa_1 = 1.01$, $\kappa_3 = 0.99$; (e) $\kappa_1 = 1.001$, $\kappa_3 = 0.99$; (f) $\kappa_1 = 1.0001$, $\kappa_3 = 0.999$.

bound-state levels are nearly degenerate. As the buckets are brought closer together, tunneling from one to the other becomes more likely with the result that the two levels split apart, the odd parity state moving up and the even parity state moving down. What is gained from the inverse scattering exercise is some insight into how the transition from nondegeneracy to degeneracy takes place.

In the presence of (N-2) additional nondegenerate bound states, the result of the collision of two levels is qualitatively the same. Two wells emerge from the N-bound-state potential, and retreat in symmetric fashion to $x=\pm\infty$ as the degeneracy becomes increasingly exact. They leave behind a symmetric reflectionless potential which supports only the N-2 nondegenerate levels. If κ_p approaches κ_{p+1} , the retreating buckets are calculated in the general case to be centered at

$$x_0 = \pm \frac{1}{2\kappa_p} \log \left(\frac{4\kappa_p}{|\kappa_p - \kappa_{p+1}|} \prod_{n \neq p, p+1} \left| \frac{\kappa_n + \kappa_p}{\kappa_n - \kappa_p} \right| \right). \quad (2.8)$$

To illustrate this in a simple case, we show in Fig. 2 the evolution of a three-bound-state potential with $\kappa_1 = 1.3$ and $\kappa_2, \kappa_3 \rightarrow 1$. The potential well that remains behind after the

degeneracy has been attained is the one-level potential (1.5).

Variations of this behavior may be observed when more than two levels are made to approach one another. As an example, Fig. 3 depicts the development of a three-bound-state potential as the lowest and highest levels converge on the middle one. The potential decomposes into three buckets, two of which recede symmetrically to $x = \pm \infty$. The third bucket remains centered at x = 0 and approaches the form (1.5). Each of the bound-state wave functions also becomes trichotomous. After the receding lumps have disappeared, the remaining parts of the wave functions are all proportional, as required by the Wronskian argument. A single linearly independent solution thus survives.

III. SUMMARY

Potentials and bound-state wave functions constructed using inverse scattering techniques have been shown to provide a novel perspective upon the question of degeneracy in one-dimensional quantum mechanics. Examples have been given to show how bound-state solutions to the Schrödinger equation become linearly dependent and, in

the case of coincident levels of opposite parity, may disappear entirely. The procedures described here for constructing potentials supporting prescribed bound-state spectra may themselves be of instructional value, when implemented on computer systems with graphics capabilities. In such a setting, many possibilities for independent study at the undergraduate level suggest themselves. An obvious extension of the examples we have presented would involve the study of bands of several nearly degenerate levels.

ACKNOWLEDGMENTS

Part of the work reported here was carried out when J.L.R. and J.F.S. were visitors in the Theoretical Physics Department at Fermilab. J.F.S. also wishes to acknowledge the hospitality of the University of Minnesota. We wish to thank H. Miyazawa for helpful discussions. This research was supported in part by the U.S. Department of Energy under Contract No. E(11-1)-1764. Fermilab is operated by Universities Research Association under contract with the U.S. Department of Energy.

- ^aOn leave of absence from School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455.
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