Bounds on Scattering Phase Shifts: Static Central Potentials*

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It has recently been shown that rigorous upper bounds on scattering lengths can be obtained by adding to the Kohn variational expression certain integrals involving approximate wave functions for each of the negative-energy states. For potentials which vanish identically beyond a certain point, it is possible to extend the method to positive-energy scattering; one obtains upper bounds on $(-k\cot\eta)^{-1}$, where η is the phase shift. In addition to the negative-energy states one must now take into account a finite number of states with positive energies lying below the scattering energy. The states in this associated energy eigenvalue problem are defined by the imposition of certain boundary conditions on the wave functions. A second approach, involving an associated potential-strength eigenvalue problem, is also used. The second method includes the first as a special case and, more significantly, can be extended to scattering by compound systems. If some states are not accounted for, a bound on $\cot\eta$ is not obtained; nevertheless it is still possible to obtain a rigorous lower bound on η. Upper bounds on η may also be obtained, but in a way which is probably not too useful for many-body scattering problems.

1. INTRODUCTION

A VARIATIONAL expression which provides a rigorous upper bound on the scattering length has recently been obtained for the scattering of one compound system by another where only one channel is open and where a finite number of composite bound states exist.[1–4] The method consisted of expressing the scattering length as a variational estimate plus an error term which is of second order, and then bounding the error term. This term is of the form $\int w(H-E_g)wd\tau$, where H is the Hamiltonian, E_g is the sum of the unperturbed ground-state energies of the two colliding systems, and w is the difference between the exact and the trial wave function, each appropriately normalized. It is first recognized that if there are no composite bound states, the integral is non-negative, i.e., one has a bound immediately.[1] The extension[2] to the case where there are N composite bound states, represented by the functions ϕ_i with eigenvalues E_i, proceeds with the observation that the function

$$w-\sum_{i=1}^{N}(w,\phi_i)\phi_i$$

has no components with an energy less than E_g. It follows that the expectation value of $H-E_g$ with respect to the above function is non-negative. Evaluating this expectation value, one then immediately finds that

$$\int w(H-E_g)wd\tau\geqq\sum_{i=1}^{N}\frac{1}{(E_i-E_g)}\times\left[\int\phi_i(H-E_g)u_id\tau\right]^2, \quad (1.1)$$

where u_i is the trial scattering function. Now of course the ϕ_i are not generally known. It proved to be possible, however, to show that the bound is rigorous even though the bound-state functions employed in the calculation are not exact solutions of the Schrödinger equation; the only requirement, essentially, is that they be sufficiently accurate to give binding. If then one can find N orthonormal trial functions, ϕ_{it}, which have the property that the N eigenvalues of the Hamiltonian matrix formed from them all lie below E_g, the inequality given by Eq. (1.1) remains valid when the ϕ_i are replaced by the ϕ_{it}.

It would be extremely useful to generalize the above result to the case for which the initial relative kinetic energy of the systems is greater than zero. More precisely, we seek bounds on $\tan\eta$, where η is one of the phase shifts. [Actually, it will prove convenient as well as useful to seek bounds on $\cot(\eta-\theta)$, where $0\leqq\theta<\pi$.] For purposes of simplicity, the present paper is confined to consideration of the zero angular momentum scattering of a spinless particle by a short-range central potential. (The case of a short-range central potential plus a Coulomb potential will also be treated. See Sec. 2B.) As in the zero-energy case, many of the results are applicable to a wider class of problems, and in fact throughout the present paper stress is placed upon those methods which do indeed allow extensions. The wider class of problems, which are always restricted to

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[1] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); **117**, 1095 (1960).

[2] L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **118**, 184 (1960).

[3] Though the papers deal primarily with applications, some slight extensions of the method are included in L. Spruch and L. Rosenberg, Nuclear Phys. **17**, 30 (1960); and L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **119**, 164 (1960).

[4] The question of bounds on scattering lengths has also been considered by T. Ohmura, J. Math. Phys. **1**, 27 (1960). As the author notes, however, the variational estimate obtained is guaranteed to be a bound only for trial functions which differ infinitesimally from the true function, and is therefore not a rigorous bound for arbitrary trial functions. Further, considerations are limited to cases for which no bound state exists.

those for which only one channel is open, include the scattering of one system by another, with the effects of the Pauli principle taken fully into account.[5] The results can also be extended to the case of an arbitrary angular momentum. On the other hand, in contrast to the zero-energy case, the inclusion of tensor forces would require a major modification.[6] The origin of this difference is that the mixing parameter, the parameter which characterizes the relative admixtures of states of different orbital angular momentum, vanishes in general only at zero energy.

Henceforth, then, we restrict our attention to the one-body problem, for zero angular momentum. Since the initial kinetic energy, to be denoted by E, is greater then 0, there are now an *infinite* number of solutions of the Hamiltonian with energies less the energy of the system under consideration, the N bound states and the continuum below E. If, however, we restrict ourselves to potentials which vanish identically beyond $r=R$, it will prove possible by the imposition of appropriate boundary conditions to require the subtraction of only a *finite* number of states with energies less than E. The problem is then almost identical in form with that at zero energy.

The technique involved utilizes a connection between the *scattering* problem at energy E for a potential $V(r)$ which cuts off beyond $r=R$, and the *bound-state* problem for the potential $V(r)$ for $0\leqq r<R$ followed by an infinitely repulsive potential for $r\geqq R$. The spectrum of the bound-state problem is of course discrete, and a bound on $\int w(H-E)wdr$ may be obtained by performing a subtraction that involves the N negative-energy states[7] and the finite number of positive-energy eigenstates of the bound-state problem which lie below the energy E. This is shown in Secs. 2 and 3.

The reduction of the positive-energy problem to a form similar to that of the zero-energy problem previously studied has of course been achieved only at a price, namely, the restriction on the potential. One would expect, however, that in practice, for low-energy scattering, R can be chosen to be sufficiently large so that the neglect of the potential tail which exists beyond $r=R$ gives rise to a negligible error in η; it may be possible, in fact, to make reasonably reliable estimates of the error incurred. Of course at higher scattering energies the labor involved in the calculation is increased, due to the larger number of states to be subtracted off, for R fixed. At higher scattering energies, therefore, one would have to strike a balance in the choice of R; it would have to be sufficiently large so as to give reasonable accuracy, but not so large as to unduly increase the necessary labor.

The results of Secs. 2 and 3 lead to a lower bound on η. Two methods of obtaining an upper bound on η are discussed in Sec. 4.

The method of Secs. 2 and 3 involves the introduction of an associated bound-state energy eigenvalue problem. It is shown in Sec. 5 that a more general result (which includes the above as a special case) can be obtained by the introduction of an associated eigenvalue problem in which the eigenvalues are certain appropriate strengths of an auxiliary arbitrarily chosen positive-definite potential, $\rho(r)$; this will be referred to as the associated potential-strength eigenvalue problem. The significant feature of this alternate approach is not that its greater generality leads to an improved bound on $\cot(\eta-\theta)$ and on η. Rather, it is that it makes possible the extension of the determination of a bound on η to the scattering of one system by another, with the Pauli principle fully accounted for.[5]

The technique of the associated potential-strength eigenvalue problem was introduced into scattering theory some time ago by Kato,[8,9] who obtained some rather striking results for zero angular momentum scattering by a static central potential. He was able to get both bounds on $\cot(\eta-\theta)$, and he did not need to cut off the potential. The differences between the present approach and that of the original work of Kato, for the one bound that we obtain, are however essential, as matters both of practice and of principle, if results are to be obtained for compound systems. The matter of practice is that we need only calculate matrix elements of H while the Kato method requires the calculation of matrix elements of H^2; the former is difficult enough while the latter is all but impossible for even the simplest compound systems. The matter of principle is that the result deduced by Kato will be less accurate, for the same choice of trial scattering function, than the result obtained in Sec. 5.

2. UPPER BOUND ON $\cot(\eta-\theta)$ USING ENERGY EIGENFUNCTIONS

A. Potentials Which Vanish Identically Beyond $r=R$

The scattering problem is defined by the differential equation

$$(H-E)u(r)=\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)-\frac{\hbar^2k^2}{2\mu}\right)u(r)=0,$$

with boundary conditions

$$u(0)=0,$$

$$u(r)=\cos(kr+\theta)+\cot(\eta-\theta)\sin(kr+\theta), \quad r\geqq R.$$

[5] A paper treating the extension to the many-body problem is in preparation.

[6] The modification should be possible. Bounds on the elements of the scattering matrix for some simple multichannel problems have been obtained by L. Spruch and R. Bartram (to be published).

[7] Here, and in the following, we assume that R has been chosen to be sufficiently large so that no negative-energy bound states are "lost" when the barrier is introduced. In those cases where the number of negative-energy states has been determined experimentally one can really check whether or not any such states have been lost.

[8] T. Kato, Progr. Theoret. Phys. (Kyoto) **6**, 394 (1951).

[9] See also L. Spruch and M. Kelly, Phys. Rev. **109**, 2144 (1958); L. Spruch, Phys. Rev. **109**, 2149 (1958); L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960).

The last result follows from the restriction, in line with the previous discussion, to potentials $V(r)$ which vanish identically for $r>R$.

We introduce the trial function $u_t(r)$ which satisfies

$$u_t(0)=0,$$
$$u_t(r)=\cos(kr+\theta)+\cot(\eta_t-\theta)\sin(kr+\theta), \quad r\geqq R. \tag{2.1}$$

We then have the identity

$$k\cot(\eta-\theta)=k\cot(\eta_t-\theta)+(2\mu/\hbar^2)\int_0^R u_t(H-E)u_t dr - (2\mu/\hbar^2)\int_0^R w(H-E)w dr, \tag{2.2}$$

where the difference function,

$$w(r)=u_t(r)-u(r),$$

has the properties

$$w(0)=0,$$
$$w(r)=[\cot(\eta_t-\theta)-\cot(\eta-\theta)]\sin(kr+\theta), \quad r\geqq R$$
$$(H-E)u_t(r)=(H-E)w(r), \quad \text{for all } r, \tag{2.3}$$

and where we have made use of the fact that

$$(H-E)u_t(r)=(H-E)w(r)=0, \quad r>R.$$

The identity is due to Kato, but is here specialized to the case of a cutoff potential. The last term in Eq. (2.2) is of second order; if it is dropped we remain with a one-parameter family of variational principles. It is our present purpose, however, to bound this term.

One procedure for doing so is to adjust θ and R such that

$$kR+\theta=(P+1)\pi,$$

where P is an arbitrary non-negative integer.[10] It then follows from Eqs. (2.3) that $w(r)$ vanishes at $r=R$ as well as at $r=0$. These boundary conditions are precisely those that would be placed on an energy eigenfunction for a particle in a spherical box, with a rigid wall at a radius R, within which a potential may exist. The desired bound on

$$\int_0^R w(H-E)w dr$$

may then be obtained by considering the associated energy eigenvalue problem in which the potential is $V(r)$ for $r<R$ and is $+\infty$ for $r>R$. Suppose this potential supports M states with energies below E. (These M states include N negative-energy states.) Denote the normalized eigenfunctions by $\phi_i(r)$ with corresponding eigenvalues E_i. We now assume that we have been able to find M trial functions $\phi_{it}(r)$ with the properties

$$\phi_{it}(0)=\phi_{it}(R)=0,$$
$$(\phi_{it},\phi_{st})=\delta_{is}, \tag{2.4}$$
$$(\phi_{it},H\phi_{st})=E_{it}\delta_{is}, \quad E_{it}<E,$$

where i and s each run from 1 through M. The bound on the error integral is obtained in terms of these quantities in a manner which is formally identical to that described previously for the zero-energy case,[2] and we omit the details. Inserting the bound in Eq. (2.2), we find

$$k\cot(\eta-\theta)\leqq k\cot(\eta_t-\theta)+(2\mu/\hbar^2)\int_0^R u_t(H-E)u_t dr + (2\mu/\hbar^2)\sum_{i=1}^M \frac{1}{(E-E_{it})}\left(\int_0^R u_t(H-E)\phi_{it}dr\right)^2. \tag{2.5}$$

It may be worth stressing that this bound is at the same time a variational approximation, so that for reasonably good trial functions u_t and ϕ_{it}, one would expect the bound obtained to be quite close to the true value. Further, the form of the trial functions as well as the choice of the variational parameters which appear in them may be chosen according to an *optimum* procedure, namely, one which minimizes the right-hand side of the inequality, Eq. (2.5), subject to the requirements stated in Eqs. (2.1) and (2.4). Finally, as noted earlier, we must evaluate matrix elements of H but *not* of H^2.

The inequality of Eq. (2.5) reduces, for $k\to 0$, to the zero-energy result of reference 2. This may be verified by dividing Eq. (2.5) through by k^2 and letting $k\to 0$ and $R\to\infty$ such that $kR+\theta=\pi$, with $\theta\neq 0$. To complete the proof it need only be recognized that since kR is a fixed number less than π and since $\eta\to N\pi$ as $k\to 0$, there exists a $k_{\max}$, independent of R (provided R is large enough so that N negative-energy bound states exist), such that for all $k<k_{\max}$ we have $kR+\eta<(N+1)\pi$, implying that no positive-energy states exist in this range. (See Fig. 1.)

B. Potentials Which are Solvable Beyond $r=R$

The analysis of the previous subsection depended not on the fact that the potential vanish identically for $r>R$ but rather, more generally, that the Schrödinger equation be solvable in that region. The extension to the solvable potential is straightforward, but rather than demonstrate this in all of its generality, we will illustrate the point by a brief outline of the procedure in the particularly important case for which a pure Coulomb field exists for $r>R$; $V(r)$ is arbitrary for $r<R$. In the pure Coulomb region, the wave function may be written

$$u(r)=G_\theta(r)+\cot(\eta-\theta)F_\theta(r), \quad r>R, \tag{2.6}$$

[10] This choice can be restated as the condition that $w(r)$ must have an infinite logarithmic derivative at $r=R$. More generally, θ and R may be chosen such that the logarithmic derivative of $w(r)$ at $r=R$ has an arbitrarily specified value.

where $F_\theta(r)$ and $G_\theta(r)$ are defined in terms of the regular and irregular Coulomb functions, $F(r)$ and $G(r)$, respectively,[11] by the relations

$$F_\theta(r)=\cos\theta F(r)+\sin\theta G(r),$$
$$G_\theta(r)=-\sin\theta F(r)+\cos\theta G(r).$$

The choice of the normalization of $F(r)$ and of $G(r)$ is such that the asymptotic forms of $F_\theta(r)$ and $G_\theta(r)$ are

$$F_\theta(r)\to\sin(kr-\xi\ln 2kr+\sigma_0+\theta),\quad r\to\infty,$$
$$G_\theta(r)\to\cos(kr-\xi\ln 2kr+\sigma_0+\theta),\quad r\to\infty,$$

where

$$\xi=Z_1Z_2e^2/\hbar v,\quad \exp(2i\sigma_0)=\Gamma(1+i\xi)/\Gamma(1-i\xi).$$

The charges, Z_1e and Z_2e, can each be either positive or negative.

Introducing a trial function, $u_t(r)$, which, for $r>R$, is of the form given by Eq. (2.6) with η replaced by η_t, and introducing the difference function $w\equiv u_t-u$, we again obtain the Kato identity, Eq. (2.2).

With the choice of θ and of R such that

$$\tan\theta=-F(R)/G(R),$$

we have $F_\theta(R)=0$, whence $w(R)=0$. The problem is then the by now familiar one of obtaining a (lower) bound on

$$\int_0^R w(H-E)w\,dr,$$

where $w(0)=w(R)=0$. Since, in the *finite* domain, $0<r<R$, the operator H has a finite number of bound states, even though we allow for attractive Coulomb potentials,[12] the bound can be obtained in a manner identical to that used for the cutoff potential.

3. LOWER BOUND ON η

There is one weakness in the procedure described in Sec. 2, namely, one must assume that the correct number of states with energies less than E, which we have taken to be M, is precisely the number calculated in the process of diagonalizing the Hamiltonian matrix. In fact, it may be more, though it cannot be less. If the assumption is incorrect, that is, if one or more states have not been accounted for, there is no justification for the bound. The question of the correctness of the number of states is a rather more serious one at positive scattering energies that it was for the zero-energy case, for the number of positive-energy states will not be known experimentally. It is, therefore, of some interest that one can still extract some information which is of a rigorous nature. The results so obtained concern η, rather than $\cot(\eta-\theta)$. We will now describe a method for obtaining a rigorous lower bound on η, and we will then show that this result contains, as a special case, the one previously obtained by Risberg and by Percival. Further, the new result should always be used rather than the old one. [While the discussion could be carried through for $V(r)$ solvable beyond $r=R$ we will, for simplicity, consider cutoff potentials in the following.]

A. Use of the Conditional Inequality

We begin by recalling a theorem due to Wigner concerning the dependence of the phase shift on the scattering energy. Wigner showed[13] that if $V(r)$ vanishes identically for $r>R$, the identity

$$\frac{d\eta}{dk}=-R+\left(\frac{1}{2k}\right)\sin 2(kR+\eta)+2\int_0^R u^2dr \quad (3.1)$$

obtains, where $u(0)=0$ and where

$$u(r)=\sin(kr+\eta),\quad r\geqq R.$$

The integral is clearly non-negative. For $E\neq 0$, which is the concern of the present paper, it is in fact positive. It follows that for those values k_j for which

$$\zeta(k_j)\equiv k_jR+\eta(k_j)=j\pi, \quad (3.2)$$

where j is an integer (actually, as is shown below, j must be greater than N), we have

$$\left.\frac{d\zeta}{dk}\right|_{k_j}=R+\left.\frac{d\eta}{dk}\right|_{k_j}>0. \quad (3.3)$$

We will also have occasion to use a slight generalization of this last result, which also follows from Eq. (3.1), namely, that for $\zeta(k)$ in the range

$$j\pi\leqq\zeta(k)\leqq(j+\tfrac{1}{2})\pi,$$

the inequality $d\zeta(k)/dk>0$ is satisfied. A typical graph of $\zeta(k)$ *versus* k is given in Fig. 1. The relationship $\zeta(0)=N\pi$ which has been used is simply Levinson's theorem.[14]

Let the energy eigenvalues for the problem in which a particle is confined to the region $r\leqq R$, in the presence of the potential $V(r)$, be arranged in increasing order. We label the general positive-energy term in the se-

[11] See, for example, J. M. Blatt and L. C. Biedenharn, Phys. Rev. **86**, 399 (1952).

[12] A previous discussion of the zero-energy problem [see L. Spruch and L. Rosenberg, *Proceedings of the International Conference on Nuclear Forces and the Few Nucleon Problem, London, July, 1959*, Pergamon Press (to be published)] was restricted to the scattering of systems with like net charges. The present extension to include attractive Coulomb potentials (and nonzero scattering energies) is of course made possible by the additional restriction that the non-Coulombic component must vanish identically beyond a certain point.

[13] E. P. Wigner, Phys. Rev. **98**, 145 (1955). Alternative derivations of this causal inequality were subsequently given by M. A. Martin, Compt. rend. **243**, 22 (1956), and by E. Corinaldesi and S. Zienau, Proc. Cambridge Phil. Soc. **52**, 599 (1956). See also F. Smith, Phys. Rev. **118**, 349 (1960).

[14] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949).

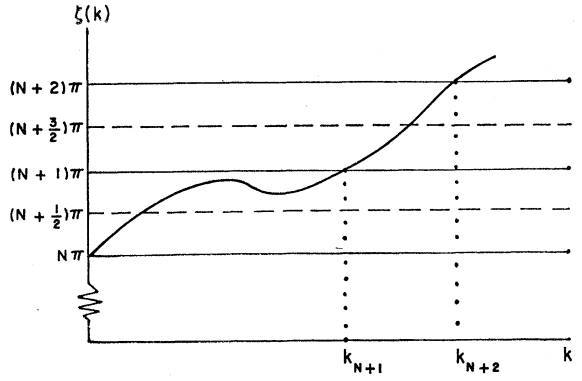

FIG. 1. A schematic plot of $\zeta(k)\equiv kR+\eta(k)$ *versus* k; $\zeta(k)$ need be defined only for non-negative energies. Since there are N negative-energy states, Levinson's theorem gives $\zeta(0)=N\pi$. By Wigner's causal inequality, $d\zeta(k)/dk>0$ for any interval of k which satisfies $j\pi\leqq\zeta(k)\leqq(j+\frac{1}{2})\pi$, where j is an integer, which, from the above discussion, must be greater than N. By continuity the slope will be positive for $\zeta(k)$ less than but sufficiently close to $(j+1)\pi$. The eigenvalues k_j are defined by $\zeta(k_j)=j\pi$. Once $\zeta(k)$ has passed through the value $j\pi$, which occurs at $k=k_j$, it can never return to that value. The k_j as defined above determine the positive-energy eigenstates, E_j, of the particle constrained to the interval 0 to R in the presence of the potential, $V(r)$, by the relationship $E_j=\hbar^2k_j^2/2\mu$.

quence by E_j $(j>N)$, and write

$$E_j=\hbar^2k_j^2/2\mu. \tag{3.4}$$

The sequence then is $E_1, \cdots, E_N, \cdots, E_j, \cdots$. The bound states are characterized by the requirement that the function vanish at $r=R$. Now consider that function which is identical with the jth bound state solution for $r\leqq R$ and which is a solution of the free wave equation for the energy E_j for $r>R$, with continuous value and slope at $r=R$. From uniqueness, this must be identical with the scattering solution, which is a multiple of $\sin[k_jr+\eta(k_j)]$ in the external region. Since this must vanish at $r=R$, it follows that $k_jR+\eta(k_j)$ must be a multiple of π.

To prove the equivalence of the two different definitions of k_j, Eqs. (3.2) and (3.4), it must still be shown that the multiple of π is in fact j itself. To see this, we note firstly that by Levinson's theorem, $\zeta(0)=\eta(0)=N\pi$. Further, it follows from Eqs. (3.2) and (3.3) that once $\zeta(k)$ has passed through a given multiple of π, it can never return to that value.[15] Thus $\zeta(k)$ starts, at $k=0$, at $N\pi$; at the first positive-energy bound state, which is the state labelled by $N+1$, it has the value $(N+1)\pi$. In general, then, we do in fact have that

$$k_jR+\eta(k_j)=j\pi, \quad j=N+1, N+2, \cdots,$$

and that $E_j=\hbar^2k_j^2/2\mu$ represents the jth bound state. It follows that if $j\pi<\zeta(k)<(j+1)\pi$, precisely j bound states of the associated energy eigenvalue problem exist with energies less than $\hbar^2k^2/2\mu$.

The fact that the k_j defined by Eq. (3.2) are identical with the k_j defined by Eq. (3.4) can also be proved,[16] with the aid of continuity arguments (the case $E=0$ must therefore be excluded in this particular proof), by studying the phase shift as the potential strength is built up from zero to its true strength.

We are now in a position to obtain a rigorous lower bound on η. Thus, suppose that M' bound states have been found with energies below the energy E. If $M'=M$, where M is the true number of such states, then the inequality satisfied by $k\cot(\eta-\theta)$, Eq. (2.5), is valid. If, however, $M'<M$, the above mentioned inequality, in which M' trial bound-state functions, ϕ_{tt}, are employed need not be valid. We may, however, simply *assume* that $M'=M$, which implies that

$$M'\pi\leqq kR+\eta(k)\leqq(M'+1)\pi.$$

If the assumption is correct, Eq. (2.5) will provide a lower bound on η, namely η_L, where η_L is a known number which is less than $(M+1)\pi-kR$. If, on the other hand, the assumption is incorrect we have $\eta>(M'+1)\pi-kR$. Therefore, the inequality $\eta>\eta_L$ is correct, independent of the validity of the original assumption, and we then have a rigorous lower bound on η.

In summary then, we have, if we have proved the existence of at least M' eigenstates of our bound-state problem with energies less than the scattering energy E, that

$$\eta>\eta_L, \tag{3.5a}$$

where η_L is defined by the relations

$$k\cot(\eta_L-\theta)=\text{right-hand side of Eq. (2.5)}, \tag{3.5b}$$

and

$$M'\pi-kR\leqq\eta_L\leqq(M'+1)\pi-kR. \tag{3.5c}$$

The technique of treating Eq. (2.5) as a conditional inequality which leads nevertheless to a rigorous lower bound on the phase shift is closely analogous to a procedure used earlier[17] in a study of the Kato method.

It should be remarked that while the lower bound on η is rigorous even when one has not accounted for all of the bound states, a situation quite different from that for the upper bound on $\cot(\eta-\theta)$, the lower bound on η deduced when $M\neq M'$ is a very poor one, being too small by roughly $(M-M')\pi$.

B. Comparison with Risberg-Percival Result

During the course of the last derivation, we arrived at the result that $\zeta(k)>j\pi$ if $k>k_j$. This inequality

[15] Actually, the fact that $\zeta(k)$ has a positive slope at *zero* energy does not follow from the Wigner inequality, which reduces to a trivial identity at $k=0$, but rather can be established directly. We first observe that $d\zeta/dk|_{k=0}=R-A$, where A is the scattering length. Now if R were less than A the existence of a zero-energy scattering function which vanishes at $r=A$ would imply that a zero-energy bound state exists in a box of radius A. This state would disappear if the radius of the box were reduced to R, which, however, runs counter to the condition mentioned in reference 7, which we have placed on R.

[16] I. C. Percival, Phys. Rev. **119**, 159 (1960).

[17] See the second paper mentioned in reference 9, and Sec. 5 of the present paper.

itself clearly provides a lower bound on the phase shift for a scattering energy which lies above the appropriate level. With the method of Hylleraas and Undheim[18] upper bounds, E_{jU}, may be found, yielding a discrete set of scattering energies for which a lower bound on the phase shift is determined. This method for getting a bound on $\eta(k)$ is essentially that given earlier by Risberg[19] and by Percival.[20] The similarity between their result and that deduced in the previous subsection, which grew out of a quite different approach, is rather striking and it may be of some interest to compare the two. We first note that their result can be derived using Eq. (2.5) and the concept of the "conditional inequality." The question then arises whether the present technique affords any improvement. While it is perhaps not appropriate here to present the analysis in detail we might indicate that an improvement does exist, and may be traced to the fact that the inequality, Eq. (2.5), is based on the use of a sharper form of the Hylleraas-Undheim theorem than they used. Thus, suppose a set of orthonormal functions, ϕ_{it}, where $1\leqq i\leqq M'+1$, has been found which diagonalizes the $(M'+1)\times(M'+1)$ Hamiltonian matrix. The functions ϕ_{it} will, in general, still contain some free variational parameters. According to the Hylleraas-Undheim theorem we have

$$E_{M'+1}\leqq\int\phi_{M'+1,t}H\phi_{M'+1,t}dr;$$

the best result, for a given form of functions ϕ_{it}, is obtained by choosing the variational parameters to minimize the right-hand side of the inequality. Clearly, a lower value of the bound on $E_{M'+1}$ can be determined by dropping the restriction that $\phi_{M'+1,t}$ be orthogonal to the remaining M' trial functions. It may be claimed that this lower value is better only if it is still guaranteed to lie above the exact value, $E_{M'+1}$. To see that this guarantee *can* be made, provided $(\phi_{kt},H\phi_{kt})<E_{M'+1}$, where $1\leqq k\leqq M'$, we note that the inequality we have obtained for $\int w(H-E)wdr$ may be rewritten as

$$\int\phi_{M'+1,t}(H-E)\phi_{M'+1,j}dr\geqq 0,\quad E<E_{M'+1},$$

where

$$\phi_{M'+1,t}\equiv w-\sum_{k=1}^{M'}\frac{(\phi_{kt},[H-E]w)}{(\phi_{kt},[H-E]\phi_{kt})}\phi_{kt}.$$

Here, for the purpose of the present discussion, w is an arbitrary function which satisfies the appropriate boundary conditions. While the $(M'+1)\times(M'+1)$ matrix, formed from the operator $H-E$ using functions ϕ_{kt}, where $1\leqq k\leqq M'$, and $\phi_{M'+1,t}$ as defined above, is diagonal, no orthogonality restrictions exist for $\phi_{M'+1,t}$.

[18] E. A. Hylleraas and B. Undheim, Z. Physik **65**, 759 (1930).
[19] V. Risberg, Arch. Math. Naturvidenskab **53**, 1 (1956).
[20] I. C. Percival, Proc. Phys. Soc. (London) **70**, 494 (1957).

We have, therefore, an improved form of the Hylleraas-Undheim theorem. The improvement carries over to the scattering problem by virtue of the Wigner inequality, from which we conclude that an estimate of $j\pi$ for $\zeta(k)$ will have increased accuracy as k approaches k_j from above, at least for k sufficiently close to k_j such that $\zeta(k)<(j+\frac{1}{2})\pi$.

Had the sharpened form of the Hylleraas-Undheim method been used in the Risberg or Percival derivation, the superiority of our method, as discussed above, would disappear for the scattering energies E_{jU} obtained from the Hylleraas-Undheim method. There is however an inherent advantage, which is primarily one of convenience, associated with the present method. The point is that their results, while rigorous, are reasonably accurate only for energies equal to or slightly greater than the energies E_{jU}. Thus, for any energy E greater than E_{jU}, it follows that $E>E_j$ and hence that $\zeta(k)>\zeta(k_j)=j\pi$, that is, that $\eta(k)>j\pi-kR$; however, while rigorous, the accuracy of this last estimate diminishes rapidly as the difference between E and E_j increases. In order to obtain reasonably accurate phase shifts over a range of energies, it would then be necessary to repeat the calculation for various values of R. On the other hand, Eq. (3.5a) is explicitly rigorous and variational for a range of energies above $E_{M'U}$, and one would have to perform the calculation for only one value of R.

4. UPPER BOUND ON η

The fact that a lower bound on η can be obtained using a minimum principle, so that a well-defined procedure exists for improving the calculation, has the consequence that quite accurate estimates of the phase shift should often be obtainable. Nevertheless, since both bounds on η are required to obtain an absolute measure of the accuracy of the calculation it is of interest to examine the question of determining an upper bound. Again we exploit the connection between the scattering and bound-state problems. We shall describe two methods, both of which involve a determination of a lower bound on an energy eigenvalue. The practical utility of the results obtained is considerably diminished, as compared to the methods described in the previous sections for obtaining the other bound on η, since it is far more difficult, in general, to obtain a lower bound than an upper bound on an energy eigenvalue.

A. Use of Wigner Inequality

To find then an upper bound on η, first observe that according to the discussion in Sec. 3, the inequality

$$\zeta(k)<(M+1)\pi$$

is valid for energies $E<E_{M+1}$, where k is the wave number corresponding to the scattering energy E. Thus, if $E_{M+1,L}$ is a lower bound on E_{M+1}, and if $k_{M+1,L}$ is

the corresponding wave number, we have

$$\eta(k_{M+1,L})<(M+1)\pi-k_{M+1,L}R.$$

The accuracy of this bound will generally increase as the estimate of the lower bound on E_{M+1} is improved. Since we are now operating in the region in which the slope of $\zeta(k)$ can be negative, this last statement cannot be made more precise; the best that one can say is that the accuracy of the bound will necessarily increase with increasing accuracy for the lower bound on E_{M+1} if $\zeta(k)$ is sufficiently close to an integral multiple of π.

B. Use of Energy Eigenfunction Expansion

We again employ the difference function, $w(r)$, as a trial function in the energy eigenvalue problem introduced in Sec. 2A. Thus, with $w(r)$ satsifying the boundary conditions

$$w(0)=w(R)=0,$$

we have

$$\int_0^R w(H-E-c)^2wdr=\sum_{i=1}^{\infty} a_i^2(E_i-E-c)^2,$$

where the expansion coefficients, a_i, are defined by

$$a_i=(w,\phi_i),$$

and where c is an energy value as yet unspecified. The sum is clearly larger than

$$[\min(E_i-E-c)^2]\sum_{i=1}^{\infty} a_i^2=[\min(E_i-E-c)^2]\int_0^R w^2dr.$$

Now let $c=\frac{1}{2}(E_{M+1}-E)$, where E_{M+1} is the smallest eigenvalue which lies above E. Then we may write

$$\min(E_i-E-c)^2=\min[E_i-\tfrac{1}{2}(E_{M+1}+E)]^2 =[\tfrac{1}{2}(E_{M+1}-E)]^2,$$

the minimum value being achieved for $E_i=E_{M+1}$, so that

$$\int_0^R w[H-E-\tfrac{1}{2}(E_{M+1}-E)]^2wdr \geqq[\tfrac{1}{2}(E_{M+1}-E)]^2\int_0^R w^2dr,$$

which may be rewritten as

$$\int_0^R w(H-E)^2wdr\geqq(E_{M+1}-E)\int_0^R w(H-E)wdr.$$

Using the Hermiticity of $H-E$, we obtain the inequality

$$\int_0^R w(H-E)wdr\leqq(E_{M+1}-E)^{-1}\int_0^R[(H-E)u_t]^2dr.$$

If then we can find a lower bound $E_{M+1,L}$ on E_{M+1} which at the same time satisfies $E<E_{M+1,L}$, we have the sought-for inequality

$$\int_0^R w(H-E)wdr\leqq(E_{M+1,L}-E)^{-1}\int_0^R[(H-E)u_t]^2dr.$$

While both methods described in this section for obtaining an upper bound on η require that one find a lower bound on an energy eigenvalue, the second method has the advantage that an accurate upper bound on η may be obtained if one can choose a sufficiently accurate trial scattering function, even if a quite crude lower bound on the energy eigenvalue is employed.

In a similar manner, the other bound on the error integral may be obtained as

$$\int_0^R w(H-E)wdr\geqq(E_{MU}-E)^{-1}\int_0^R[(H-E)u_t]^2dr.$$

Here E_{MU} is an upper bound on E_M which is in turn the largest eigenvalue below E. This latter result is of little interest, however, since it is inferior to the result obtainable from the inequality of Eq. (2.5). The proof of this statement is quite similar to a proof given in Sec. 5.

C. Lower Bound on Energy Eigenvalue

We will discuss very briefly the question of determining a lower bound on E_{M+1}. One possibility would be to use a solvable comparison problem. A more general method would be to use a technique that involves

$$G(r,r';R;E)=(1/k)\sin kr_<(\cos kr_>-\cot kR\sin kr_>),$$

which represents the Green's function for a particle confined to a spherical box of radius R within which there is no potential. $r_<$ and $r_>$ represent the smaller and the larger, respectively, of the quantities r and r'. Thus, let $k_{M+1,L}$ represent the wave number corresponding to the lowest value of the energy, to be denoted by $E_{M+1,L}$, which satisfies

$$\left(\frac{2\mu}{\hbar^2}\right)\int_0^R G(r,r;R;E_{M+1,L})|V(r)|dr=M.$$

If

$$k_{M+1,L}R<\pi, \tag{4.1}$$

it can be shown[21] that $E_{M+1,L}$ is in fact a lower bound on E_{M+1}.

[21] The above results are generalizations of the result due to Bargmann [V. Bargmann, Proc. Natl. Acad. Sci. U. S. **38**, 961 (1952)] that the necessary condition for the existence of N (negative energy) bound states of angular momentum zero in the full range 0 to ∞ is

$$\left(\frac{2\mu}{\hbar^2}\right)\int_0^{\infty} r|V(r)|dr>N.$$

A paper on the use of Green's functions in the derivation of necessary conditions for the existence of bound states of given angular momentum and below a specified energy, for a particle in a center of force, is in preparation.

If Eq. (4.1) is not satisfied, one can still obtain a lower bound $E_{M+1,L}$ on E_{M+1} (at least in principle) by finding the smallest value $E_{M+1,L}$ which satisfies

$$(2\mu/\hbar^2)\ \mathrm{Trace}[G(E_{M+1,L})|V|]^2=M.$$

We omit further discussion of the possibilities of this technique.

We might note that the fact that the potential exists only in a finite range considerably enhances the likelihood of being able to obtain a lower bound on an energy eigenvalue.

5. UPPER BOUND ON $\cot(\eta-\theta)$ USING POTENTIAL EIGENFUNCTIONS

We now consider an alternate approach to the problem of finding an upper bound on $k\cot(\eta-\theta)$ for cutoff potentials. Instead of the energy eigenvalue problem of Sec. 2 we introduce an associated potential-strength eigenvalue problem, with an auxiliary potential $\rho(r)$ which satisfies $\rho(r)\geqq 0$ for $r\leqq R$ and $\rho(r)=0$ for $r>R$, but which is otherwise arbitrary and which will be chosen for convenience. We then consider the equation

$$(H-E)\varphi=\mu\rho\varphi,$$

with boundary conditions

$$\varphi(0)=0,\quad \varphi(r)=\text{const}\sin[kr+\delta(\mu)]\quad \text{for}\quad r\geqq R.$$

The eigenfunctions φ_n and their corresponding potential-strength eigenvalues, μ_n, are defined by the condition

$$\delta(\mu_n)=\theta+n\pi.$$

The fact that $\rho(r)$ vanishes for $r>R$ implies the existence of a lowest eigenvalue. Thus, by comparison with the infinitely repulsive square well of range R we have

$$\delta(\mu)\geqq -kR\quad \text{for all } \mu,$$

so that, if

$$\theta-(P+1)\pi\leqq -kR<\theta-P\pi,$$

then

$$\mu_n\geqq\mu_{-(P+1)}\quad \text{for all } n.$$

Here we have made use of the monotonicity of $\delta(\mu)$ with respect to μ. (It may be of interest to note that in the associated energy eigenvalue problem, the potentials which one considers are those for which there exists a lowest energy eigenvalue; the potential had to be cut off to make the energy eigenvalues everywhere discrete. In the associated potential-strength eigenvalue problem, on the other hand, the potential strength eigenvalues are automatically discrete for $E\neq 0$, and one had to cut off the potential in order that there should be a lowest potential strength eigenvalue.)

The bound on $\cot(\eta-\theta)$ that will be deduced will utilize the Hylleraas-Undheim theorem again. This time, however, the theorem is applied not to the eigenstates with energy eigenvalues less than the energy E under consideration, but rather to potential strength eigenstates with potential strength eigenvalues less than the potential strength under consideration, namely, $\mu=0$. [It is to be recalled that $\eta(k)=\delta(0)$.] In other words, eigenstates for which μ_n is negative are involved. In this connection it may be noted that for the specific choice

$$kR+\theta=(P+1)\pi, \tag{5.1}$$

the relevant number of states with negative eigenvalues μ_n is equal to the number of states which appear using the energy eigenfunction approach. To see this we recall (see Sec. 3) that

$$M\pi-kR\leq\delta(0)=\eta(k)\leqq(M+1)\pi-kR,$$

or

$$(M-P-1)\pi+\theta\leqq\delta(0)\leqq(M-P)\pi+\theta.$$

The negative eigenvalue, smallest in absolute value, is then μ_{M-P-1}. Since, from Eq. (5.1), the lowest eigenvalue is $\mu_{-P-1}(\mu_{-P-1}=-\infty)$ there are in all $M+1$ negative eigenvalues. However, the eigenfunction φ_{-P-1} vanishes for $0\leqq r\leqq R$ and is therefore orthogonal, with respect to the weight factor $\rho(r)$, to the other eigenfunctions, so that the number of relevant eigenfunctions is M, for arbitrary $\rho(r)$.

We now return to the case for which R and θ are arbitrary, and we let T denote the exact (unknown) number of negative-value eigenvalues μ_n for this case. [We have just seen that for the choice of R and of θ which satisfies Eq. (5.1), T is equal to M.] Let us now assume that we have found T' trial functions φ_{nt} which satisfy the conditions

$$\varphi_{nt}(0)=0,\quad \varphi_{nt}(r)=C_{nt}\sin(kr+\theta)\quad \text{for}\quad r\geqq R,$$

$$\int_0^R\varphi_{nt}\varphi_{mt}\rho dr=\delta_{nm},$$

$$\int_0^R\varphi_{nt}(H-E)\varphi_{mt}dr=\mu_{nt}\delta_{nm},\quad \mu_{nt}=\mu_{nt}(T')<0. \tag{5.2}$$

The indices n and m, here and below (except where specifically indicated otherwise) each run through the T' integers $-P$ to $-P+T'-1$. The C_{nt} are independent of r. By the Hylleraas-Undheim theorem, the $\mu_{nt}(T')$, when put into an ordered sequence, satisfy the inequalities $\mu_{nt}(T')\geqq\mu_n$, where μ_n is the corresponding member of the ordered sequence of exact eigenvalues. Further, if a $(T'+1)\times(T'+1)$ matrix of $(H-E)$ is formed, with the first T' functions φ_{nt} the same as before, and if the eigenvalues of this matrix are labelled $\mu_{nt}(T'+1)$, then for the first T' values of n, we have $\mu_{nt}(T')\geqq\mu_{nt}(T'+1)$. The situation is then similar to that which obtained at zero energy, and at nonzero energies with the introduction of an associated energy eigenvalue problem. It follows that *if* $T'=T$, then we may deduce a bound on $\int_0^R w(H-E)wdr$ which, when

inserted into the Kato identity, yields the inequality

$$k\cot(\eta-\theta)\leqq k\cot(\eta_t-\theta)+\left(\frac{2\mu}{\hbar^2}\right)\int_0^R u_t(H-E)u_t dr$$

$$-\left(\frac{2\mu}{\hbar^2}\right)\sum_{n=-P}^{-P+T'-1}\frac{1}{\mu_{nt}}\left[\int_0^R \varphi_{nt}(H-E)u_t dr\right]^2. \quad (5.3)$$

The trial scattering function, u_t, and the difference function, w, satisfy Eqs. (2.1) and (2.3). In particular, the logarithmic derivative of $w(r)$ at $r=R$ is just that assumed by the φ_{nt} which allowed us to use $w(r)$ as a trial eigenfunction in the application of the Hylleraas-Undheim theorem (in its sharpened form).

The bound given by Eq. (5.3) is very much simpler to calculate than the corresponding bound deduced by Kato. Further, it will lead to a more accurate bound for the same trial scattering function u_t. The proof of this statement follows from the observation that the φ_{nt} may be considered to be the first T' functions of a complete set of functions, which we denote by $\{\varphi_{nt}\}$, with $-P\leqq n\leqq\infty$. We then have

$$\sum_{n=-P}^{-P+T'-1}\frac{1}{\mu_{nt}}\left[\int_0^R \varphi_{nt}(H-E)u_t dr\right]^2$$

$$\geqq\frac{1}{\mu_{-P+T'-1,t}}\sum_{n=-P}^{-P+T'-1}\left[\quad\right]^2$$

$$\geqq\frac{1}{\mu_{-P+T'-1,t}}\sum_{n=-P}^{\infty}\left[\quad\right]^2$$

$$=\frac{1}{\mu_{-P+T'-1,t}}\int_0^R\frac{[(H-E)u_t]^2}{\rho(r)}dr,$$

where in the last step we have used the closure property of the set $\{\varphi_{nt}\}$. If we identify $-\mu_{-P+T'-1,t}$ with the trial value of β to be used in the calculation of the Kato bound then the superiority of Eq. (5.3) is established, since in reducing it to the Kato result we have employed inequalities which decrease the accuracy of the bound. It might be mentioned that the Hylleraas-Undheim theorem is a general method for obtaining a bound on β; it is however restricted to cutoff potentials, and it must always be assumed that the correct number of negative eigenvalues μ_n have been obtained.

The weakness of Eq. (5.3) is that we cannot in general be certain that $T'=T$. Proceeding as in Sec. 3, we can once again use the conditional inequality technique to obtain a rigorous bound on η. Thus, *assuming* that $T'=T$, it follows that

$$T'\pi<\delta(0)-\delta(\infty)<(T'+1)\pi,$$

or that

$$T'\pi-kR<\eta(k)<(T'+1)\pi-kR.$$

We have, as a rigorous consequence, that

$$\eta>\eta_L', \quad (5.4a)$$

where η_L' is defined by

$$k\cot(\eta_L'-\theta)=\text{right-hand side of Eq. (5.3)} \quad (5.4b)$$

$$T'\pi-kR<\eta_L'<(T'+1)\pi-kR. \quad (5.4c)$$

The point is, of course, that if T' is less than T, then the inequality of Eq. (5.4a) is *a fortiori* true.

We now wish to compare the results based on the associated energy eigenvalue problem and on the associated potential-strength eigenvalue problem. It can be shown, in fact, that the latter result includes the former as a special case. To see this we simply choose $\rho(r)=\rho_0$, for $r\leqq R$, where ρ_0 is a positive constant with the dimensions of energy, and choose R and θ such that $kR+\theta$ is an integral multiple of π. Since the inequality, Eq. (5.3), is independent of the normalization of the φ_{nt} the orthonormality condition given in Eqs. (5.2) may be replaced by

$$\int_0^R \varphi_{nt}\varphi_{mt}dr=0, \quad n\neq m.$$

Therefore, the form of the inequality for the error integral, and the conditions satisfied by the functions $w(r)$, $u_t(r)$, and the $\varphi_{nt}(r)$ (there is a trivial difference in the normalization of the φ_{nt} and of the ϕ_{it}) are the same as those of Sec. 2.