

was not observed in the inelastic proton-proton scattering experiments the momentum transfers were larger than those included in the ( $p, p\pi^+$ ) reaction.

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## Intermediate-State Theory of Single-Particle Resonances\*

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The  $d_{3/2}$  state in oxygen is observed as a very sharp scattering resonance in  $O^{16}(n,n)O^{16}$ . The state is a "virtual" state, therefore, and its inclusion among the single-particle discrete states employed in the shell-model description of states of  $O^{16}$  requires some justification. In this paper a unified reaction theory recently given by one of the authors is used as the basis of a description in which the resonance is described as arising from the virtual transitions into a true bound state. The continuum states of this description are nonresonant because the continuum  $d_{3/2}$  resonance is replaced by a bound  $d_{3/2}$  state which plays the role of a new "doorway state." This description leads to the conventional shell-model description of the particle-hole resonances of  $O^{16}$  and simplifies the description of the interaction between virtual and bound states.

### I. INTRODUCTION

THE relationship between the single-particle resonance of a shell-model potential and resonances associated with particle-hole states is extremely crucial to a consistent, indeed a correct, calculation of a nuclear-reaction cross section. In fact, a considerable amount of insight into the correctness or the usefulness of a particular formulation of reaction theory can be gained from the way in which single-particle resonances are handled, particularly when they occur near thresholds. A resonance associated with any nonzero value of angular momentum becomes increasingly narrow if the resonance energy is decreased. Not only does the resonance then become more difficult to distinguish experimentally from a "compound nuclear resonance," but appreciable configuration mixing with discrete shell-model states may make this distinction less meaningful. The single-particle resonance is parceled out among more complex levels (e.g., two-particles, one-hole states) in precisely the manner discussed by Lane, Thomas, and Wigner.<sup>1</sup> We shall learn from our analysis of a low-lying resonance that in this situation the "doorway state" is a single-particle state, or one quasiparticle state.

The considerations of this paper are based on the shell-model reaction theory outlined in earlier papers,<sup>2</sup> and the results of a specific calculation will be presented for the  $d_{3/2}$  resonance in the elastic scattering of neutrons on  $O^{16}$ . For the purpose of testing a reaction theory the situation which obtains in the nuclei with  $A=15$ , 16, and 17 is nearly ideal and this paper is preliminary to a more extensive survey of the reactions involving these nuclei.

The  $d_{3/2}$  resonance observed in  $O^{16}(n,n)O^{16}$  occurs at 0.934 MeV with a width of only 90 keV. This width is approximately what one should expect for a  $d$ -wave resonance produced by the average Hartree field in this nucleus. A corresponding resonance also occurs in proton scattering on  $O^{16}$ . Since these resonances arise from the average potential generated by  $O^{16}$ , we should also expect to find  $d_{3/2}$  resonances in the nucleon scattering on  $O^{15}$  and  $N^{15}$ . In the simplest shell model these nuclei are described as belonging to the configuration  $1p_{1/2}^{-1}$ , a hole in the  $1p_{1/2}$  shell. Overlooking the distinction between bound and continuum states for the moment, we could describe the resonance observed in nucleon scattering on  $N^{15}$  and  $O^{15}$  as "belonging to the configuration  $p_{1/2}^{-1} d_{3/2}$ ." Similarly if elastic scattering could be performed on  $O^{15}$  and  $N^{15}$  in their first excited state

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<sup>1</sup> A. M. Lane, R. G. Thomas, and E. P. Wigner, *Phys. Rev.* **98**, 693 (1955).

<sup>2</sup> W. M. MacDonald, *Nucl. Phys.* **54**, 393 (1964); **56**, 636, 647 (1964).

( $p_{3/2}^{-1}$  in the shell model), resonances would be observed which could be described as "belonging to  $1p_{3/2}^{-1} d_{3/2}$ ."

Now actually a central potential can only describe nucleon scattering in the lowest approximation, and therefore even the continuum states  $p_{1/2}^{-1} d_{3/2}$  and  $p_{3/2}^{-1} d_{3/2}$  are not eigenstates of the complete Hamiltonian with a real two-body interaction. A diagonalization of the full Hamiltonian using just these continuum states will yield eigenstates which are a linear superposition of these two configurations. Such a calculation is equivalent to finding the inelastic scattering which is produced by the two-body interaction in a direct interaction.

The calculation of the nucleon scattering is further complicated, however, by the fact that discrete bound states belonging to the configurations  $p_{1/2}^{-1} d_{5/2}$ ,  $p_{3/2}^{-1} d_{5/2}$ ,  $p_{1/2}^{-1} 2s_{1/2}$ , and  $p_{3/2}^{-1} 2s_{1/2}$  also interact strongly with the resonant continuum states (which have large amplitudes over the nuclear volume). In the shell-model calculations of the bound and the "resonant states" of  $O^{16}$  a  $d_{3/2}$  state is included among the particle states from which the particle-hole states are constructed. Since a bound  $d_{3/2}$  state does not actually exist in  $O^{17}$ , it is clear that such a state is actually a representative of the  $d_{3/2}$  single-particle resonance. The conventional shell-model diagonalization can then be viewed in some sense as an approximate diagonalization of the full Hamiltonian on the discrete shell-model states and on certain resonant continuum states.<sup>3</sup>

This description of the role of resonant continuum states is accurate, but it does not readily lend itself to an accurate calculation of the detailed shape of resonances, particularly when two or more resonances overlap. Therefore we shall develop another formulation which does provide a basis for such analyses. The motivation for the development of the next section is provided by the observation that a slightly deeper  $d_{3/2}$  potential would provide a bound  $d_{3/2}$  state. This state would then give discrete states of the configurations  $p_{1/2}^{-1} d_{3/2}$  and  $p_{3/2}^{-1} d_{3/2}$ . The interaction of these states would then easily be found by diagonalizing the Hamiltonian on this discrete set. We shall now proceed to show how to remedy the failure of nature to present us with this simpler situation.

## II. RESONANCE THEORY OF SINGLE-PARTICLE SCATTERING

We apply the formalism of the shell-model reaction theory<sup>2</sup> to the analysis of low-energy single-particle resonance. Let  $U$  be a central potential which describes the elastic scattering and which therefore fits the resonance. For the purpose of the subsequent analysis we regard the cross section given by  $U$  as exact. The  $T$ -matrix element is

$$T(\mathbf{k}', \mathbf{k}) = \langle \Phi_{\mathbf{k}'} | U | \chi_{\mathbf{k}}^+ \rangle, \quad (1)$$

<sup>3</sup> R. A. Ferrell, *Eastern Theoretical Physics Conference*, edited by M. E. Rose (Gordon and Breach Science Publishers, New York, 1963).

where  $\Phi_{\mathbf{k}'}$  is a plane wave of momentum  $\mathbf{k}'$  and  $\chi_{\mathbf{k}}^+$  is the exact scattering wave function for the potential  $U$  with outgoing scattered waves at infinity.

Introduce now the potential  $\hat{U}$  which is sufficiently deeper than  $U$  to possess a bound single-particle state of the same quantum numbers as the sharp resonance of  $U$ . The energy of this state will be denoted by  $E_d (= -E_B$ , the binding energy). Let  $\hat{H} = K + \hat{U}$  be the "model Hamiltonian," and use the scattering states  $\hat{\chi}_{\mathbf{k}}^+$  of  $\hat{H}$  to calculate  $T(\mathbf{k}', \mathbf{k})$ .

Using the equation

$$\chi_{\mathbf{k}}^+ = \hat{\chi}_{\mathbf{k}}^+ + (E^+ - \hat{H})^{-1} \Delta \chi_{\mathbf{k}}^+, \quad (2)$$

where

$$\Delta \equiv U - \hat{U},$$

we can obtain by operator algebra<sup>4</sup>

$$T(\mathbf{k}', \mathbf{k}) = \langle \Phi_{\mathbf{k}'} | \hat{U} | \hat{\chi}_{\mathbf{k}}^+ \rangle + \langle \hat{\chi}_{\mathbf{k}}^- | \mathcal{T} | \hat{\chi}_{\mathbf{k}}^+ \rangle. \quad (3)$$

The "reduced transition operator"  $\mathcal{T}$  is given by the equation

$$\mathcal{T} = \Delta + \Delta (E^+ - \hat{H})^{-1} \mathcal{T}. \quad (4)$$

This equation is the starting point for our development of a resonance theory of single-particle scattering.

Since the potential  $\hat{U}$  will not have a resonance at low energy,  $\mathcal{T}$  is the quantity which introduces a resonance into the scattering amplitude. This resonance can be exhibited explicitly by separating  $\mathcal{T}$  into a nonresonant "effective interaction"  $\mathcal{T}_e$  and a resonant term of the Breit-Wigner form. The  $\mathcal{T}_e$  is defined by the equation

$$\mathcal{T}_e = \Delta + \Delta (E^+ - \hat{H})^{-1} P_e \mathcal{T}_e, \quad (5)$$

where  $P_e$  projects on the continuum states of  $\hat{H}$ . From Eqs. (4) and (5) it follows that

$$\mathcal{T} = \mathcal{T}_e + \mathcal{T}_e P_d (E^+ - \hat{H} - P_d \mathcal{T}_e P_d)^{-1} P_d \mathcal{T}_e, \quad (6)$$

where  $P_d$  projects on the discrete bound state of  $\hat{H}$  which corresponds to the narrow resonance of  $H$ . The  $T$ -matrix amplitude is then given by

$$T(\mathbf{k}', \mathbf{k}) = \langle \Phi_{\mathbf{k}'} | \hat{U} | \hat{\chi}_{\mathbf{k}}^+ \rangle + \langle \hat{\chi}_{\mathbf{k}'}^- | \mathcal{T}_e | \hat{\chi}_{\mathbf{k}}^+ \rangle + \frac{\langle \hat{\chi}_{\mathbf{k}'}^- | \mathcal{T}_e | d \rangle \langle d | \mathcal{T}_e | \hat{\chi}_{\mathbf{k}}^+ \rangle}{E - E_d - S + i(\Gamma_d/2)}. \quad (7)$$

The denominator of the resonance term is defined by

$$S - i\Gamma_d/2 \equiv \langle d | \mathcal{T}_e | d \rangle \quad (8)$$

with  $S$  being called the level shift and  $\Gamma_d$  being the level width of the state. Both  $S$  and  $\Gamma_d$  are dependent upon the energy of the incident nucleon, but at resonance  $E_d + S(E_R) = E_R$ , the resonance energy, and  $\Gamma_d(E_R)$  is the width of the single-particle resonance.

The effective interaction, which determines the resonance energy and width through Eq. (9), is itself non-resonant. In a lowest approximation  $\mathcal{T}_e$  is just equal to

<sup>4</sup> M. Gell-Mann and M. Goldberger, *Phys. Rev.* **91**, 398 (1953).

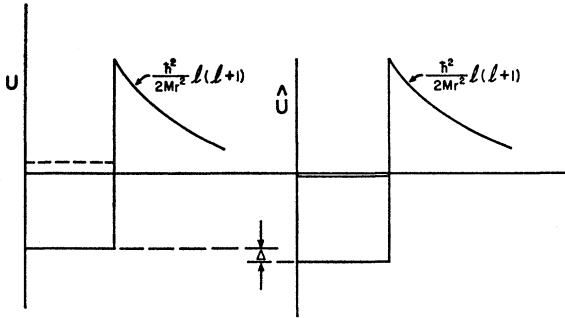


FIG. 1. The potential  $U$  provides the resonant  $d_{3/2}$  scattering cross section which is regarded as exact. The potential  $\hat{U}$  possesses the bound  $d_{3/2}$  state whose displacement by the perturbation  $\Delta = U - \hat{U}$  gives rise to the scattering resonance of  $U$ .

$\Delta$ , the perturbation which pushes the bound state of  $H$  into the continuum and mixes it with the continuum levels of  $H$ . The deviation of  $\mathcal{T}_e$  from  $\Delta$  arises from virtual transitions into continuum states with a consequent modification of the perturbing interaction. The optical theorem for  $\mathcal{T}_e$ ,

$$\text{Im} \mathcal{T}_e = -\pi \mathcal{T}_e P_c \delta(E^+ - \hat{H}) P_c \mathcal{T}_e^\dagger \quad (9)$$

leads to the familiar expression for  $\Gamma_d$

$$\Gamma_d(E) = 2\pi |\langle d | \mathcal{T}_e | \hat{\chi}^+(E) \rangle|^2 \rho(E), \quad (10)$$

where  $\rho(E)$  is the density of states.

As should be anticipated from this view of matters, there is a simple relation between  $S$  and  $\Gamma_d$ . This is easily found by writing the explicit equation for  $\mathcal{T}_e$

$$\mathcal{T}_e = \Delta + \Delta P_c (E^+ - P_c H P_c)^{-1} P_c \Delta. \quad (11)$$

One finds the states  $\psi^+(E)$  which diagonalize  $P_c H P_c$ , i.e.,

$$\langle \psi^+(E') | P_c H P_c | \psi^+(E) \rangle = E \delta(E - E') \quad (12)$$

and uses these to deduce from Eq. (8)

$$\Gamma_d(E) = 2\pi |\langle d | \Delta | \psi^+(E) \rangle|^2 \rho(E), \quad (13)$$

$$S(E) = \langle d | \Delta | d \rangle + (2\pi)^{-1} \mathcal{P} \int dE' \frac{\Gamma_d(E')}{E - E'}, \quad (14)$$

where  $P$  denotes "principal part." The second of these two equations leads to an extremely simple way of calculating the energy-dependent level shift to second order in  $\Delta$ .

### III. NUMERICAL EXAMPLE

This approach was used to describe the  $d_{3/2}$  resonance at 0.934 MeV in elastic neutron scattering from  $O^{16}$ . For simplicity  $U$  was chosen to be a square well whose depth of 29.905 MeV and radius of 3.75 F were chosen to fit the resonance energy and the width at half-maximum, respectively. The well  $\hat{U}$  was also chosen as a square well, and with the same radius as  $U$ . The depth of  $\hat{U}$ , however, was chosen to give a bound state whose

energy was varied from  $E_d = 0$  to  $E_d = -10$  MeV as a check on the sensitivity of the calculation to the choice of  $E_d$ . The results were found to be very insensitive to this quantity and we quote only the results for the calculation with  $E_d = -0.1$  MeV, for which the depth of  $\hat{U}$  was 31.723 MeV. (See Fig. 1.)

After determining  $U$  and  $\hat{U}$ , we first calculated the resonance energy  $E_R = E_d + S$  and  $\Gamma(E_R)$  in the lowest approximation for  $\mathcal{T}_e = \Delta$ . The resonance energy  $E_R^{(1)}$  was found to be  $E_R = 1.009$  MeV and the width at resonance was approximately 100 keV. Since  $\Gamma_d^{(1)}(E)$  is a function of energy from which the second-order correction to the level shift is calculated, its dependence on  $E$  was calculated for the range  $0 \leq E \leq 50$  MeV and is shown in Fig. 2.

The energy shift was then calculated to second order, using the equation

$$S^{(2)} = \langle d | \Delta | d \rangle + (2\pi)^{-1} \mathcal{P} \int dE' \frac{\Gamma_d^{(1)}(E')}{E - E'}. \quad (15)$$

Since the second-order correction given by the last term of this equation is a function of energy, we plot it in Fig. 3. Notice that it is very small and is smoothly varying through the resonance region around 1 MeV. The dependence of  $S^{(2)}$  on the energy, however, means that the resonance energy  $E_R^{(2)}$  must be found by solving the equation

$$E_R^{(2)} - E_d - S(E_R^{(2)}) = 0. \quad (16)$$

The resonance energy is found to be  $E_R^{(2)} = 0.937$  MeV. Within the accuracy of our calculation this is the exact resonance energy.

The width is much more difficult to calculate to second order in  $\Delta$ . Therefore we adopted another method of estimating the effect upon  $\Gamma_d$  of the second-order correction to  $\mathcal{T}_e$ . Make the approximation

$$\mathcal{T}_e = \theta \Delta, \quad (17)$$

where  $\theta$  is a constant whose magnitude is fixed by the exact resonance energy.

$$E_R = 0.934 \text{ MeV} = E_d + \theta \langle d | \Delta | d \rangle. \quad (18)$$

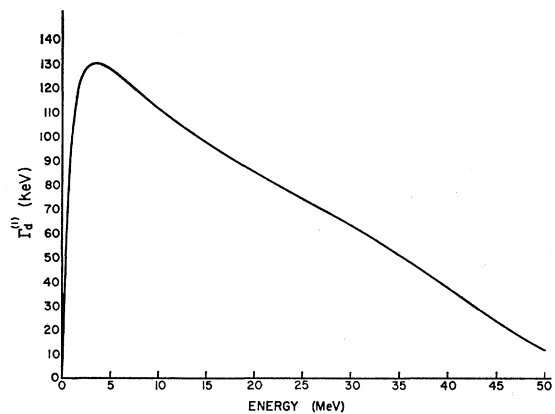


FIG. 2. The width function  $\Gamma_d^{(1)}$  calculated with  $\mathcal{T}_e = \Delta$ .

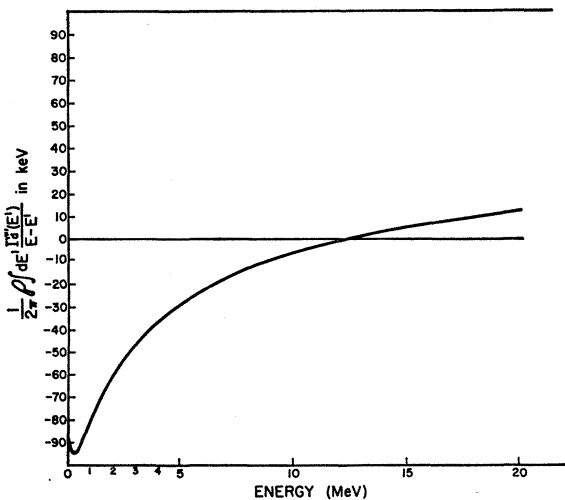


FIG. 3. The second-order correction to the energy of the intermediate state [cf. Eq. (14)] is given as a function of the excitation energy.

The width is then calculated with this approximation to  $\mathcal{T}_e$  and is found to be 90 keV at resonance.

The scattering cross section is proportional to  $\sin^2\delta_{3/2}$ . As a further check on the intermediate-state representation of the resonance cross section, the quantity  $\sin^2\delta_{3/2}$  was calculated from Eq. (7) using  $E_d + S = 0.934$  MeV and  $\Gamma_d(E) = 2\pi |\langle d | \theta \Delta | \chi^+ \rangle|^2 \rho(E)$  for all energies. The result agreed with the exact calculation of  $\sin^2\delta_{3/2}$  to better than 1% except where the cross section was small or rapidly varying. Maximum errors of 3% at such places are obviously a consequence of the crude approximations used in evaluating the resonance amplitude.

#### IV. SUMMARY

The significance of our work is that we have shown that narrow, single-particle resonances are easily treated by introducing a bound state which plays the role of an intermediate state in a Breit-Wigner resonance amplitude. The resonance energy and the width of the state are determined by a one-body effective interaction which is nonresonant. This means that the  $d_{3/2}$  resonance observed in nucleon scattering on  $O^{16}$  can be incorporated into the shell model by introducing a  $d_{3/2}$  bound state, which is then treated on the same footing as the other bound single-particle states. In  $O^{16}$  this  $d_{3/2}$  state can be combined with the  $1p_{3/2}^{-1}$  hole states in the same way as are the  $1d_{5/2}$  and  $2s_{1/2}$  bound states.

The shell-model diagonalization which is to be carried out with a particle-hole interaction will then include in a relatively simple way the effect of configuration interaction between all the resonant continuum states (associated with the  $d_{3/2}$  single-particle resonance) and the bound states.

The only essential modification required of the particle-hole treatment of  $O^{16}$  is the addition of the one-body interaction in the  $1d_{3/2}$  state. In the shell-model diagonalization which leads to the resonant energies and the compound states the only effect of this additional interaction is to "restore" the  $d_{3/2}$  single-particle energy to the position of the resonance observed in  $O^{17}$ . The shell-model calculation is then of same form as that of Elliott and Flowers,<sup>5</sup> Brown,<sup>6</sup> and others.<sup>7</sup>

In the calculation of particle widths for the states of  $O^{16}$  the one-body interaction in the  $d_{3/2}$  state is a direct consequence of the fact that this state is not bound. Consequently, even in the absence of a particle-hole interaction the 24.8-MeV state of  $O^{16}$ , which belongs mostly to  $p_{3/2}^{-1} d_{3/2}$ , would decay. This contribution to the particle width of the compound states is properly included by the procedure of this paper.

Finally, we wish to point out that the  $d_{3/2}$  intermediate state introduced to describe the scattering resonance in  $O^{17}$  is properly regarded as a "doorway state" although this state does not satisfy the definition of such states given by Block and Feshbach.<sup>8</sup> Such states are commonly thought of as being states which differ from the initial state by the excitation of a nucleon. In current parlance, "doorway states" differ by two quasi-particles from the initial state. More properly, however, a doorway state should be regarded as merely a resonant configuration which is directly coupled to the incident channel and also to more complex excitations of the compound system. The  $d_{3/2}$  state clearly meets this criterion.

The application of this formalism to a complete analysis of the states of  $O^{16}$  is being carried out and will be reported in another paper.

The computations for this paper were carried out at the Computer Science Center of the University of Maryland under NASA Grant Nsg-398.

<sup>5</sup> J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) **A242**, 57 (1957).

<sup>6</sup> G. E. Brown, L. Castillejo, and J. A. Evans, Nucl. Phys. **22**, 1 (1961).

<sup>7</sup> V. Gillet and N. Vinh-Mau, Phys. Letters **1**, 25 (1962).

<sup>8</sup> B. Block and H. Feshbach, Ann. Phys. (N. Y.) **23**, 47 (1963).