

## Redundant states, reduced potentials, and extra nodes in the radial wave function

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First-principle scattering calculations which include antisymmetrization of a projectile with respect to identical particles in the target result in a nonsymmetric nonlocal effective potential. Such a potential can lead to redundant states in the scattering wave function. In this case the potential is required to satisfy a consistency condition. We discuss this condition and the manner in which it can be imposed. We also discuss the replacement of this potential by a reduced symmetric nonlocal effective potential which does not produce redundant states. This reduced potential generates a scattering wave function orthogonal to the redundant states. If the original equation has one redundant state, the phase shift at zero energy is  $\pi$ , resulting in an extra node in the zero-energy wave function. The reduced effective potential must retain this extra node. This characteristic of the reduced effective potential is illustrated with an example. We show that the extra node produced by the potential in the example comes either from a spurious state or a bound state of that potential.

[NUCLEAR REACTIONS Scattering by a nonlocal potential, extra nodes, Fredholm determinants and their zeros, redundant states, continuum bound states, spurious states.]

### I. INTRODUCTION

Scattering formalisms that incorporate antisymmetrization of the projectile with respect to particles in the target identical to the projectile or any of its components result in a nonlocal effective potential<sup>1</sup> in the equation for the projectile-target relative motion. This effect of antisymmetrization has been discussed in Ref. 1 in terms of the nuclear density matrix, an overlap kernel between the total wave function of the projectile-target system and the product of the individual wave functions of the projectile and target.<sup>2,3</sup> In certain special cases this overlap kernel will have eigenvalues of unity. Such a situation occurs in nucleon-nucleus scattering if the target nucleus is assumed to be represented by a Slater determinant of single-particle nucleon states.<sup>4-6</sup> The situation also occurs when the projectile is composite and the internal structure of both the projectile and target are described by Slater determinants of pure harmonic oscillator shell model wave functions with identical oscillator parameters.<sup>7-9</sup> Under these circumstances, configurations excluded by the Pauli principle appear as solutions of the relative motion equation in addition to the scattering solution. Because these solutions can be added in any arbitrary amount, they are referred to as redundant.<sup>6,10,11</sup> Since redundant solutions behave like bound state solutions, their presence in the scattering solution does not affect the scattering phase shifts.

When incorporating antisymmetrization by means of formalisms which result in an overlap kernel with eigenvalues of unity, simplifying models have often been introduced. The essential feature of antisymmetrization retained in such simplifications traditionally has been the physical requirement of the Pauli principle that the scattering wave function be orthogonal to the occupied states. The models which have been devised accomplish this orthogonality in a variety of ways. For example, one model begins with a nonlocal potential which produces redundant states and then eliminates from that potential all terms which project onto the excluded states. The terms remaining in the potential orthogonalize the scattering solution with respect to these states. This is the technique employed by Saito<sup>3,12</sup> and by Krause and Mulligan.<sup>13</sup> Another approach is to start with scattering solutions in a space which is explicitly orthogonal to the excluded states, as is done by Shakin and Weiss,<sup>14</sup> Scheerbaum *et al.*,<sup>15</sup> and Shakin and Thaler.<sup>16</sup> Still another possibility, that discussed by Buck *et al.*,<sup>17</sup> is to recognize that the forbidden states are very similar to bound eigenfunctions of the local part of the Hamiltonian and to solve this Hamiltonian and simply disregard those states which are to be excluded. Finally, we mention the pseudopotential method, which achieves orthogonality by combining aspects of both the nonlocal potential and local potential techniques. As used by Krasnopol'skii and Kukulin<sup>18</sup> and by Kukulin

*et al.*,<sup>19</sup> this method adds a nonlocal potential to the effective local potential. The nonlocal potential is chosen to maintain orthogonality of the scattering solution with respect to the excluded states while allowing the binding energy of those local potential eigenfunctions excluded by the Pauli principle to be assigned an arbitrary energy.

Saito,<sup>12</sup> Okai *et al.*,<sup>20</sup> and Krasnopol'skii and Kukulin<sup>18</sup> all have emphasized that in any model the essential feature for maintaining orthogonality is providing for extra nodes in the scattering wave function. The necessity for extra nodes sufficient to insure orthogonality with respect to filled states has also been discussed in detail by Swan.<sup>21</sup>

A well-investigated example of the need for extra nodes for orthogonality occurs in  $\alpha$ - $\alpha$  scattering.<sup>7,9,20,22,23</sup> The behavior of the  $\alpha$ - $\alpha$  relative wave function must exhibit effects of excluded radial configurations. This is expressed in terms of orthogonality of the radial wave function with respect to the states excluded. The states excluded for the relative motion of two  $\alpha$  particles are the 1S, 2S, and 1D radial configurations. Thus the radial wave functions for the  $s$  and  $d$  states must exhibit sufficient nodal structure to be orthogonal to the 1S and 2S states and 1D states, respectively.

The purpose of the present paper is to present a unified description and summary of the mechanisms by which a potential can ensure the required orthogonality in terms of extra nodes in the scattering wave function. In the case of a local potential it is well known that the only circumstance which causes an extra node is the presence of a bound state. This is analyzed in detail, for example, in Ref. 24. As we shall discuss, in the case of a nonlocal potential two additional mechanisms which are unique to nonlocal potentials are also possible. In the following sections we describe these mechanisms in terms of the zeros of a system of Fredholm determinants. In this regard, the discussion will make use of definitions given in a recent paper<sup>25</sup> in which we examined the relationship between nonlocality, extra nodes, and the zero-energy phase shift.

## II. FREDHOLM DETERMINANTS AND EXTRA NODES

In the Introduction we discussed the requirement that if a radial wave function is to satisfy the Pauli principle it must be orthogonal to the redundant states. Extra nodes in the wave function are required for this orthogonality.<sup>21</sup> In this section of the paper we show how the required orthogonality and the presence of the extra nodes can be expressed in terms of zeros of Fredholm determinants. The analysis applies to nonlocal potentials which are symmetric and real. For simplicity, we

consider the  $l=0$  partial wave; similar considerations also apply for  $l>0$ .

For  $l=0$  the radial equation for a nonlocal potential  $V$  is

$$u(k,r)'' + k^2 u(k,r) = \int_0^\infty V(r,r') u(k,r') dr'. \quad (1)$$

The physical wave function  $\psi^+(k,r)$  and its conjugate  $\psi^-(k,r)$  are defined to be the solutions of the pair of integral equations

$$\psi^\pm(k,r) = \sin kr + \int_0^\infty \int_0^\infty G^\pm(k,r,r') V(r',s) \psi^\pm(k,s) ds dr' \quad (2)$$

with

$$G^\pm(k,r,r') = -k^{-1} e^{\pm ikr} \sin kr'. \quad (3)$$

The Fredholm determinants associated with the kernels of Eq. (2) are referred to as  $D^\pm(k)$ . The solutions of Eq. (2) will be regular at the origin and  $\psi^+(k,r)$  will satisfy the boundary condition that, as  $r \rightarrow \infty$ ,

$$\psi^+(k,r) \rightarrow \frac{1}{2}i [e^{-ikr} - S^+(k)e^{ikr}]. \quad (4)$$

The regular solution of Eq. (1) is defined to be the solution of the integral equation

$$\varphi(k,r) = k^{-1} \sin kr + \int_0^r \int_0^\infty G(k,r,r') V(r',s) \varphi(k,s) ds dr' \quad (5)$$

with

$$G(k,r,r') = k^{-1} \sin k(r-r'). \quad (6)$$

The Fredholm determinant associated with the kernel of Eq. (5) is  $D(k)$ . The regular solution  $\varphi(k,r)$  is real and is governed by the boundary conditions

$$\varphi(k,0) = 0 \quad (7)$$

and

$$\varphi(k,0)' = 1. \quad (8)$$

The Jost solutions  $f^\pm(k,r)$  satisfy the integral equations

$$f^\pm(k,r) = e^{\pm ikr} - \int_r^\infty \int_0^\infty G(k,r,r') V(r',s) f^\pm(k,s) ds dr'. \quad (9)$$

The Fredholm determinant associated with the kernel of Eq. (9) is denoted by  $\Delta(k)$  and is equal to  $D(k)$  for a symmetric potential. The boundary conditions on  $f^\pm(k,r)$  are imposed at  $\infty$  and are

$$\lim_{r \rightarrow \infty} e^{\mp ikr} f^\pm(k,r) = 1. \quad (10)$$

There are three methods by which an effective potential can introduce an extra node into a wave function:

a. *Zero of  $D^+(ik)$ .* When a potential has a bound

state, the wave function for scattering from that potential is orthogonal to the bound state wave function. In this case, the scattering wave function will have the extra node characteristic of scattering by a potential which has a bound state. The presence of the bound state is also characterized by a zero of the Fredholm determinant  $D^*$  on the positive imaginary  $k$  axis,  $D^*(ik)=0$ . Thus, a zero of the Fredholm determinant  $D^*(ik)$  requires an extra node in the scattering wave function. This is true for an effective potential which is either local or nonlocal. The relationship between zeros of  $D^*(ik)$  and bound states is well known in the case of a local potential.<sup>24</sup>

*b. Zero of  $D^*(k)$ .* A nonlocal potential can have a zero of  $D^*(k)$  on the real  $k$  axis. A zero of this kind is not possible for a short-range local potential.<sup>24</sup> For a symmetric nonlocal potential, such a zero is referred to as a continuum bound state. It has been demonstrated in Ref. 25 that a continuum bound state is characterized by an extra node in the scattering wave function. Thus, a second method by which an effective potential which is nonlocal can produce a wave function exhibiting an extra node is for  $D^*(k)$  to be zero for some real value of  $k$ .

*c. Zero of  $D(k)$ .* For a local potential, the integral equation for the regular solution is a Volterra equation; thus the Fredholm determinant associated with this equation is unity.<sup>24</sup> When the potential is nonlocal, the equation becomes a Fredholm integral equation, with a determinant which depends upon the wave number of the incident particle. This determinant, usually denoted by the symbol  $D(k)$ , may have a zero on the real  $k$  axis. It has been demonstrated<sup>26</sup> for a symmetric nonlocal potential that if  $D^*(k)$  is zero,  $D(k)$  is also zero. However, a zero of  $D(k)$  can occur for which  $D^*(k) \neq 0$ . Such a zero of  $D(k)$  is known as a spurious state.<sup>26</sup> In Ref. 25 it is shown that for all wave numbers below that at which a spurious state occurs, the scattering wave function has an extra node. For wave numbers above the spurious state wave number, the extra node is not present. Thus, a third method by which an effective potential which is nonlocal can produce a wave function which exhibits an extra node is for  $D(k)$  to be zero for some real value of  $k$ .

### III. REDUNDANT STATES AND THE CONSISTENCY CONDITION

When circumstances require antisymmetrization, the nonlocality of the effective potential results in an integrodifferential Schrödinger equation. Depending upon the method of construction of the effective potential, the associated overlap kernel

may or may not have eigenvalues unity. However, the work of Saito *et al.*<sup>2,3</sup> suggests that the complicated nonlocal potential which appears in the case of an overlap kernel with eigenvalues which are not unity can be very well approximated by a simpler nonlocal potential associated with an overlap kernel with all eigenvalues unity. Such an overlap kernel gives rise to redundant states.

Thus, a clear physical connection exists between antisymmetrization and the presence of redundant states. Saito,<sup>12</sup> for example, has suggested a model that starts with a symmetric nonlocal potential which produces redundant states. On the other hand, first principle calculations such as those of Schenter and Thaler<sup>27</sup> or of Feshbach<sup>1</sup> result, in the limit of an overlap kernel with all eigenvalues unity,<sup>6</sup> in a potential which is not symmetric. From the point of view of integral equation theory, the symmetry or nonsymmetry of a potential which produces redundant states has important implications.

A redundant state has been shown<sup>6</sup> to be a continuum bound state present at all energies. Thus, when a redundant state is present  $D^*(k)=0$  for all real  $k$  and the redundant state is a solution at all energies of the homogeneous integral equation associated with Eq. (2). However, from Fredholm's third theorem, if a homogeneous solution,  $\psi_h^*(k,r)$ , exists, then a solution of Eq. (2) exists if and only if

$$\int_0^\infty \sin kr \bar{\psi}_h^*(k,r) dr = 0, \quad (11)$$

where  $\bar{\psi}_h^*(k,r)$  is the solution of the transposed homogeneous integral equation associated with Eq. (2), namely

$$\bar{\psi}_h^*(k,r) = \int_0^\infty \int_0^\infty V(r',r) G^*(k,r',s) \bar{\psi}_h^*(k,s) ds dr'. \quad (12)$$

For a symmetric nonlocal potential, condition (11) is always satisfied.<sup>26</sup> On the other hand, if a nonlocal potential which produces redundant states is not symmetric, condition (11) may or may not be satisfied.<sup>13</sup> Thus Eq. (11) is a consistency condition which must be imposed if a scattering solution is to exist; this can be accomplished either by imposing condition (11), if necessary, or by starting with a symmetric nonlocal potential, such as Saito does.

Because first-principle effective potentials which produce redundant states are nonsymmetric, the question of the existence of a scattering solution must be examined. For an effective nonlocal potential calculated from a complete microscopic picture, it would be expected that the consistency condition would be fulfilled and thus that the solution would exist. However, for a potential con-

structured at least in part phenomenologically, the existence of a scattering solution can be guaranteed only by the application of Eq. (11). That is, since the consistency condition arises from the Pauli principle, only certain interaction potentials are physically meaningful. Although imposing the consistency condition does not affect the structure of the integrodifferential scattering equation, it must be incorporated in determining parameters of nonlocal phenomenological potentials.

In this paper we follow previous convention and designate redundant states by  $\xi_i(r)$ . An important aspect of all model potentials which produce such states is that terms appear in the potential which project onto these states. If the potential meets the consistency condition, then dropping these terms will eliminate the redundant states and yield a scattering equation with a solution  $\psi^*(k, r)$  which is orthogonal to the states  $\xi_i(r)$ . The phase shift of this scattering solution is the same as that of the original equation with redundant states. Suppose, on the other hand, that the potential did not conform to the consistency condition. No scattering solution would be possible. However, throwing away the terms which project onto the redundant states would result in an equation which does have a scattering solution. But this scattering solution would not have the same phase shift as that of the original equation with redundant states. Thus it is imperative that the consistency condition be fulfilled before the terms which project onto the states  $\xi_i(r)$  are discarded.

Even if the consistency condition is satisfied, dropping terms which project onto  $\xi_i(r)$  requires further consideration. Dropping the terms in the potential which project onto the states  $\xi_i(r)$  is justified if one wishes to obtain only the scattering solutions  $\psi^*(k, r)$ . However, the altered potential may no longer be used in off-shell calculations.

The equation with the terms which project onto the  $\xi_i(r)$  removed we refer to as the reduced equation for the scattering wave function; the potential in this equation is the reduced potential. As the above discussion implies, solutions of Eq. (1) with the reduced potential are also solutions of Eq. (1) with the original potential. As far as the two wave functions are concerned, they differ only by the presence of redundant states. Redundancies  $\xi_i(r)$  have been eliminated from the solutions of the reduced equation; these solutions are orthogonal to the states  $\xi_i(r)$ .

From the Fredholm determinant point of view,<sup>26</sup> there are also basic differences in the structure of the complete and reduced equations. With the full potential, the Fredholm determinant  $D^*(k)$  associated with the kernel of the integral equation for

the physical wave function is zero for all wave numbers  $k$  of the incident particle; with the reduced potential, this is no longer the case. That is, the Fredholm determinant  $D^*(k)$  associated with this reduced equation will not, in general, be zero. Thus, while the fact that  $D^*(k)$  was zero for the full equation ensured that its solution would have an extra node, this mechanism is not present for the reduced equation. However, the requirement of antisymmetrization demands that the extra node be present. Thus the extra node must occur as a result of one of the other processes discussed in the previous section. For example, in the case of the Saito potential (which is a reduced potential) the extra node results from a zero of  $D^*(k)$  at  $k=0$ .<sup>28</sup> In general, however, any one of the processes may ensure the retention of the extra node. That this is the case will now be demonstrated by discussing a simple analytic example.

#### IV. EXAMPLE

In this example, we consider the  $l=0$  radial wave equation

$$\left(\frac{d^2}{dr^2} + k^2\right)u(r) = \int_0^\infty \langle r | \mathcal{V} | s \rangle u(s) ds. \quad (13)$$

We construct the potential  $\langle r | \mathcal{V} | s \rangle$  such that it will have a single redundant solution given by

$$\xi(r) = 2\alpha^{3/2} r e^{-\alpha r}. \quad (14)$$

It has been shown<sup>6,13</sup> that a nonlocal potential which produces a redundant solution assumes a particular form, namely

$$\langle r | \mathcal{V} | s \rangle = \left[ \left( \frac{d^2}{dr^2} + k^2 \right) \xi(r) \right] \xi(s) + \langle r | \mathcal{V}_2 | s \rangle, \quad (15)$$

where

$$\int_0^\infty \langle r | \mathcal{V}_2 | s \rangle \xi(s) ds = 0. \quad (16)$$

In order to have a potential that satisfies Eq. (16) and for which a simple analytic solution of Eq. (13) is possible,  $\langle r | \mathcal{V}_2 | s \rangle$  is chosen to be

$$\langle r | \mathcal{V}_2 | s \rangle = \int_0^\infty \lambda e^{-\beta r} e^{-\beta r'} \langle r' | \Lambda | s \rangle dr', \quad (17)$$

with

$$\langle r' | \Lambda | s \rangle = \delta(r' - s) - 4\alpha^3 r' e^{-\alpha r'} s e^{-\alpha s}. \quad (18)$$

The potential  $\langle r | \mathcal{V} | s \rangle$  then assumes the form

$$\langle r | \mathcal{V} | s \rangle = 4\alpha^3 [(\alpha^2 + k^2)r - 2\alpha] e^{-\alpha r} s e^{-\alpha s} + \lambda e^{-\beta r} \left( e^{-\beta s} - \frac{4\alpha^3 s}{(\alpha + \beta)^2} e^{-\alpha s} \right). \quad (19)$$

Direct substitution shows  $\xi(r)$  as given by Eq. (14) to be a solution at all  $k$  of Eq. (13) with this potential. Thus,  $\xi(r)$  is indeed a redundant state and a solution of the homogeneous integral equation associated with Eq. (2). Direct calculation of  $D^*(k)$  also demonstrates it to be zero at all  $k$ .

Since the potential of Eq. (19) is not symmetric,

$$a = \frac{2\lambda\beta(\beta^2 + k^2)[(\alpha + \beta)^2(\alpha^2 - k^2) - (\alpha^2 + k^2)^2 \pm i2\alpha k(\alpha + \beta)^2]}{(\alpha + \beta)^2(\alpha^2 + k^2)^2 [2\beta(\beta^2 + k^2)^2 + \lambda(\beta^2 - k^2 \pm i2\beta k)]} \quad (21)$$

and  $N$  is an arbitrary constant of normalization. Substituting this expression into the consistency condition integral yields

$$\int_0^\infty \sin kr \bar{\psi}_h^*(k, r) dr = Nk \left( \frac{2\alpha}{(\alpha^2 + k^2)^2} - \frac{a}{\beta^2 + k^2} \right). \quad (22)$$

This expression, in general, is not equal to zero. Therefore, in general,  $\psi^*(k, r)$  will not exist for the potential given by Eq. (19). The consistency condition of Eq. (11) can be satisfied for all  $k$  and solutions  $\psi^*(k, r)$  made to exist for all  $k$  by setting the right hand side of Eq. (22) equal to zero. This yields

$$\lambda = -\frac{2\alpha\beta(\beta^2 + k^2)(\alpha + \beta)^2}{\beta(\alpha^2 + k^2) - \alpha(\alpha^2 - \beta^2)}. \quad (23)$$

Equation (13) with the potential given by Eq. (19) will have a scattering solution if, and only if, Eq. (23) is satisfied.

The value of  $\lambda$  given by Eq. (23) ensures that the consistency condition is fulfilled. We now drop from Eq. (19) for  $\langle r | \psi \rangle$  those terms which project onto the redundant state  $2\alpha^{3/2}se^{-\alpha s}$ , and which thus give zero when acting on the scattering wave function. Equation (13) then reduces to

$$\left( \frac{d^2}{dr^2} + k^2 \right) u(r) = \lambda e^{-\beta r} \int_0^\infty e^{-\beta s} u(s) ds. \quad (24)$$

As long as the  $\lambda$  in Eq. (24) is given by Eq. (23), the solution of Eq. (24) will be orthogonal to the redundant state. This would not be the case if some other value of  $\lambda$  were taken. Equation (24) is an appropriate reduction of Eq. (13) only if the  $\lambda$  which appears in Eq. (24) is given by Eq. (23).

The symmetric nonlocal potential which appears in Eq. (24) is of the Yamaguchi form<sup>29</sup>; the coordinate space solution of Eq. (24) is well known.<sup>30</sup> For this potential the Fredholm determinant  $D(k)$  is

$$D(k) = 1 - \frac{\lambda}{2\beta(\beta^2 + k^2)}, \quad (25)$$

while the Fredholm determinant  $D^*(k)$  is

the scattering solutions  $\psi^*(k, r)$  will not necessarily exist.<sup>13</sup> In order to apply the consistency condition we solve Eq. (12) for  $\bar{\psi}_h^*(k, r)$ . We get

$$\bar{\psi}_h^*(k, r) = N[re^{-\alpha r} - ae^{-\beta r}], \quad (20)$$

where

$$D^*(k) = D(k) + \frac{\lambda\beta}{(\beta^2 + k^2)^2} \pm \frac{i\lambda k}{(\beta^2 + k^2)^2}. \quad (26)$$

The value of  $\alpha$  determines the wave function of the redundant state. Since the choice of the redundant state is arbitrary, the choice of  $\alpha$  is arbitrary, but  $\alpha$  should not be energy dependent ( $k$  dependent). From Eq. (23) it is clear that the consistency condition requires that at least one of the two parameters  $\lambda$  and  $\beta$  of the effective potential  $\mathcal{U}$  depend upon the energy. The form of Eq. (23) suggests that we assume that  $\beta$  not be energy dependent, and satisfy the consistency condition by incorporating all energy dependence of the effective potential into the strength parameter  $\lambda$ .

Since the full potential of Eq. (19) produces a single redundant state, the phase shift at zero energy will be  $\pi$ .<sup>21</sup> Evidence of this phase shift will be an extra node in the zero-energy wave function of the zero-energy effective potential in Eq. (24). It should be noted that the Fredholm determinant

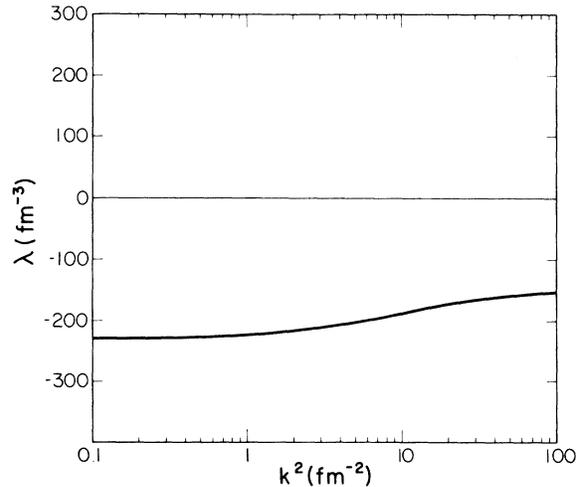


FIG. 1. Variation of the effective strength parameter  $\lambda$  with  $k^2$  for  $\alpha = 2 \text{ fm}^{-1}$  and  $\beta = 4 \text{ fm}^{-1}$ . In this case  $\lambda < -2\beta^3$ , yielding an effective potential with a bound state.

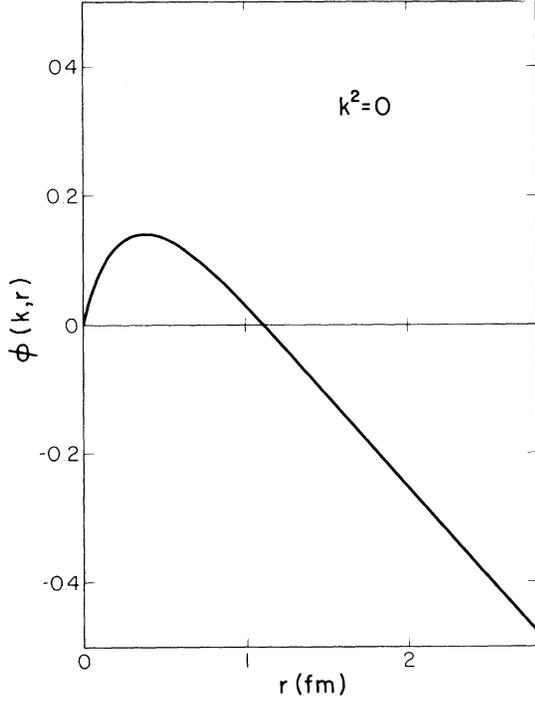


FIG. 2. Wave function  $\phi(k, r)$  at  $k^2=0$  for  $\alpha=2 \text{ fm}^{-1}$  and  $\beta=4 \text{ fm}^{-1}$ . The zero-energy effective strength parameter  $\lambda$  is  $-230.4 \text{ fm}^{-3}$ . The zero-energy wave function shows an extra node due to a bound state at  $k^2=-1.87 \text{ fm}^{-2}$ .

$D^*(k)$  given by Eq. (26) is not zero for any real value of the wave number greater than zero.<sup>26</sup> Thus, as expected, this potential cannot produce a continuum bound state and the required extra node must be generated by a spurious state [ $D(k)=0$ ] or a bound state [ $D^*(ik)=0$ ].

From Eq. (25) we see that a zero of  $D(k)$  will occur only for  $\lambda \geq 2\beta^3$ , with the equality holding only

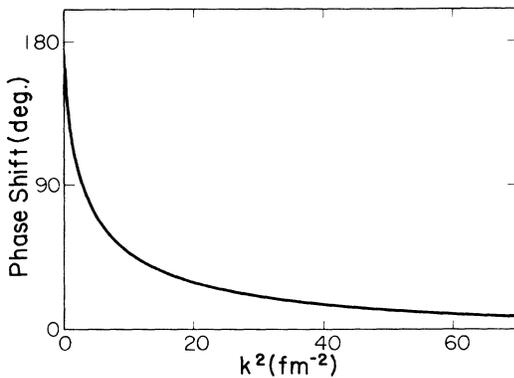


FIG. 3. Variation of the phase shift with  $k^2$ . Note that the change in the effective strength parameter with  $k^2$  is a necessary part of this variation.

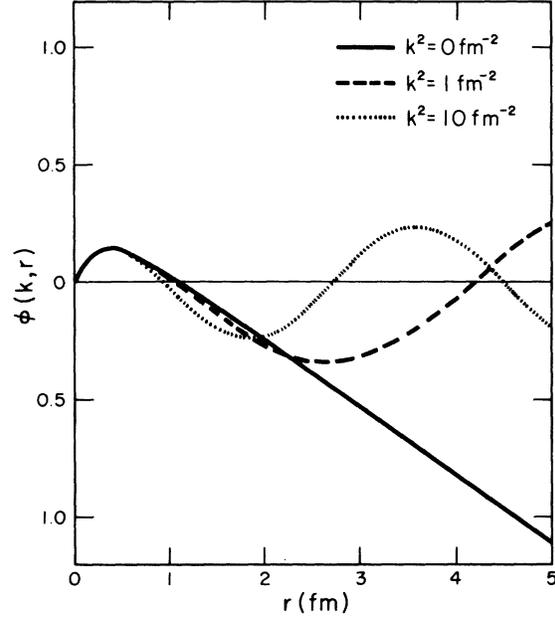


FIG. 4. Wave function at  $k^2=0, 1,$  and  $10 \text{ fm}^{-2}$  for  $\alpha=2 \text{ fm}^{-1}$  and  $\beta=4 \text{ fm}^{-1}$ . Note the small variation with energy of the position of the inner node. This almost energy independence of the extra node is similar to that of the extra node due to the Saito potential (Ref. 20).

for a spurious state at zero energy. Likewise, from Eq. (26) it follows that a zero of  $D^*(ik)$  can occur only for  $\lambda \leq -2\beta^3$ , with the equality holding only for a zero-energy bound state. Thus, for values of  $\lambda$  with  $k=0$  which satisfy  $-2\beta^3 < \lambda < 2\beta^3$ , we should expect no zero of  $D(k)$  or  $D^*(ik)$  and thus no extra node by any mechanism. In the Appendix it is shown that for all  $\alpha$  and  $\beta$  greater than zero the values of  $\lambda$  with  $k=0$  given by Eq. (23) cannot lie between  $\pm 2\beta^3$ . Furthermore,  $\lambda = \pm 2\beta^3$  will occur only for nonphysical values of  $\alpha$  and  $\beta$ , namely zero and infinity. Thus, for any physical values of  $\alpha$  and  $\beta$ , the zero-energy wave function always will exhibit an extra node due either to a spurious state or to a bound state.

It also follows from Eq. (23) that as  $k^2 \rightarrow \infty$ ,  $\lambda$  approaches the negative value  $-2\alpha(\alpha + \beta)^2$ . For  $\beta > \frac{1}{2}(\sqrt{5} - 1)\alpha$ ,  $\lambda$  will be negative for all values of  $k^2$ . On the other hand, if  $\beta < \frac{1}{2}(\sqrt{5} - 1)\alpha$ ,  $\lambda$  will be positive for  $k^2=0$  and change sign at some positive value of  $k^2$ . Thus, there are two distinct circumstances which must be considered. As examples of these two circumstances we fix the redundant state parameter  $\alpha$  at the value  $\alpha=2 \text{ fm}^{-1}$ , picking  $\beta=4 \text{ fm}^{-1}$  in the first case and  $\beta=1 \text{ fm}^{-1}$  in the second case.

*Case 1.* A plot of  $\lambda$  as a function of  $k^2$  is given in Fig. 1 for  $\alpha=2 \text{ fm}^{-1}$ ,  $\beta=4 \text{ fm}^{-1}$ . As expected,  $\lambda$  is negative for all values of  $k^2$ . Neither  $D(k)$

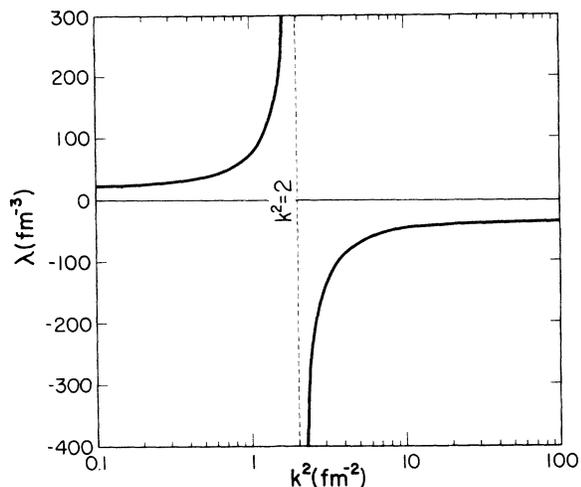


FIG. 5. Variation of the effective strength parameter  $\lambda$  with  $k^2$  for  $\alpha = 2 \text{ fm}^{-1}$  and  $\beta = 1 \text{ fm}^{-1}$ . Note that  $\lambda$  is discontinuous at  $k^2 = 2 \text{ fm}^{-2}$ .

nor  $D^*(k)$  can be zero for positive, real  $k$ . The zero-energy wave function is given in Fig. 2. This wave function has an extra node, indicating that this Yamaguchi potential has one bound state. It is easy to verify by direct calculation that the potential with  $\alpha = 2 \text{ fm}^{-1}$ ,  $\beta = 4 \text{ fm}^{-1}$ ,  $\lambda = -230.4 \text{ fm}^{-3}$  has

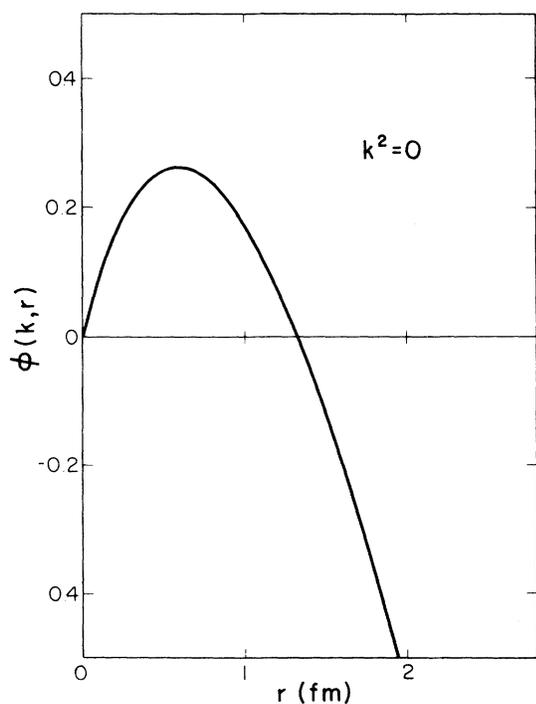


FIG. 6. Wave function  $\phi(k, r)$  at  $k^2 = 0$  for  $\alpha = 2 \text{ fm}^{-1}$  and  $\beta = 1 \text{ fm}^{-1}$ . The zero-energy effective strength parameter  $\lambda$  is  $18.0 \text{ fm}^{-3}$ . The zero-energy wave function shows an extra node due to a spurious state at  $k^2 = 8.0 \text{ fm}^{-2}$ .

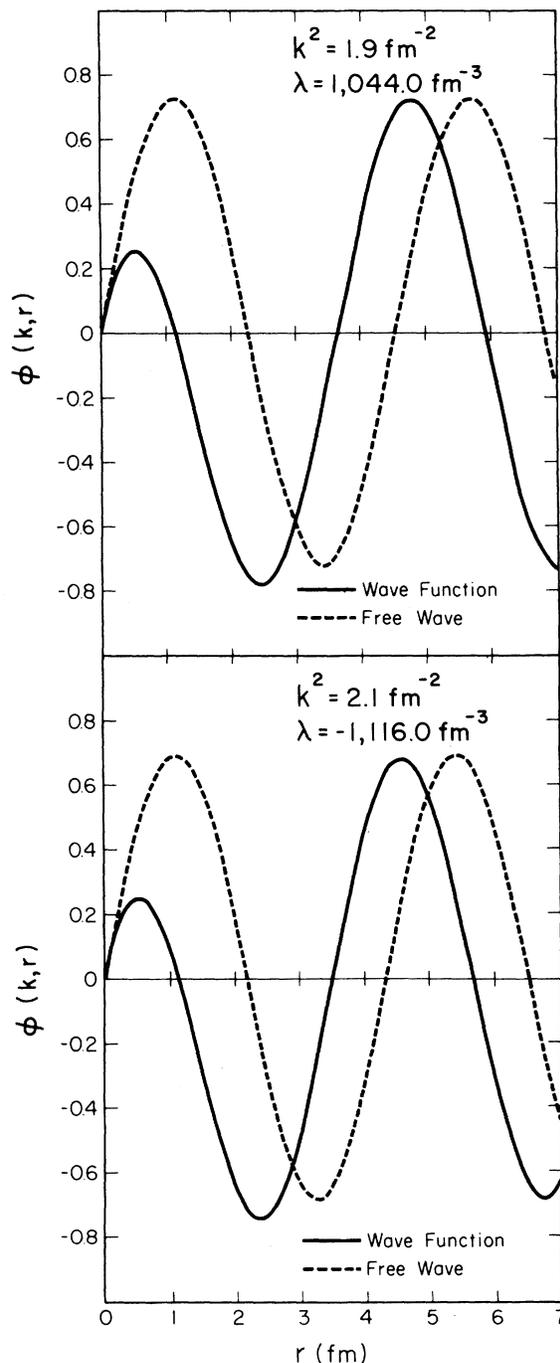


FIG. 7. Wave function  $\phi(k, r)$  at  $k^2 = 1.9 \text{ fm}^{-2}$  and at  $k^2 = 2.1 \text{ fm}^{-2}$  for  $\alpha = 2 \text{ fm}^{-1}$  and  $\beta = 1 \text{ fm}^{-1}$ . These parameters yield an effective strength parameter of  $1044.0 \text{ fm}^{-3}$  at  $k^2 = 1.9 \text{ fm}^{-2}$  and of  $-1116.0 \text{ fm}^{-3}$  at  $k^2 = 2.1 \text{ fm}^{-2}$ . For comparison, the free wave function  $k^{-1} \sin kr$  is shown in each case as a dashed line. The phase shift at  $k^2 = 1.9 \text{ fm}^{-2}$  is  $72.2^\circ$  and at  $k^2 = 2.1 \text{ fm}^{-2}$  is  $68.9^\circ$ .

a bound state at  $k^2 = 1.87 \text{ fm}^{-2}$ . In Fig. 3 we plot the phase shift versus  $k^2$ . This figure clearly illustrates the  $k^2 = 0$  phase of  $\pi$ . It is important to see that the extra node is present not only at  $k = 0$ , but for larger values of  $k$  as well. Also note that the position of the extra node is almost independent of  $k$ . This is demonstrated in Fig. 4, where the wave function is plotted for different values of  $k^2$ .

*Case 2.* A plot of  $\lambda$  as a function of  $k^2$  is given in Fig. 5 for  $\alpha = 2 \text{ fm}^{-1}$ ,  $\beta = 1 \text{ fm}^{-1}$ . This diagram shows the change in sign of the potential strength  $\lambda$  at  $k^2 = 2 \text{ fm}^{-2}$ . It is important to recognize that this singularity of the potential does not affect the scattering wave function but is, in fact, necessary in order for the wave function to exhibit the proper continuity and nodal behavior. To see this, we plot in Fig. 6 the zero-energy wave function. This wave function has an extra node, as is required for the phase shift to be  $\pi$  at  $k^2 = 0$ . However, in this case the extra node is due to a spurious state of the potential and not to a bound state; since the potential is repulsive, it cannot have a bound state. Using the  $k = 0$  value of  $\lambda$ , namely  $\lambda = 18 \text{ fm}^{-3}$ , direct calculation from Eq. (25) shows  $D(k) = 0$  at  $k^2 = 8 \text{ fm}^{-2}$ . Thus, an extra node will appear at all energies below  $k^2 = 8 \text{ fm}^{-2}$  for the potential with these parameters.<sup>25</sup>

As is clear from Fig. 5, this potential has a singularity and changes sign at  $k^2 = 2 \text{ fm}^{-2}$ . The scattering wave function at values of  $k^2$  below the singularity contains an extra node due to a spurious state, while the scattering wave function for  $k^2 > 2 \text{ fm}^{-2}$  possesses an extra node due to a bound state. The scattering wave function, however, is continuous through  $k^2 = 2 \text{ fm}^{-2}$ . To see this we show in Fig. 7 the scattering wave function for  $k^2 = 1.9 \text{ fm}^{-2}$  ( $\lambda = 1044 \text{ fm}^{-3}$ ) and for  $k^2 = 2.1 \text{ fm}^{-2}$

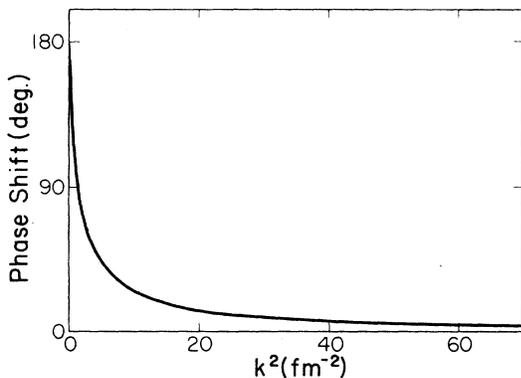


FIG. 8. Variation of the phase shift with  $k^2$ . Note that at  $k^2 = 2 \text{ fm}^{-2}$  there is no discontinuity of the phase shift despite the discontinuity in the strength parameter of the effective potential.

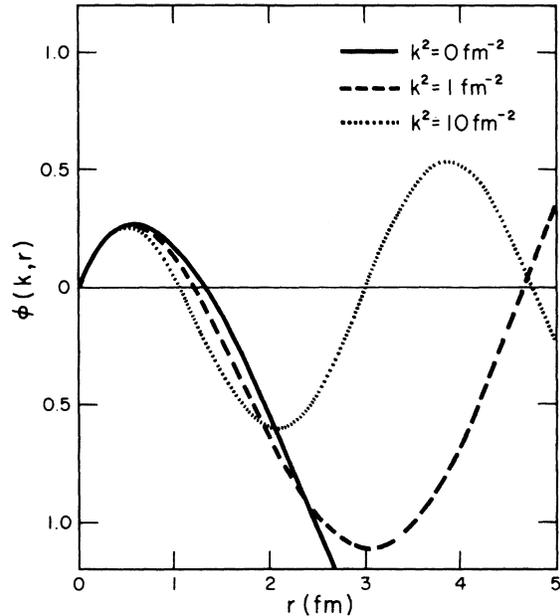


FIG. 9. Wave function at  $k^2 = 0, 1,$  and  $10 \text{ fm}^{-2}$  for  $\alpha = 2 \text{ fm}^{-1}$  and  $\beta = 1 \text{ fm}^{-1}$ . The small variation with energy of the position of the extra node is similar to that found for the wave function for scattering by the Saito potential (Ref. 20).

( $\lambda = -1116 \text{ fm}^{-3}$ ). This figure shows the continuity of the scattering wave function despite the enormous difference in the potential strength parameter. This continuity is also demonstrated in Fig. 8, in which the phase shift is plotted as a function of  $k^2$ . It is clearly continuous through  $k^2 = 2 \text{ fm}^{-2}$ , and the zero-energy phase shift is  $\pi$ . To see again that the extra node is present not only at  $k = 0$  but for larger values of  $k$  as well, and that the position of the extra node is almost independent of  $k$ , the wave function for different values of  $k^2$  is plotted in Fig. 9.

## V. CONCLUSION

In this paper, we have discussed techniques for including effects of antisymmetrization in scattering formulations. We conclude that all of these techniques ultimately reduce to methods for ensuring an extra node in the scattering wave function by requiring an isolated zero of  $D^*(ik)$ ,  $D(k)$ , or  $D^*(k)$ . Such a zero of the Fredholm determinant corresponds to a bound state, a spurious state, or a continuum bound state, respectively. An exception is a formalism which includes redundant states. In this case  $D^*(k)$  is equal to zero at every energy. However, because of the rather complicated nature of potentials which produce redundant states, most techniques depend upon potentials which result in an isolated zero.

We have given an example in Sec. IV which shows that an isolated zero of a Fredholm determinant can result directly from a simplification of an approach using redundant states. Obtaining a "reduced potential" from a potential with redundant states can, depending on the circumstances, yield a potential with a bound state, a spurious state, or a continuum bound state. In the example, the reduced potential retains the extra node through a zero of  $D^*(ik)$  or of  $D(k)$ . In the case of the Saito potential, it has been shown<sup>28</sup> that the extra node is due to a zero of  $D^*(k)$  at  $k=0$ . The pseudopotential method<sup>18,19</sup> also relies on a continuum bound state for supporting the required extra node. This continuum bound state is a bound state which has been moved into the continuum by the insertion of an extra term into the scattering potential.

The example of Sec. IV also discusses the consistency condition required when redundant states are present. Potentials which produce extra nodes without using redundant states are not subject to this constraint. However, it is crucial to realize that if the potential resulted from a reduction of an original scattering equation containing redundant states, then the consistency condition should be imposed if the effects of antisymmetrization are to be properly incorporated.

It should again be emphasized that all of the methods discussed have similar on-shell effects in that they all produce scattering wave functions with the proper number of nodes. Off-shell effects, however, may vary widely and have not been investigated thoroughly. Off-shell effects are currently under study in terms of the system of Fredholm determinants discussed here.

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#### APPENDIX

For  $k^2=0$ , the depth parameter  $\lambda$  given by Eq. (23) becomes

$$\lambda(k^2=0) \equiv \lambda_0 = \frac{2\beta^3(\alpha+\beta)^2}{\alpha^2 - \alpha\beta - \beta^2}. \quad (\text{A1})$$

In this Appendix we demonstrate that  $\lambda_0$  satisfies either the condition

$$\gamma_0 \leq -2\beta^3, \quad (\text{A2a})$$

or the condition

$$\lambda_0 \geq 2\beta^3. \quad (\text{A2b})$$

For this purpose we set

$$\lambda_0 = -2\beta^3 + \eta. \quad (\text{A3})$$

Comparison with Eq. (A1) yields

$$\eta = \frac{2\alpha\beta^3(\beta+2\alpha)}{\alpha^2 - \alpha\beta - \beta^2}. \quad (\text{A4})$$

From (A3) all negative values of  $\eta$  are consistent with condition (A2a). We now show that if  $\eta$  is positive, it must be at least as great as  $4\beta^3$ , which is consistent with condition (A2b).

From Eq. (A4) it follows that if  $\eta$  is to be positive, the inequality

$$\alpha > \beta \quad (\text{A5})$$

must hold. We now assume the inequality

$$\eta < 4\beta^3. \quad (\text{A6})$$

Using condition (A5) we see that this implies

$$3\alpha < -\frac{2}{3}\beta. \quad (\text{A7})$$

Since, by assumption, both  $\alpha$  and  $\beta$  are greater than zero, condition (A7) cannot be met. Thus  $\eta$  cannot be both greater than zero and less than  $4\beta^3$ .

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