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## A simple model for inelastic scattering

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A simple model for inelastic scattering may be obtained by suitably generalizing scattering from a square well. The generalization introduces matrices into the quantum-mechanical scattering equations. These equations may be solved exactly to give an explicit expression for the scattering matrix. In this paper we first describe and solve the model, and then discuss the results it predicts for a simple example. We will see that even a simple inelastic system can exhibit rich scattering behavior.

### I. INTRODUCTION

In a simple collision, two particles approach each other, interact or react in some way, and then fly apart. The scattering event may be designated elastic, inelastic, or reactive, depending on what changes take place during the collision. Elastic scattering, in which at most the directions of motion of the two particles change, is the easiest to study, and most elementary scattering theory is concerned with elastic collisions. Reactive scattering, in which the identities of the colliding particles change, is the most complex and interesting process, but is quite difficult to treat. Between the elastic and reactive limits lies inelastic scattering, in which the internal states of one or both particles change. The particles might be nuclei, atoms, or molecules. Thus typical inelastic scattering processes involve Coulomb excitation of nuclei, electronic excitation of atoms, and rotational or vibrational excitation of molecules.

In this paper we will develop a model for the inelastic scattering of two particles. It is not meant to simulate the features of specific inelastic processes like those mentioned above, but rather to incorporate the important features shared by all inelastic problems. One specific model for inelastic scattering has already been discussed in this Journal<sup>1</sup>; it treated the colinear scattering of a particle and a harmonic oscillator. By foregoing detailed specification of the system, we obtain a model that is much more general, yet no more complex.

Basically, the model we will consider is a generalization of scattering from a finite radial square well<sup>2</sup> in which the equations are rewritten in terms of matrices. The necessary background for this development is an acquaintance with elementary matrix operations (diagonalization and inversion)<sup>3</sup> and with the basic concepts of scattering in three dimensions.<sup>4</sup> Optionally, with some previous computer experience it is not hard to write a program to evaluate the expressions for the scattering behavior that we will derive; the problem is ideal for computer study. It is hoped that this treatment can serve as a pedagogically sound way of

introducing inelastic scattering at the advanced undergraduate level.

The square well is perhaps the simplest model for elastic scattering. It is straightforward to formulate and solve exactly the quantum-mechanical scattering equations. The model displays several important quantum effects, such as interference and tunneling; it also serves as a good example for some standard approximation techniques, such as the perturbation and semiclassical methods. For these reasons the square well is, along with the harmonic oscillator and the hydrogen atom, one of the most important examples in elementary quantum mechanics.<sup>5</sup>

The inelastic square well also serves as an illuminating example, but for somewhat different reasons. Its value lies in the fact that it combines several different familiar techniques to achieve an understanding of a relatively complex and physically interesting system.<sup>6</sup> Like the anharmonic oscillator and the helium atom, the inelastic square well builds upon a simpler system, and like them it both demands some extra work and offers some new insights.

To construct the model, we start with an ordinary three-dimensional square well, which is used to approximate the basic radial potential between two particles. However, these particles are now understood to have internal states that are coupled during a collision. To keep the model as simple as possible, we take the coupling to be proportional to the radial potential—hence zero outside the well and constant within. The inelastic square-well model is therefore completely specified by the depth and width of the well, the particle energy levels, and the coupling coefficients of the internal states.

The coupling coefficients form a matrix, with row and column numbers specifying the initial and final states. We can form another matrix, labeled in the same way, whose entries are the probability amplitudes for transitions between states as the result of a collision. This is the so-called scattering matrix, or *S* matrix. It can be derived from the solutions to the Schrödinger equation, and is closely connected to the observed scattering behavior (e.g., cross

sections).

An explicit expression for the  $S$  matrix of the inelastic square well will be obtained below. It is recommended that a simple computer program be written to do the algebra for some sample cases. This program can then be used to survey the scattering behavior as a function of the system parameters, such as the total energy and the depth of the potential well. To complement such numerical studies, it is instructive to locate the sources of the major features of the scattering behavior in the explicit expressions. We will carry out such an analysis for a simple example later in this paper. First, however, we devote Sec. II to the formulation of the scattering problem for the inelastic square well, and Sec. III to its solution.

## II. SCHRÖDINGER EQUATION

In an inelastic collision the internal state of the pair of particles changes. We start by considering these internal states in the absence of translational motion and the interaction energy. The states are eigenfunctions of an internal Hamiltonian  $h(\mathbf{r})$ :

$$h(\mathbf{r})\Gamma_n(\mathbf{r}) = \epsilon_n\Gamma_n(\mathbf{r}), \quad (1)$$

where  $\mathbf{r}$  stands for a complete set of internal coordinates and  $n$  designates the internal state or "channel" of the system. (Note that we are considering the pair of particles as one system.) For purposes of the model, this is as far as we have to go in describing the internal problem, as will become clear below. We therefore proceed immediately to the scattering problem.

The complete Schrödinger equation, in the center-of-mass coordinate frame, reads

$$H(\mathbf{R},\mathbf{r})\Psi_n(\mathbf{R},\mathbf{r}) = E\Psi_n(\mathbf{R},\mathbf{r}), \quad (2)$$

where

$$H(\mathbf{R},\mathbf{r}) = h(\mathbf{r}) - (\hbar^2/2\mu)\nabla_{\mathbf{R}}^2 + V(\mathbf{R},\mathbf{r}). \quad (3)$$

Here  $\mathbf{R} = (R, \theta, \phi)$  is the relative separation vector,  $E$  is the total energy, and  $\mu$  is the reduced mass. The first term in the Hamiltonian describes the internal motions, the second gives the relative translational energy, and the third is the interaction potential that is responsible for the inelastic scattering. We assume the following form for this potential:

$$V(\mathbf{R},\mathbf{r}) = V_{\text{well}}(R)V_{\text{couple}}(\mathbf{r}), \quad (4)$$

where

$$V_{\text{well}}(R) = \begin{cases} V_0 & (R < R_0) \\ 0 & (R > R_0). \end{cases} \quad (5)$$

These equations define the model. They describe a spherically symmetric well (for  $V_0 < 0$ ), within which the internal states are coupled by a function that shows no further dependence on the distance between the particles.

Now consider the wave functions  $\Psi_n$ . The index  $n$  is used to indicate that this solution corresponds to scattering from channel  $n$ . Of course, because of the coupling, the total wave function will in general have contributions from all channels. It is convenient to separate these contributions by making an expansion in terms of the internal states  $\Gamma_m(\mathbf{r})$ :

$$\Psi_n(\mathbf{R},\mathbf{r}) = \sum_m \Gamma_m(\mathbf{r})\chi_{m'n}(\mathbf{R}). \quad (6)$$

We may interpret  $\chi_{m'n}$  as the component of the total wave function in channel  $m'$ , assuming an incident wave in chan-

nel  $n$ . We immediately make a further expansion, this time in terms of the Legendre polynomials  $P_l(\cos\theta)$ , in order to separate contributions from different angular momenta:

$$\chi_{m'n}(\mathbf{R}) = \frac{1}{R} \sum_{l=0}^{\infty} \psi'_{m'n}(R) P_l(\cos\theta). \quad (7)$$

Such a "partial wave" expansion is also used in the treatment of elastic scattering from spherically symmetric potentials.<sup>4</sup>

These two expansions will enable us to perform a separation of variables that reduces the original many-dimensional Schrödinger equation to a set of one-dimensional equations. To perform this reduction, insert Eqs. (3)–(7) into Eq. (2), multiply by  $\Gamma_m^*(\mathbf{r})P_l(\cos\theta)$ , and integrate over all coordinates except  $R$ . The result, after a little work, is<sup>1,7</sup>

$$\left( \frac{d^2}{dR^2} + k_m^2 - \frac{l(l+1)}{R^2} \right) \psi'_{mn}(R) = \begin{cases} V_0 \sum_m U_{mm'} \psi'_{m'n}(R) & (R < R_0) \\ 0 & (R > R_0). \end{cases} \quad (8a)$$

$$(8b)$$

Here  $k_m^2 = (2\mu/\hbar^2)(E - \epsilon_m)$  is the square of the wave vector for internal state  $m$ , and  $U_{mm'} = (2\mu/\hbar)(m'|V_{\text{couple}}|m)$  is the matrix element coupling internal states  $m$  and  $m'$ . Note that the term  $l(l+1)/R^2$  is a centrifugal potential that arises from the angular part of  $\nabla_{\mathbf{R}}^2$ . At this point we can forego explicit reference to both the internal states  $\Gamma_m$  and the coupling potential  $V_{\text{couple}}$ , retaining only a constant coupling matrix  $U$ . Quantum mechanics assures us that specification of the matrix elements alone still uniquely prescribes the problem.

The Schrödinger equation for  $\Psi(\mathbf{R},\mathbf{r})$  has been transformed into sets of coupled equations for the  $\psi'_{mn}(R)$ —one set for each  $l$ . We now proceed to solve these equations.

## III. SCATTERING MATRIX

Perhaps the most straightforward way to solve the elastic square-well problem is the following: First, write the wave function in each region ( $R < R_0$  and  $R > R_0$ ) as a linear combination of independent solutions with unknown coefficients; then impose conditions (boundary, normalization, and continuity) in order to fix these coefficients. The same method can be used here, but it must be combined with a method for handling the inelastic coupling.

Coupling is most easily dealt with by expressing the problem in terms of matrices. We can construct matrices from objects with two subscripts in the obvious way, by letting the first subscript designate the row and the second the column; this gives us  $U$  and  $\psi'(R)$ , for example. We can also construct diagonal matrices from objects with one subscript, by placing these along the diagonal and zeros elsewhere; in this way we obtain  $k^2$  and  $\Gamma(\mathbf{r})$ . There will be no confusion if we omit reference to  $l$  and  $R$  in our matrix notation, and write, for example,  $\psi$  in place of  $\psi'(R)$ . We will need to perform one matrix diagonalization and one matrix inversion in order to solve the inelastic square-well problem.

Before proceeding we give a precise definition for the  $S$  matrix<sup>7</sup>: An element  $S_{nm}^l(E)$  is the probability amplitude for scattering between incoming channel  $n$  and outgoing channel  $m$  at angular momentum  $l$  and energy  $E$ .

Explicitly,

$$\psi'_{mn}(R) \rightarrow \delta_{nm} F'_m(R) + S'_{nm} G'_m(R), \quad (9)$$

where  $F'_m$  and  $G'_m$  are incoming and outgoing solutions to Eq. (8b),

$$F'_m(R) \rightarrow k_m^{-1} e^{-i(k_m R + \delta_l)}, \quad (10)$$

$$G'_m(R) \rightarrow k_m^{-1} e^{+i(k_m R + \delta_l)}.$$

Here the factor  $k_m^{-1}$  normalizes the flux, or rate of collisions, and the phase  $\delta_l = -(l+1)\pi/2$  arises from the centrifugal potential. (We will present more explicit forms for  $F'_m$  and  $G'_m$  later.) With this definition of the  $S$  matrix, the partial cross sections  $\sigma'_{nm}$  and total measurable cross sections  $\sigma_{nm}$  are given by<sup>7</sup>

$$\sigma_{nm} = \sum_{l=0}^{\infty} \sigma'_{nm} = (\pi/k_n^2) \sum_{l=0}^{\infty} (2l+1) |S'_{nm} - \delta_{nm}|^2. \quad (11)$$

We now return to the problem of solving Eqs. (8). Denoting differentiation with respect to  $R$  by a prime, we can rewrite them in matrix form

$$\psi'' + W\psi - \frac{l(l+1)}{R^2} \psi = 0 \quad (R < R_0), \quad (12)$$

$$\psi'' + k^2 \psi - \frac{l(l+1)}{R^2} \psi = 0 \quad (R > R_0), \quad (13)$$

where  $W = k^2 - V_0 U$ . The off-diagonal elements of  $W$  have the effect of coupling the entries of  $\psi$  in the interior region. However, we can uncouple them by an appropriate change of basis.<sup>3</sup> Indeed, we can always find an orthogonal matrix  $P$  such that  $d^2 = P^T W P = P^{-1} W P$  is a diagonal matrix. If we now let

$$\varphi = P^T \psi, \quad (14)$$

then we can rewrite Eq. (12) in its diagonalized or uncoupled form

$$\varphi'' + d^2 \varphi - \frac{l(l+1)}{R^2} \varphi = 0 \quad (R < R_0). \quad (15)$$

We must now solve Eqs. (13) and (15). These are second-order differential equations, so their solutions can be written as linear combinations of two independent functions. For the last equation we take these to be

$$\begin{aligned} J'_m(R) &= \sqrt{(d_m) R} j_l(d_m R), \\ N'_m(R) &= \sqrt{(d_m) R} n_l(d_m R), \end{aligned} \quad (16)$$

where  $j_l$  and  $n_l$  are spherical Bessel functions, the same ones that arise in the elastic scattering problem<sup>4</sup>; they differ from the usual Bessel functions. The only specific information we will need about them is that the  $n_l$  diverge at the origin, while the  $j_l$  do not. Away from the origin  $J'_m$  and  $N'_m$  behave like cosines and sines. In the exterior region it is more convenient to use functions that behave like plane waves. These may be written in terms of the complex functions  $h_l^+ = j_l + in_l$  and  $h_l^- = j_l - in_l$ :

$$F'_m(R) = \sqrt{(k_m) R} h_l^+(k_m R), \quad (17)$$

$$G'_m(R) = \sqrt{(k_m) R} h_l^-(k_m R).$$

We can now solve Eqs. (13) and (15) by analogy with an ordinary square-well problem. We start by writing the wave function in each region as a linear combination of independent solutions with unknown coefficients:

$$\begin{aligned} \varphi'_{mn}(R) &= A'_{nm} J'_m(R) + B'_{nm} N'_m(R) \quad (R < R_0), \\ \psi'_{mn}(R) &= C'_{nm} F'_m(R) + D'_{nm} G'_m(R) \quad (R > R_0). \end{aligned} \quad (18)$$

Next we impose conditions to fix the coefficients. First, the boundary condition that the wave functions not diverge at the origin requires that  $B'_{nm} = 0$ . Second, from Eq. (9) we obtain the normalization condition  $C'_{nm} = \delta_{nm}$  and the identification  $D'_{nm} = S'_{nm}$ . So far, then, we have reduced Eqs. (18) to the following:

$$\begin{aligned} \varphi &= J A^T \quad (R < R_0), \\ \psi &= F + G S^T \quad (R > R_0). \end{aligned} \quad (19)$$

Finally, to relate the equations for  $\varphi$  and  $\psi$  and finish our derivation, we must invoke the continuity condition that the wave functions and their first derivatives be continuous at the boundary between the two regions. Denoting evaluation at  $R = R_0$  by a subscript 0, this double condition reads

$$P\varphi_0 = \psi_0, \quad (20)$$

$$P\varphi'_0 = \psi'_0.$$

Substituting in the expressions from Eqs. (19) we find

$$P J_0 A^T = F_0 + G_0 S^T, \quad (21)$$

$$P J'_0 A^T = F'_0 + G'_0 S^T.$$

This is a set of two matrix equations in two matrix unknowns,  $A$  and  $S$ . They can be solved like ordinary algebraic equations, provided we remember that matrices do not in general commute. Solving for  $S$ , we have the final result

$$S = -(Q F_0 - F'_0)(Q G_0 - G'_0)^{-1}, \quad (22)$$

where  $Q = P J' J^{-1} P^T$ .

#### IV. APPLICATION

In this section we will look at the scattering behavior exhibited by a weakly coupled two-state system specified by the conditions

$$\begin{aligned} R_0 &= 1, & -500 < V_0 < 0, \\ \epsilon_1 &= 0, & U = \begin{pmatrix} 1.0 & 0.1 \\ 0.1 & 1.0 \end{pmatrix}, \\ \epsilon_2 &= 200, & \end{aligned} \quad (23)$$

(Throughout this section, lengths are given in units of  $R_0$  and energies in units of  $\hbar^2/2\mu R_0^2$ .) The total energy of the system is taken to be 400. Because the off-diagonal (inelastic) elements of the coupling matrix  $U$  are small compared to the diagonal (elastic) ones, elastic scattering will dominate, and inelasticity will act as a perturbation. Keeping this in mind will simplify the interpretation of the observed scattering behavior. This set of parameters was chosen for purposes of illustration; other choices could be used to simulate real inelastic collisions.

To calculate the scattering behavior we must evaluate the expression in Eq. (22). In the example all matrices are  $2 \times 2$ , so that the diagonalization and inversion that are required could be performed by hand. However, a computer program is almost indispensable for repeated evaluations, and for problems with more than two channels. Given subroutines to diagonalize and invert matrices and to evaluate Bessel functions (all of which are usually included in libraries of numerical algorithms), it is not difficult to write such a program. Below we will present some typical results from such a program. We will look at both elastic and inelastic scattering, in each case calculating the partial

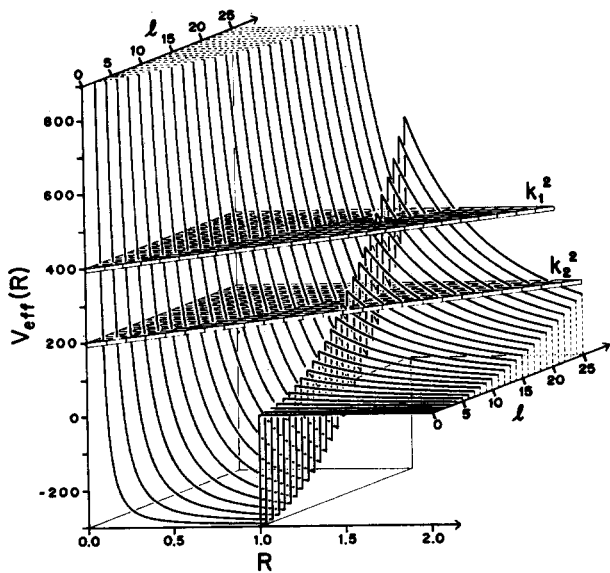


Fig. 1. Effective potentials for  $0 < l < 25$ ,  $V_0 = -300$  along with surfaces at  $k_1^2 = 400$  and  $k_2^2 = 200$  representing the energy available in each channel.

cross sections  $\sigma_{nm}^l$  as functions of the angular momentum  $l$  and well depth  $V_0$ . It is convenient to think of these parameters as determining an effective potential that includes a centrifugal term<sup>7</sup>:

$$V_{\text{eff}}(R) = V_{\text{well}}(R) + V_{\text{cent}}(R) = \begin{cases} V_0 + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{R^2} & (R < R_0) \\ \frac{\hbar^2}{2\mu} \frac{l(l+1)}{R^2} & (R > r_0). \end{cases} \quad (24)$$

Some effective potentials are plotted in Fig. 1; also shown are sections of planes representing the energies  $k_m^2$  available in the two channels. Note that as the angular momentum is increased, the centrifugal barrier surrounding the well eventually exceeds the available energy, rendering scattering classically forbidden; another way of saying this is that the impact parameter  $b = l/k_m$  eventually exceeds the well radius, so that the particles simply miss each other. This first happens for  $l = 20$  in channel 1 and for  $l = 14$  in channel 2. Wave functions in both channels for the inter-

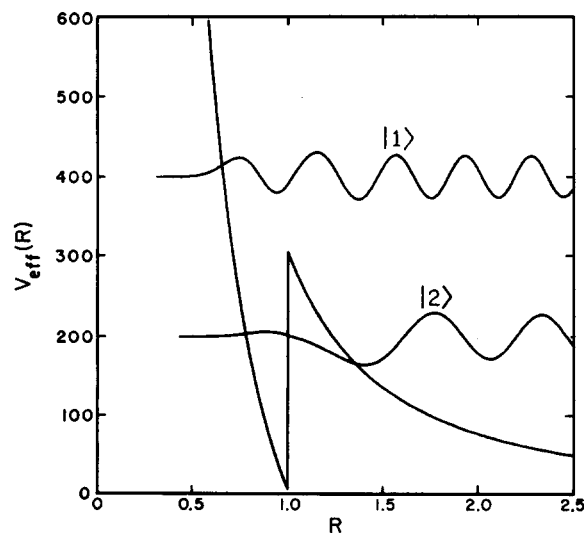


Fig. 2. Effective potential for  $l = 17$ ,  $V_0 = -300$  along with real-valued wave functions in each channel.

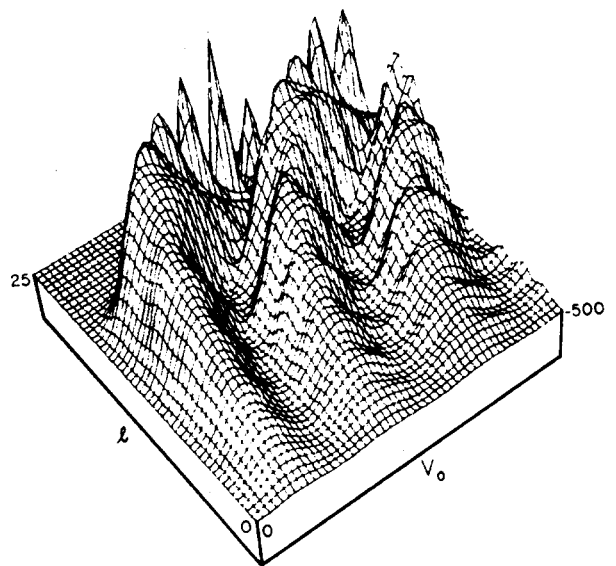


Fig. 3. Elastic partial cross sections  $\sigma'_{11}$  as a function of  $l$  and  $V_0$ ; maximum value plotted is  $1.386R_0^2$ .

mediate case  $l = 17$  are plotted in Fig. 2. The nonzero amplitude of the channel-2 wave function in the classically forbidden well region is evidence of quantum-mechanical tunneling.

The elastic scattering behavior in channel 1 is plotted in Fig. 3. We may ignore the effects of inelasticity in discussing the general features of this plot. The overall waviness—that is, the variation in the magnitudes of the partial cross sections as the angular momentum and well depth are varied—may be attributed to an oscillation between constructive and destructive interference of the incident and scattered waves.<sup>8,9</sup> Modulating this oscillatory behavior is an amplitude factor, which appears to increase steadily with the angular momentum until it falls rather abruptly to zero. The steady increase is a geometrical effect, arising because the effective target area corresponding to an angular momentum  $l$  increases as  $2l + 1$ .<sup>10</sup> The abrupt drop occurs around  $l = 20$  at the transition from classically allowed to classically forbidden scattering.

The two factors just discussed fail to account for the large spikes in the background of Fig. 3. These are located in the domain of classically forbidden scattering, which means that scattering is achieved only by tunneling of the

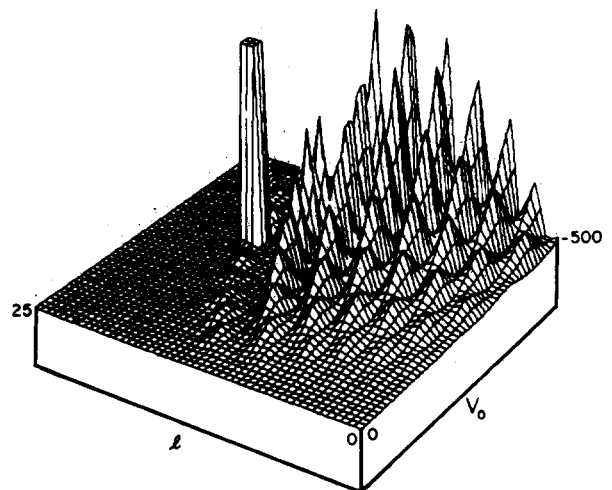


Fig. 4. Inelastic partial cross sections  $\sigma'_{12}$  as a function of  $l$  and  $V_0$ ; maximum value (at  $l = 18$ ,  $V_0 = 300$ ) is  $0.1608R_0^2$ ; maximum value plotted is  $0.0237R_0^2$ .

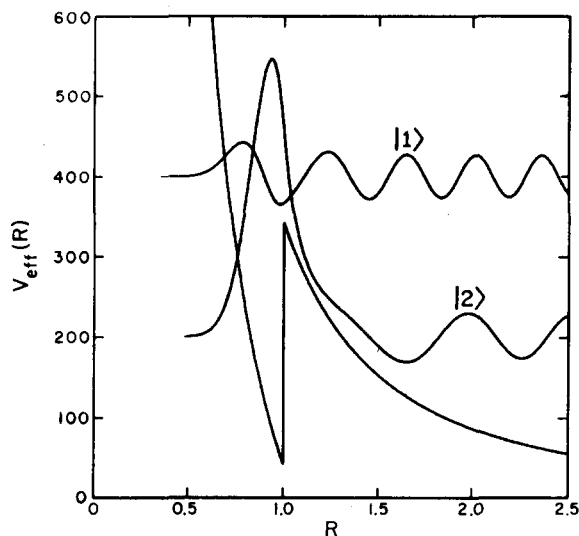


Fig. 5. Effective potential for  $l = 18$ ,  $V_0 = -300$  along with wave functions in each channel plotted at their respective energies. The wave function in channel 2 clearly demonstrates resonant behavior.

incident wave through the centrifugal barrier to the region of the well. Nevertheless, for some combinations of  $l$  and  $V_0$ , there is a tendency for the incident wave to excite a standing wave in the well, leading to a large amplitude in this forbidden region. This effect, which is sometimes described as resonance with a "quasibound level" of the effective potential, accounts for the spikes.<sup>11</sup>

The inelastic scattering behavior is plotted in Fig. 4. Again we can interpret the behavior by considering inelasticity to be a small perturbation; now, however, it is precisely the value of this perturbation that we are interested in. The regular array of maxima on the right results from simultaneous oscillatory behavior in two different directions of the  $l$ - $V_0$  plane. This can be traced to the perturbation theory result that the cross sections depend on the overlap of the unperturbed undulating wave functions in the two channels. The envelope of the peaks is now governed by two amplitude factors: a factor  $2l + 1$ , as in the elastic cross sections, and a factor  $V_0^2$  from perturbation theory.

Again in Fig. 4 there is resonant behavior in the classically forbidden domain, in this case in the form of one very large partial cross section at  $l = 18$ ,  $V_0 = -300$ . (The spike has been truncated at about 15% of its full height in the figure.) Like the forbidden spikes in the elastic cross section plot, it is a consequence of a resonance with a quasibound level of the effective potential. This resonant situation is illustrated in Fig. 5, which should be compared with Fig. 2. In both cases the high centrifugal barrier renders the well region classically inaccessible to channel 2, but quantum-mechanical tunneling temporarily overrides this classical restriction in the case of resonance.

This concludes our brief survey of the two-state example. Among the avenues available for further investigation, we recommend the following: First, there are many insights to be gained by varying other important system parameters, such as the total collision energy and the inelastic

coupling strength. At a more formal level, the expression for the  $S$  matrix, Eq. (22), can be manipulated to reveal its properties (e.g., unitarity) and its limiting cases (e.g., small inelastic coupling).<sup>6</sup> The model can also be used to study approximation techniques; this can be done either empirically, by comparing approximate with exact results, or analytically, by observing the modifications to the exact expressions introduced by the approximations.

## V. CONCLUSION

In this paper we have studied a model for inelastic scattering that can be solved by combining a few techniques familiar from elementary quantum mechanics. The simplicity of the problem and its solution, however, do not preclude interesting scattering behavior. Indeed, many phenomena observed in real inelastic collisions are already exhibited by this model. The inelastic square well is useful at both the educational and research levels, and can be used as a means to bridge the two.

## ACKNOWLEDGMENT

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<sup>7</sup>M. S. Child, *Molecular Collision Theory* (Academic, New York, 1974), pp. 91-97.

<sup>8</sup>This can be understood more fully by considering the phase shifts  $\eta'_n$ . These are related to the diagonal elements  $S'_{nn}$  of the  $S$  matrix by  $S'_{nn} \approx \exp(2i\eta'_n)$ . Substituting this into Eq. (11), we find that  $\sigma'_{nn} \propto \sin^2 \eta'_n$ . Hence the valleys in Fig. 3 correspond to phase shifts of  $0, \pi, 2\pi, \dots$ , while the ridges correspond to phase shifts of  $\pi/2, 3\pi/2, \dots$

<sup>9</sup>P. H. E. Meijer and J. L. Repace, *Am. J. Phys.* **43**, 428 (1975).

<sup>10</sup>The "effective target" is an annulus whose inner and outer radii are the minimum and maximum impact parameters leading to angular momentum  $l$ . These are  $b_{\min} = l/k_1$  and  $b_{\max} = (l+1)/k_1$ . The area of this annulus is  $\pi b_{\max}^2 - \pi b_{\min}^2 = (2l+1)\pi/k_1^2$ . This accounts for the remaining factors in Eq. (11).

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*Equipped with his five senses, man explores the universe around him and calls the adventure Science.*

Edwin Powell Hubble