Positive energy Weinberg states for the solution of scattering problems

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Positive energy Weinberg states are defined and numerically calculated in the presence of a general complex Woods-Saxon potential. The numerical procedure is checked for the limit of a square well potential for which the Weinberg states and the corresponding eigenvalues are known. A finite number M of these (auxiliary) positive energy Weinberg states are then used as a set of basis functions in order to provide a separable approximation of rank M, V_M, to a potential V, and also to the scattering matrix element S which obtains as a result of the presence of V, S_M. Both V_M and S_M are obtained by means of algebraic manipulations which involve the matrix elements of V calculated in terms of the auxiliary positive energy Weinberg states. Next, expressions are derived which enable one to iteratively correct for the error in $V-V_M$. These expressions are a modified version of the quasiparticle method of Weinberg. The convergence of S_M to S, as well as the first order iteration of the error in S_M, is examined as a function of M for a numerical example which uses a complex Woods-Saxon potential for V and assumes zero angular momentum. With $M=5$ and one iteration an error of less than 10% in S is achieved; for $M=8$ the error is less than 1%. The method is expected to be useful for the solution of large systems of coupled equations by matrix techniques or when a part of the potential is nonlocal.

[NUCLEAR REACTIONS Scattering theory, expansions on a basis set of positive energy Weinberg states, removal of truncation error by the quasiparticle method. Normal mode effective scattering channels.]

I. INTRODUCTION

Weinberg states, also called Sturmian functions, were introduced many years ago into the physics literature.[1-6] Negative energy Weinberg states, which asymptotically decrease exponentially (like bound states) have been used as a discrete basis set in the case of scattering of composite particles,[1,3] in order to evaluate the effect of the breakup of a target, consisting of a bound state of two or more particles, by the scattering of a third particle.

The positive energy Weinberg states also form a discrete set. Asymptotically they have only outgoing waves, all with the same wave number corresponding to the physical scattering energy. They are regular at the origin, and they differ from each other by the number of nodes within the scattering region. These functions have been used as an aid in the solution of scattering equations, particularly as a way to extend shell model methods into the continuum.[5] However, since the exact Weinberg states are as hard to calculate as the scattering solution itself, only rough approximations to the positive energy Weinberg states have been found practical thus far. These approximations consist of Gamow states (complex energy), scattering states (at the physical energy), or resonance states (at a nearby energy), calculated for a much simplified Hamiltonian, as reviewed by Romo.[6] Or approximations to the Weinberg states have been simply guessed.[2]

The advantage of using such states, even though approximate, is to obtain a finite rank separable approximation for a potential whose effect is hard to calculate exactly or a separable expression for the Green's function. The separability enables one to approximate the solution by means of algebraic equations, and the correction to the approximation can then be found, within the quasiparticle formal-

ism,[2] by iterations which converge.

It is the purpose of the present paper to provide a method of obtaining systematic approximations to the positive energy Weinberg states, by solving only local uncoupled Schrödinger equations in the presence of an auxiliary potential $\bar{V}(r)$ and then by inverting algebraic equations. The hope is to eventually provide a systematic way of solving either large systems of coupled equations, or nonlocal equations,[7] by methods which are numerically faster than the ones used until now. These methods either solve numerically the N coupled equations N times, or use a set of expansion functions.[8,9] The present method also uses a set of expansion functions, which are the Weinberg states, but requires no division into interior and exterior regions, and rests on the well developed theoretical foundation of the quasiparticle formalism.[2]

In Sec. II, the Weinberg states will be defined and their properties reviewed, in the present context, even though Weinberg[2] has already given an extensive discussion of their properties. In Sec. III a numerical calculation is described and comparison is made with results based on analytical expressions obtained for the square well potential.

In Secs. IV and V the scattering solution is expanded in Weinberg states, convergence for the scattering matrix elements is examined, and a Green's function which corrects for the truncation errors is written down.

In Sec. VI the eigenstates of the operator G_0V are discussed, and a relation established with the functions encountered in Sec. IV. In Sec. VII expressions needed for the quasiparticle iterative method are derived, and a numerical example of the first order iteration in $G_M(V-V_M)$ is given. Section VIII contains the summary and conclusions.

II. THE AUXILIARY WEINBERG STATES

The auxiliary Weinberg states are denoted as $\phi_j(r)$ with $j=1,2\ldots$. They obey the equation

$$(H_0-E)\phi_j(r)=-\alpha_j\bar{V}(r)\phi_j(r)\ , \tag{2.1}$$

where

$$H_0=-\frac{\hbar^2}{2m}d^2/dr^2+V_0(r)\ . \tag{2.2}$$

The distorting potential V_0 is assumed to be local. It contains the centrifugal potential as well as a Coulomb potential, should it be present. The α's are the Weinberg eigenvalues. The potential $\bar{V}$ is an auxiliary potential, to be chosen such that its range is similar to the nonlocal or off diagonal coupling potential to be introduced later. In case there is coupling between several channels, one $\bar{V}_n$ will be introduced in each channel n so that Eq. (2.1) remains uncoupled. The boundary conditions for the ϕ_j are

$$\phi_j(r)=0,\quad r=0\ , \tag{2.3a}$$

$$\phi_j(r)\approx\beta_jH_L^{(+)}(r),\quad r\to\infty\ , \tag{2.3b}$$

where $H_L^{(+)}$ is the usual outgoing radial Coulomb wave function corresponding to angular momentum L and energy E. If the latter is negative one obtains the usual negative energy Weinberg states, which decay exponentially at large distances. If the energy is positive, the complex constants α_j are such that the net potential $V_0+\alpha_j\bar{V}$ has a positive imaginary part, such that it becomes "emissive," rather than what is usually the case in optical model applications, where it is absorptive. The constants β_j are fixed by the normalization of the ϕ's, which is

$$\int_0^\infty\phi_i(r)\bar{V}(r)\phi_j(r)\,dr=(1/\alpha_j)\delta_{ij}\ . \tag{2.4}$$

A differently normalized set of Weinberg functions $\varphi_j(r)$ is also convenient. They obey the same equation as the ϕ's, in particular the eigenvalues α_i are the same, but asymptotically they are all equal to $H_L^{(+)}(r)$

$$\phi_j(r)=\beta_j\varphi_j(r);\quad \varphi_j\approx H_L^{(+)}\ . \tag{2.5}$$

As a result of Eq. (2.4) one obtains

$$\beta_j=\left[\alpha_j\int_0^\infty\varphi_j\bar{V}\varphi_j\,dr\right]^{-1/2}\ . \tag{2.6}$$

The normalization, Eq. (2.4) for the ϕ's is so chosen as to make a matrix $\underline{V}$, to be defined further on, symmetric.

It should be noted that if V is multiplied by a constant factor λ, then the eigenvalues α_j are divided by the same factor, and the quantities β_j, $\varphi_j(r)$, and $\phi_j(r)$ remain unchanged. One can also modify V_0 by adding to it a multiple q times $\bar{V}$

$$V_0\to V_0'=V_0+q\bar{V}\ . \tag{2.7a}$$

Then, by inspection of Eq. (2.1), one sees that the α's are all shifted by the same amount q

$$\alpha_j\to\alpha_j'=\alpha_j-q\ , \tag{2.7b}$$

while the φ's remain unchanged. In view of Eq. (2.6), the normalization constants β_j change and thus the ϕ_j also changes.

$$\phi_j \rightarrow \phi_j' = (1-q/\alpha_j)^{-1/2}\phi_j \quad (2.7c)$$

$$= (\alpha_j - q)^{-1/2}\langle \varphi_j \bar{V} \varphi_j \rangle^{-1/2}\varphi_j \ . \quad (2.7d)$$

If $G_0(r,r')$ is the Green's function $(E-H_0+i\epsilon)^{-1}$ for the left hand side of Eq. (2.1), then this equation can also be written

$$\int_0^\infty G_0(r,r')\bar{V}(r')\phi_j(r')\,dr' = (1/\alpha_j)\phi_j(r) \ , \quad (2.8)$$

i.e., ϕ_j is an eigenstate of $G_0\bar{V}$ and the corresponding eigenvalue is $1/\alpha_j$. For values of α_j inside the unit circle iterations in $G_0\bar{V}$ do not converge.[2]

A numerical example of Weinberg eigenvalues α_j and eigenfunctions φ_j is given in Table I and Fig. 1, respectively. The numerical procedure used to calculate these quantities is described in Sec. III. The potential V_0 in Eq. (2.1) is set equal to zero and $\bar{V}$ is a real Woods-Saxon potential of depth $\bar{V}_0 = -50$ MeV, radius $\bar{R}_0 = 3$ fm, and diffuseness $\bar{a}_0 = 0.5$ fm. The projectile is a neutron of 15 MeV laboratory energy, incident on a nucleus of ^{16}O. This example is the same as that used by Soper[10] in his study of the Born and Sasakawa-Austern[11] series.

As the table shows, for a depth of 50 MeV for $\bar{V}$, not all eigenvalues lie outside the unit circle and hence the Born series will not converge. If the depth of $\bar{V}$ is changed from 50 MeV to $50\times 0.255 = 12.75$ MeV the first eigenvalue would just lie on the unit circle, and all others would be outside, i.e., the Born series would just cease to converge. This is close to the value of ~ 15 MeV estimated by Soper to be the convergence limit. If the depth of $\bar{V}$ is changed to $50\times 0.806 = 40.3$ MeV, then the first two eigenvalues α lie within the unit circle and the Born series diverges strongly while the Sasakawa-Austern series[11] still converges. (The latter begins to diverge at 55 MeV.[10]) In Fig. 1 the first four eigenfunctions φ_j are displayed. One sees how for each increment in the index j an additional node appears in the wave function, and that beyond the range of $\bar{V}$ all functions become identical. The first of these functions is qualitatively similar to the expression $[1-\exp(-r/a)]\exp(ikr)$ given by Weinberg for the Hulthen potential.[2] It has no node within the range of $\bar{V}$.

III. THE NUMERICAL CALCULATION

The numerical code solves the Schrödinger equation by the Numerov method, for an initially guessed value of α_j. The corresponding potential is $V_0 + \alpha_j\bar{V}$. A matching radius R_{int} is chosen somewhere inside the radial region where the potential is appreciable. The function φ_j is started as a regular function at the origin and is integrated out towards R_{int}. Next, the function is independently started at an asymptotic radius R_M, where it obeys the boundary conditions given by Eq. (2.3b), and is integrat-

TABLE I. Values of α_j[a] and $|\beta_j|$[a] for a 50 MeV deep Woods-Saxon potential.[b]

j	$R_e\alpha_j$	$I_m\alpha_j$	$\lvert\alpha_j\rvert$	$\lvert\beta_j\rvert^{-1}$
1	−0.100	−0.235	0.255	3.61
2	0.652	−0.474	0.806	3.96
3	2.103	−0.710	2.22	5.25
4	4.196	−0.963	4.30	6.17
5	6.930	−1.218	7.04	6.91
6	10.31	−1.473	10.41	7.57
7	14.32	−1.730	14.43	8.16
8	18.98	−1.986	19.09	8.71
9	24.29	−2.242	24.39	9.23
10	30.23	−2.498	30.34	9.72
11	36.82	−2.754	36.92	10.18
12	44.05	−3.010	44.15	10.62
13	51.92	−3.267	52.02	11.04

[a]The α_j are potential eigenvalues defined in Eq. (2.1). The asymptotic value of the Weinberg states is given in terms of β_j, defined in Eqs. (2.3b) and (2.6).

[b]The potential V_0 in Eq. (2.2) is set equal to zero. The potential $\bar{V}$ is of a real Woods-Saxon form with depth radius and diffuseness given by −50 MeV, 3 fm, 0.50 fm. This potential has also been used by Soper (Ref. 10) as a test of convergence of the Sasakawa-Austern series.

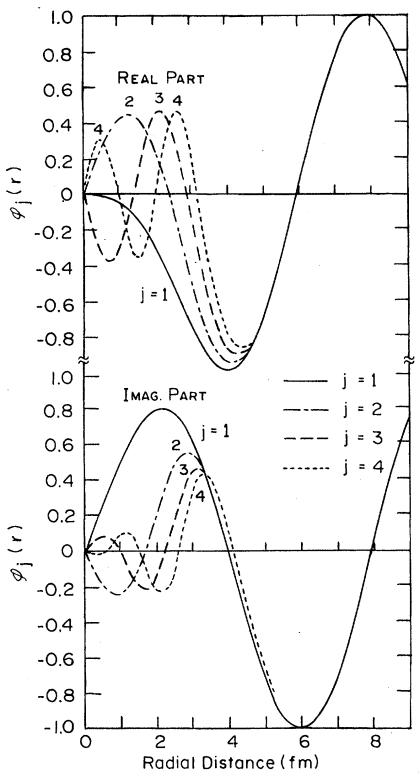

FIG. 1. Real and imaginary parts of positive energy Weinberg states, defined in Eq. (2.1) for 15 MeV neutrons incident on ^{16}O. The eigenvalues are given in Table I, the potential V_0 is set equal to zero, $\bar{V}$ is a real Woods-Saxon potential of radius $R=3$ fm, diffuseness $a=0.5$ fm, and depth -50 MeV. The angular momentum L is zero.

ed inward towards the radius $R_{\rm INT}$. From the discrepancy between the two derivatives at $R_{\rm INT}$ a correction for α is determined.

If the incorrect value of α is denoted as α_n, and the corresponding solutions of Eq. (2.1) are $\varphi^n_{\rm out}$ and $\varphi^n_{\rm in}$, respectively, and if the correct (but unknown) quantities are denoted by α and φ, then one obtains for the correction $\Delta\alpha=\alpha-\alpha_n$ the exact result

$$\Delta\alpha=(\hbar^2/2m)[\varphi(d\varphi^n_{\rm in}/dr-d\varphi^n_{\rm out}/dr)]_{R_{\rm INT}} \times\left[\int_0^{R_{\rm INT}}\varphi\bar{V}\varphi^n_{\rm out}dr+\int_{R_{\rm INT}}^{\infty}\varphi\bar{V}\varphi^n_{\rm in}dr\right]^{-1}. \tag{3.1}$$

Here it is assumed that $\varphi^n_{\rm out}$ is normalized such that $\varphi^n_{\rm out}=\varphi^n_{\rm in}$ at $r=R_{\rm INT}$. If φ is replaced by $\varphi_{\rm out}$ and $\varphi_{\rm in}$ in the two radial intervals $(0,R_{\rm INT})$ and $(R_{\rm INT},R_M)$, respectively, the desired iteration correction $(\Delta\alpha)_n$ to α_n is obtained.

Once convergence sets in, the error in α_n decreases approximately by one significant figure for each successive iteration. The result is, of course, independent of the choice for $R_{\rm INT}$. The initial guess for α_j is taken from a treatment of the square well case,[5] where j is taken to have a value larger than ten.

For large values of j one obtains for the square well case

$$r_0^2(m/\hbar^2)W_j\simeq kr_0+O(j^{-2}), \tag{3.2}$$

$$r_0^2(m/\hbar^2)(E-V_j)\simeq\tfrac{1}{2}(j-\tfrac{1}{2})^2\pi^2+O(j^{-2}). \tag{3.3}$$

Here V_j+iW_j is the depth of the square well potential of radius r_0 for the energy E, which accommodates the j'th Weinberg state. The corresponding value of α_j is obtained by equating V_j+iW_j to $V_0+\alpha_j\bar{V}$ at some convenient radius. One sees from the above that $|\alpha_j|$ goes to zero as j^{-2} for large values of j, and that as E increases, so does V_j. Once the value of α_j is found, the next value of α_{j-1} is searched for along the straight line in the complex plane which connects α_j to the origin. The value α_{j-2} is searched for along the straight line which connects α_j to α_{j-1}, and so on until $\alpha_{j=1}$ is found.

The results reported in Tables I and II are performed with an integration step of 0.031 25 fm between 0 and 11 fm. The overlap integrals are performed using Simpson's rule, and an accuracy of 1 part in 10^3 is obtained when the calculation is performed in single precision on an IBM 360/65. The Central Processing Unit (CPU) time required for obtaining 13 Weinberg states and performing the manipulations indicated in Table II is approximately 60 s.

A check of the code is obtained by assuming a Woods-Saxon dependence for $\bar{V}$, setting V_0 equal to zero, and decreasing the diffuseness a to successively smaller values until agreement with the square well results (the exact ones, not the asymptotic ones given in Sec. III), is obtained. The depth and radius of $\bar{V}$ are -50 MeV and 3.00 fm, respectively, and a is varied successively from 0.50 to 0.20 to 0.08 fm. The resulting values of α_j are shown in Fig. 2. One sees that the numerical values approach the square well result (open circles) in a satisfactory manner. Other internal checks are also performed, such as changing the value of $R_{\rm INT}$, making transformations on V_0 and $\bar{V}$ of the type described by Eq. (2.7), going to full double precision, etc. One important confirmation is described in the next section, where a simple application of the formalism is made to the calculation of the correction to a scattering phase shift due to $\bar{V}$. The eigenvalues α_j for the

TABLE II. The sum in Eq. (4.10) for 15 MeV $n-{}^{16}$O potential scattering. The Woods-Saxon potentials $\bar{V}$ and V_0 are real of equal depth -25 MeV, radius 3 fm, and diffuseness 0.5 fm.

i	$\lvert\langle\varphi_i\bar{V}f_0\rangle\rvert$	$\left\lvert\frac{\langle\varphi_i\bar{V}f_0\rangle}{(\alpha_i-1)\langle\varphi_i V\varphi_i\rangle}\right\rvert$	$\sum_{j=1}^{i}\langle\varphi_j\bar{V}f_0\rangle/[\langle\varphi_j\bar{V}\varphi_j\rangle(\alpha_j-1)]$ Re	Im
1	13.71	0.239	−0.016	0.238
2	17.83	1.55	−0.374	−1.273
3	5.04	0.308	−0.320	−0.968
4	2.32	0.079	−0.252	−0.927
5	1.35	0.032	−0.219	−0.926
6	0.89	0.017	−0.203	−0.931
7	0.64	0.010	−0.195	−0.937
8	0.47	0.007	−0.190	−0.942
9	0.37	0.004	−0.188	−0.946
10	0.30	0.003	−0.187	−0.949
11	0.24	0.002	−0.187	−0.952
12	0.20	0.002	−0.187	−0.953
13	0.17	0.001	−0.187	−0.955
		Exact result →	−0.186	−0.956

case of a complex Woods-Saxon potential are shown in Fig. 3.

IV. EXPANSION OF THE SCATTERING FUNCTION IN TERMS OF THE AUXILIARY WEINBERG STATES

If the scattering solution f_0 for potential V_0 is known, then the addition of a potential V will change the solution by an additional function which is regular at the origin and which is purely outgoing at large distances. The auxiliary Weinberg states ϕ_j, defined in Sec. II, have the same property and should therefore provide a good expansion basis for the addition to f_0 provided that the range of the auxiliary potential $\bar{V}$ is similar to that of V.

The equation to be solved is

$$(H_0-E)f(r)=-Vf\ . \tag{4.1}$$

Here H_0 contains local distorting potentials, as in Eq. (2.2), and V is the potential whose effect upon f_0 is to be calculated. The potential V can be either local or nonlocal, large or small. The scattering solution f_0 to H_0 is assumed to be known

$$(H_0-E)f_0=0\ . \tag{4.2}$$

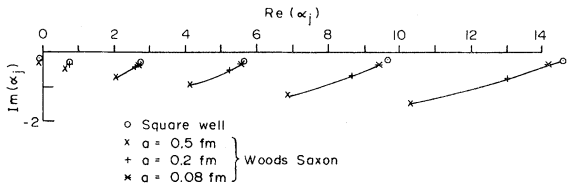

FIG. 2. Comparison of the eigenvalues α_j for $\bar{V}$ a Woods-Saxon well of varying diffuseness a with those for a square well potential (open circles). The depth of the well is -50 MeV, the radius is 3 fm, the laboratory energy of the incident neutron is 15 MeV, the mass of the target is that of ^{16}O. The result for $j=1$ is the one closest to the origin.

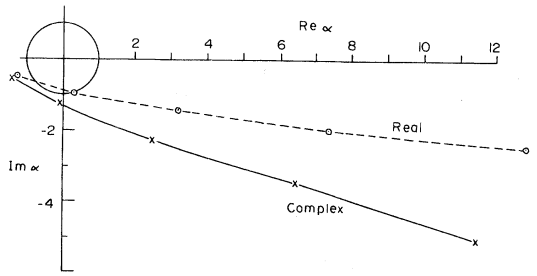

FIG. 3. Effect of an imaginary potential on the eigenvalues α_j. The potentials V_0 and $\bar{V}$ are set equal to each other. The real parts are of volume Woods-Saxon radial dependence with depth -25 MeV, radius $R=3$ fm, and diffuseness $a=0.5$ fm. The results for this potential are denoted by the open circles. If a surface derivative imaginary potential of depth -5 MeV, $R=3$ fm, and $a=0.5$ fm is added to both V_0 and $\bar{V}$, one obtains the results marked by the crosses.

The asymptotic form of f_0 is

$$f_0(r)\approx F_L(r)+(S_L^{(0)}-1)H_L^{(+)}(r)/2i \ , \tag{4.3}$$

where F_L and $H_L^{(+)}$ are the usual regular and outgoing irregular Coulomb wave functions and $S_L^{(0)}$ also written as S_0 is the scattering matrix element. The subscript L denotes orbital angular momentum. In what follows it will be suppressed. The numerical calculations presented in this paper all correspond to $L=0$.

The calculation consists in defining a local potential $\bar{V}$ whose range is approximately equal to the range of V, and obtaining a finite set of Weinberg states ϕ_j, $j=1,2\ldots M$ as in Eq. (2.1). One then expands

$$f_M(r)=f_0(r)+\sum_{j=1}^{M} C_j\phi_j(r) \ , \tag{4.4}$$

where, because of the truncation of the sum over j, f_M is an approximation to f. One can obtain algebraic equations for the C_j's by inserting Eq. (4.4) into (4.1), using Eq. (2.1) and (4.2), multiplying on the left with $<\phi_j(r)$, integrating over r and making use of the orthonormality of the ϕ's, Eq. (2.4). The result is

$$\sum_{j'=1}^{M}(\delta_{jj'}-V_{j,j'})C_{j'}=\langle\phi_j V f_0\rangle \ . \tag{4.5}$$

Here $V_{j,j'}$ are the elements of a symmetric $M\times M$ matrix $\underline{V}$, given by

$$V_{j,j'}=\langle\phi_j V\phi_{j'}\rangle \equiv\int_0^\infty \phi_j(r)V(r)\phi_{j'}(r)\,dr \ . \tag{4.6}$$

Solving Eq. (4.5) for the C's one obtains

$$f_M(r)=f_0(r)+\sum_{j,j'=1}^{M}\phi_j(r)[(\underline{1}-\underline{V})^{-1}]_{j,j'}\langle\phi_{j'}Vf_0\rangle \ . \tag{4.7}$$

One finds an expression for the S matrix elements by using the asymptotic forms for f_0 and ϕ_j, Eqs. (4.3) and (2.3b),

$$S_M^{(0)}=S_0+2i\sum_{j,j'=1}^{M}\beta_j[(\underline{1}-\underline{V})^{-1}]_{j,j'}\langle\phi_{j'}Vf_0\rangle \ . \tag{4.8}$$

The matrix $\underline{V}$ is symmetric but non-Hermitian. Such a matrix is not always diagonalizable, and the eigenstates may, in general, not be complete nor independent. This situation is not expected to occur in the present context, as is discussed further in Sec. VI, following Eq. (6.7), and in the Appendix. The equations above contain the matrix elements $\langle\phi_j V\phi_{j'}\rangle$ and $\langle\phi_j Vf_0\rangle$ which can be generalized without difficulty to the case that V is nonlocal. If V is very small, the solution of Eq. (4.5) can be obtained perturbatively. One obtains for the correction to S the result

$$S_M^{(0)}=S_0+2i\sum_j\langle\varphi_j Vf_0^{(+)}\rangle\beta_j{}^2 +2i\sum_{jj'}\beta_j{}^2\langle\varphi_j V\varphi_{j'}\rangle\beta_{j'}{}^2\langle\varphi_{j'}Vf_0\rangle+\cdots \ . \tag{4.9}$$

Note that the β_j's and the φ_j's are independent of the choice of the strength of $\bar{V}$. This series is very similar to the one obtained in conventional perturbation theory (expansion in eigenstates of H_0) for the correction to an unperturbed negative energy eigenvalue. The main difference is that the energy denominators $E_0-E_{j'}$ are replaced here by $\beta_j{}^{-2}$. By comparison the distorted wave series in $(G_0V)^n$ gives for the correction to S_0 the result

$$S=S_0-2i(2m/\hbar^2k)\times[\langle f_0Vf_0\rangle+\langle f_0VG_0Vf_0\rangle+\cdots] \ .$$

The condition for this series to converge is that

$$\langle f_0(VG_0)^nf_0\rangle\ll\langle f_0(VG_0)^{n-1}f_0\rangle \ ,$$

while for series (4.9) to converge one needs

$$\sum_{j''}\langle\varphi_j V\varphi_{j''}\rangle\beta_{j''}{}^2\langle\varphi_{j''}V\varphi_{j'}\rangle\ll\langle\varphi_j V\varphi_{j'}\rangle \ .$$

The quantities $\langle\varphi_j Vf_0\rangle\beta_j{}^2$ decrease rapidly with j (approximately like j^{-4}), as is shown further below in connection with a numerical evaluation of Eq. (4.10). Hence not many terms in j are expected to be needed in the sums in Eq. (4.9), thus making this type of perturbative approach of practical value.

If V is local and if $\bar{V}$ is chosen to be equal to V then $\underline{V}$ becomes diagonal and the eigenvalues of $\underline{V}$ are equal to $1/\alpha_j$; defined in Eqs. (2.1) or (2.8). Under these conditions Eq. (4.8) can be rewritten as

$$(S_M^{(0)}-S_0)/2i=\sum_{j=1}^{M}\langle\varphi_j\bar{V}f_0\rangle\big/[(\alpha_j-1)\langle\varphi_j\bar{V}\varphi_j\rangle] \ . \tag{4.10}$$

When $\bar{V}$ is local, S_L can be calculated by the same Numerov method as $S_L^{(0)}$ and hence $S_L-S_L^{(0)}$ is known, and thus Eq. (4.10) can be used to gain in-

sight into the accuracy of $S_M^{(0)}$ as a function of M. The result is shown in Table II, which illustrates a case similar to that of Table I. One sees that $\langle \varphi_i V f_0 \rangle$ does not decrease very rapidly with j (roughly like j^{-2}), but the denominator $(\alpha_j - 1)$ $\langle \varphi_j \bar{V} \varphi_j \rangle$ increases with j fast enough (roughly like j^2) so as to make the magnitude of each term in the sum in Eq. (4.10) decrease rapidly (roughly like j^{-4}). Most of the contribution to the sum comes from the first five or six terms, nevertheless 13 terms are needed in order to reach an accuracy of 1% in the S matrix elements. In actual calculations it would probably be preferable to choose $M=5$ or 6 and correct the result by either the quasiparticle method, or the Green's function procedure described below. A very similar conclusion is reached if both V_0 and $\bar{V}$ are made complex, or if V_0 is set equal to zero and the depth of $\bar{V}$ is increased to a value of, say, 50 MeV.

A second example for which V is different from $\bar{V}$ is given below. In this example V is chosen as differently as possible from $\bar{V}$ in order to make the test of the convergence with M as stringent as possible. The energy is again 15 MeV, the potential parameters are given in Table III. The real part of V is of the surface type, and the imaginary part is of a volume type, while the reverse is the case for $\bar{V}$. The maximum magnitude of the real part of V is either 25 or 50 MeV.

According to Eq. (4.8), the correction to S_0 is

$$S_M^{(0)} = S_0 + 2i \sum_{j=1'}^{M} d_j^{(M)} \tag{4.11}$$

with

$$d_j^{(M)} = \beta_j \sum_{j'=1}^{M} [(\underline{1} - \underline{V})^{-1}]_{jj'} \langle \phi_{j'} V f_0 \rangle \ . \tag{4.12}$$

The rate of convergence with M of $S_M^{(0)}$ to S, the exact value of the scattering matrix elements, is shown in Figs. 4 and 5, dashed lines. These lines show the absolute value of the deviation of $S_M^{(0)}$ from S. For $M=10$ that deviation is still larger than 0.04 and 0.08 for the two numerical examples, respectively, which shows that the convergence with M is slow. If the dotted line in Fig. 4 is approximated by the expression $|\Delta S| = K M^{\alpha}$ between the points $M=3$ and 14, then one obtains for α the value -2.37. In Fig. 5, a similar procedure carried out between the points with $M=5$ and 14 yields $\alpha = -2.78$. This falloff of $\Delta S_M^{(0)}$ with M is somewhat slow, and hence an iterative treatment which significantly improves the convergence is described in the next section. The method is based on a slightly modified version of the "quasiparticle" method proposed by Weinberg.[2] The improved results are shown by the solid lines in Figs. 4 and 5.

V. THE SEPARABLE POTENTIAL V_M AND THE GREEN'S FUNCTION G_M

The M approximant to the regular solution of Eq. (4.1) is given by Eq. (4.7). Similarly one can obtain the M approximant to an irregular solution, $h_M(r)$ by replacing f_0 in Eq. (4.7) by the irregular solution h_0 of Eq. (4.2). The function h_0 is defined such that asymptotically it equals the usual outgoing Coulomb wave function $H_L^{(+)}$. One obtains

$$h_M(r) = h_0(r) + \sum_{j,j'=1}^{M} \phi_j(r) [(\underline{1} - \underline{V})^{-1}]_{j,j'} \langle \phi_{j'} V h_0 \rangle \ . \tag{5.1}$$

TABLE III. Parameters for the potentials V_0, $\bar{V}$, and V.

		Real				Imaginary			
		V_0	R_v	a_v	Type[a]	W_0	R_w	a_w	Type[a]
		(MeV)	(fm)	(fm)		(MeV)	(fm)	(fm)	
	V_0	−25	3.0	0.5	Volume	−5	3.0	0.5	Surface
	$\bar{V}$	−25	3.5	0.5	Volume	−5	3.5	0.5	Surface
Case 1	V	−25	3.0	0.5	Surface	−10	3.5	0.5	Volume
Case 2	V	−50	3.0	0.5	Surface	−10	3.5	0.5	Volume

[a]The r dependence of the two types is of the form

$V = V_0/(1+e)$, volume,

$V = 4 \times V_0 e/(1+e)^2$, surface,

with $e = \exp(r-R)/a$ in both cases.

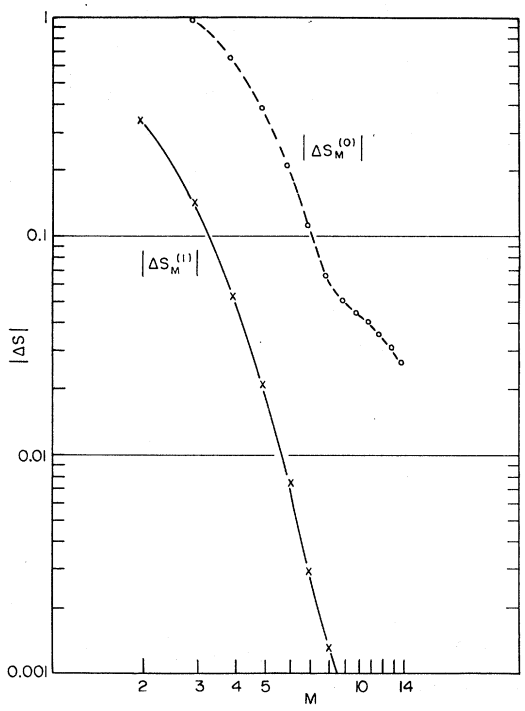

FIG. 4. Error in the scattering matrix elements, as a function of the number M of Weinberg states. The results for $|\Delta S_M^{(0)}|$ are based on Eq. (4.11) or (7.7), while $|\Delta S_M^{(1)}|$, based on Eq. (7.6). The latter contains the effect of one iteration $G_M(V-V_M)f_M$. The potentials for V_0, $\bar{V}$, and V are given by case 1 in Table III. The corresponding eigenvalues of G_0V are shown by open circles in Fig. 6.

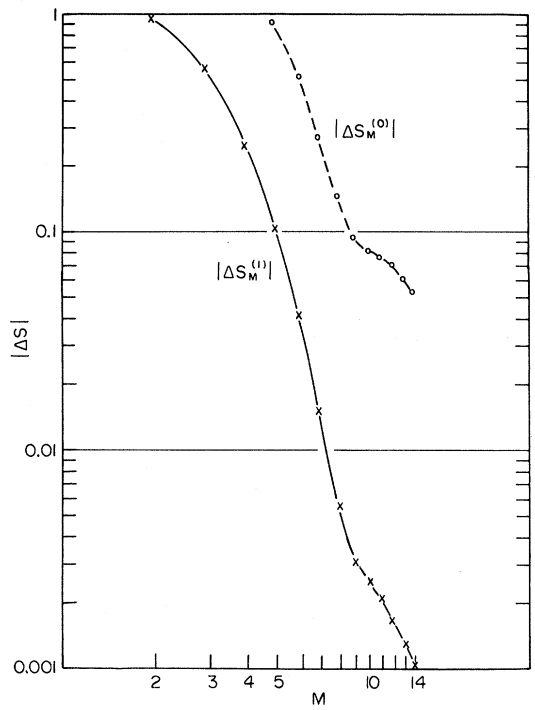

FIG. 5. Same as Fig. 4, with the potentials given by case 2. The corresponding eigenvalues of G_0V are shown by crosses in Fig. 6.

Both f_M and h_M are approximate solutions to Eq. (4.1), but they are exact solutions of the equation

$$(H_0-E+V_M)\begin{Bmatrix} f_M \\ h_M \end{Bmatrix}=0\ , \tag{5.2}$$

where V_M is a nonlocal separable potential given by

$$V_M(r,r')=\bar{V}(r)\sum_{j=1}^{M}\phi_j(r)\langle\phi_j\bar{V}\phi_j\rangle^{-1}<\phi_j(r')V(r')\ . \tag{5.3}$$

The symbol $<$ means that the integration over r' is to be performed when $V_M(r,r')$ acts upon a function $\psi(r')$. If V is a many channel potential, $<$ indicates that a sum over the first channel index is also to be carried out. The exact function f satisfies the equation

$$(H_0+V_M-E)f=-(V-V_M)f \tag{5.4}$$

or,

$$f=f_M+G_M(V-V_M)f\ . \tag{5.5}$$

Since $V-V_M$ is small, as will be seen in the next section, iterations in $G_M(V-V_M)$ should converge rapidly.

For the one channel case, the Green's function G_M can be given exactly in terms of f_M and h_M as

$$G_M(r,r')=-f_M(r_<)h_M(r_>)/W_M(r_>)\ , \tag{5.6}$$

where the Wronskian

$$W_M(r)=\frac{\hbar^2}{2m}[(dh_M/dr)f_M-h_M(df_M/dr)] \tag{5.7}$$

is not independent of r in this case because V_M is a nonlocal separable potential.

An alternate expression for G_M, more suitable for the generalization to the many channel case, is given by

$$G_M(r,r')=G_0(r,r')+\sum_{j,j'=1}^{M}\phi_j(r)[(\underline{1}-\underline{V})^{-1}]_{jj'}\langle\phi_{j'}VG_0\rangle_{r'}\ , \tag{5.8}$$

where

$$\langle \phi_{j'} V G_0 \rangle_{r'} = \int_0^\infty \phi_{j'}(r) V(r) G_0(r,r')\, dr \ . \tag{5.9}$$

The above result follows from the identity

$$G_M = G_0 + G_0 V_M G_M \tag{5.10}$$

and the fact that V_M is separable.

If the problem contains N channels, coupled to each other by the potential V, which now has the elements $V_{n,n'}$ with n and n' running from $1,2 \ldots N$ then the formalism discussed above can be easily generalized. In this case $H_0 - E$ is replaced by the diagonal operator $(H_n^{(0)} - E_n)\delta_{nn'}$, the expansion in Eq. (4.4) is replaced by

$$f_n^{(M)}(r) = f_1^{(0)}(r)\delta_{n1} + \sum_{j=1}^{M} C_{nj}\phi_{nj}(r) \ , \tag{5.11}$$

where it is understood that the only incident wave occurs in channel 1, and in each channel n a set of auxiliary Weinberg states $\phi_{n,j'} j = 1 \ldots M$ is defined. In this case the solution is

$$f_n^{(M)}(r) = f_1^{(0)}(r)\delta_{n1} + \sum_{j=1}^{M} \phi_{nj}(r) \sum_{j'=1}^{M} \sum_{n'=1}^{N} [(\underline{1} - \underline{V})^{-1}]_{jn,j'n'} \langle \phi_{n'j'} V_{n'1} f_1^{(0)} \rangle \ , \tag{5.12}$$

where $\underline{V}$ is now a $(N \times M)^2$ matrix whose elements are

$$(\underline{V})_{nj,n'j'} = \langle \phi_{nk} V_{nn'} \phi_{n'j'} \rangle \ .$$

The result for $G_{nn'}^{(M)}(r,r')$ follows from Eq. (5.8) if G_0 is replaced by $G_n^{(0)}$, $\bar{V}$ by $\bar{V}_n$, ϕ_j by ϕ_{nj}, etc. As will be seen in the next section, the matrix of the eigenvectors of the matrix $\underline{V}$ serves to define the (M) approximant to the eigenvectors of the operator $G^{(0)}V$.

The numerical examples presented in this paper refer to an orbital angular momentum L of zero. The cases of $L \neq 0$ can be treated in one of two ways. Either for each L a set of new Weinberg basis states is calculated in each channel n, and the formalism as it is described here is used—in this case there is a different V_M for each value of L—or the other alternative is to keep the potential V_M fixed as defined for $L=0$, and recalculate the functions f_0, f_M, and G_M after adding to H_0 the $L(L+1)/r^2$ term. Since V_M is separable, the effect of the centrifugal term can be incorporated without much difficulty. For example, the function f_M can be written as

$$f_{L,M} = f_L^{(0)} + G_L^{(0)} V_M f_{L,M}$$

and the quantity $\langle \phi_j V f_{L,M} \rangle$ which arises from the second term can be obtained from the solution of an algebraic equation with inhomogeneous terms $\langle \phi_j V f_L^{(0)} \rangle$ and coefficients $\langle \phi_j V G_L^{(0)} \bar{V} \phi_{j'} \rangle$. Similarly for the Green's function $G_{L,M}$.

VI. EIGENSTATES OF G_0V AND THE QUASIPARTICLE FORMALISM

The usefulness of the quasiparticle method is based on the fact that the large eigenvalues of the operator K

$$K(r,r') = G_0(r,r')V(r') \tag{6.1}$$

can be subtracted off if V is replaced by $V - V_M$ and hence iterations in $G_0(V - V_M)$ will converge if the remaining eigenvalues of $G_0(V - V_M)$ all lie inside the unit circle. This (quasiparticle) method is more transparent if it is formulated in terms of the eigenvectors $\Gamma(r)$ of the operator K. These eigenvectors and their M approximants will now be defined.

The exact eigenvalues and eigenvectors of K will be denoted as k_s and $\Gamma_s(r)$, respectively. They obey the equation

$$K\Gamma_s \equiv \langle G_0 V \Gamma_s \rangle_r = k_s \Gamma_s(r) \ , \tag{6.2a}$$

$$(H_0 - E + k_s^{-1} V)\Gamma_s = 0; \quad s = 1,2 \ldots \ , \tag{6.2b}$$

where it is understood that the Γ's are regular at the origin and are purely outgoing for positive energies E. The Γ's are V orthogonal, i.e., $\langle \Gamma_s V \Gamma_{s'} \rangle = 0$ if $s \neq s'$, and their normalization will be chosen such that

$$\langle \Gamma_s V \Gamma_{s'} \rangle = \delta_{ss'} \ . \tag{6.3}$$

The solution to Eq. (4.1) can be written in terms of the operator K as follows

$$f = f_0 + (1 - K)^{-1} K f_0 \ . \tag{6.4}$$

The iterative form of this solution,

$$f=f_0+Kf_0+K^2f_0+\cdots \tag{6.5}$$

will not converge[2] if any of the eigenvalues of K lie outside of the unit circle. There are only a finite number of such eigenvalues and they can be moved inside the unit circle by subtracting from V the separable potential V_M.[2]

In order to obtain approximations to the Γ's and k's, expansions of the Γ's in terms of the auxiliary Weinberg states ϕ will now be performed. The expansions are

$$\Gamma_s^{(M)}(r)=\sum_{j=1}^{M}\phi_j(r)e_{js}^{(M)} . \tag{6.6}$$

The ϕ's form a complete set in the region where $\bar{V}$ is nonzero, and hence the larger the value of M in the above sum, the closer $\Gamma_s^{(M)}$ should be to Γ_s. However, since the error in $\Gamma_s^{(M)}$ is corrected iteratively by the quasiparticle procedure described below, completeness of the ϕ's is not a necessary requirement in the present context. Since the Γ's and the ϕ's have the same boundary conditions at the origin and at infinity, these expansions should be well behaved. In view of Eqs. (2.8) and (2.4), one obtains, upon inserting the expansion (6.6) into Eq. (6.2b), replacing k_s by $k_s^{(M)}$, and integrating both sides over $\phi_j(r)dr$, the equations for the expansion coefficients $e_{js}^{(M)}$

$$\sum_{j'=1}^{M}V_{jj'}e_{j's}^{(M)}=e_{js}^{(M)}k_s^{(M)};j \text{ and } s=1,2\ldots M . \tag{6.7a}$$

The above equation shows that the $e^{(M)}$'s constitute eigenvectors of the matrix $\underline{V}$. Since only a finite number of j values are used, the $\Gamma_s^{(M)}$ are not eigenvectors of Eq. (6.2), but correspond to a variational approximation to the Γ_s. In matrix notation,

$$\underline{V}\,\underline{E}_M=\underline{E}_M\hat{k}_M , \tag{6.7b}$$

where $\hat{k}_M$ is the diagonal matrix of the eigenvalues and $(\underline{E}_M)_{js}=e_{js}^{(M)}$. The eigenvectors $e_{\cdot s}^{(M)}$ are mutually orthogonal if the corresponding eigenvalues $k_s^{(M)}$ are different from each other, i.e.,

$$\sum_{j=1}^{M}e_{js}^{(M)}e_{js'}^{(M)}=0 \text{ if } k_s^{(M)}\neq k_{s'}^{(M)} .$$

This follows from Eq. (6.7a) in view of the fact that the matrix $\underline{V}$ is symmetric. If in addition, all eigenvectors have nonvanishing norm, i.e., if

$$\sum_{j=1}^{M}e_{js}^{(M)}e_{js}^{(M)}\neq 0 ,$$

then the eigenvectors $e_{\cdot s}^{(M)}$ are all linearly independent from each other, the determinant of $\underline{E}_M$ is different from zero, and the inverse of $\underline{E}_M$ exists. The normalization of the eigenvectors will be chosen as

$$\sum_{j=1}^{M}e_{js}^{(M)}e_{js'}^{(M)}=\delta_{ss'}/k_s^{(M)} \tag{6.8a}$$

and as a result the normalization of the Γ's is

$$\langle\Gamma_s^{(M)}V\Gamma_{s'}^{(M)}\rangle=\delta_{ss'} \tag{6.3'}$$

and the inverse of $\underline{E}$ is given in terms of the transposed matrix $\underline{E}^T$ as

$$(\underline{E}_M)^{-1}=\hat{k}_M\underline{E}_M^T . \tag{6.8b}$$

If none of the eigenvalues $k_s^{(M)}$ are equal to unity then the inverse of the matrix $\underline{1}-\underline{V}$ also exists, and is given by

$$(\underline{1}-V)^{-1}=\underline{E}_M(\underline{1}-\hat{k}_M)^{-1}(\underline{E}_M)^{-1} .$$

Whether the conditions assumed above are valid, namely, that the eigenvalues $k_s^{(M)}$ are all different from each other and different from unity, as well as the nonvanishing of the norm of the eigenvectors, can be verified during the performance of the numerical calculations. As is mentioned after Eq. (4.8), the matrix $\underline{V}$ may not be always diagonalizable. In Appendix B it is shown that it is unlikely that diagonalization problems will be encountered. The arguments are based on the fact that the $\Gamma^{(M)}$'s approach the Γ's as $M\to\infty$. The latter exist and the former are obtained by the diagonalization of $\underline{V}$. No problems were encountered in the calculations described in Sec. VII. In this notation the matrix $\underline{V}$ can be expressed in terms of $\underline{E}_M$ and $\hat{k}$, the Weinberg states ϕ can be given in terms of the Γ's,

$$\phi_i(r)=\sum_{s=1}^{M}(\underline{E}_M\hat{k}_M)_{is}\Gamma_s^{(M)}(r) \tag{6.9}$$

and f_M, given by Eq. (4.7), can be rewritten as

$$f_M(r)=f_0(r)+\sum_{s=1}^{M}\Gamma_s^{(M)}(r)R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle \tag{6.10}$$

with

$$R_s^{(M)}=k_s^{(M)}/(1-k_s^{(M)}) . \tag{6.11}$$

Similarly, the potential V_M, defined in Eq. (5.3) can be expressed as

$$V_M(r,r')=\sum_{s=1}^{M}\bar{V}(r)\bar{\Gamma}_s^{(M)}(r)k_s^{(M)}\Gamma_s^{(M)}(r')V(r') , \tag{6.12}$$

where

$$\bar{\Gamma}_s^{(M)}(r)=\sum_{j=1}^{M}\phi_j(r)\alpha_j e_{js}^{(M)} . \tag{6.13}$$

The $\Gamma^{(M)}$'s are exact eigenvectors of the operator $K_M=G_0V_M$, i.e.,

$$\langle G_0V_M\Gamma_s^{(M)}\rangle_r=k_s^{(M)}\Gamma_s^{(M)}(r) , \tag{6.14}$$

but of course the $\Gamma^{(M)}$'s are only approximate eigenvectors of K. When $G_0\bar{V}$ operates on the $\bar{\Gamma}$'s one exactly regains the Γ's

$$\langle G_0\bar{V}\bar{\Gamma}_s^{(M)}\rangle_r=\Gamma_s^{(M)}(r) . \tag{6.15}$$

The Green's function $G_M(r,r')$, which inverts (H_0-E+V_M), and which is given by Eq. (5.8), can be rewritten as

$$G_M(r,r')=G_0(r,r')+\sum_{s=1}^{M}\Gamma_s^{(M)}(r)[k_s^{(M)}/(1-k_s^{(M)})]\langle\Gamma_s^{(M)}VG_0\rangle_{r'} . \tag{6.16}$$

This expression is exact, and is valid no matter how poorly the $\Gamma^{(M)}$'s approximate the true Γ's. However, use of Eq. (6.14) is implicit in Eq. (6.16). If instead of the choice $\Gamma^{(M)}$, as given by Eqs. (6.6)–(6.8), other arbitrary forms of Γ's, call them $\Gamma^{(W)}$'s, had been used—as was the case in the original quasiparticle method[2]—then an exact separable form for the corresponding Green's function could also have been obtained. However, in this case a double sum over s and s' would have appeared in the equations which replace Eqs. (6.10) and (6.16), and another matrix, of the form $\langle\Gamma_s^{(W)}VG_0V\Gamma_{s'}^{(W)}\rangle$, would have to be evaluated and diagonalized. Further the potential V_M would be replaced by

$$V_W(r,r')\equiv\sum_{s=1}^{M}(V\Gamma_s^{(W)})_r(\Gamma_s^{(W)}V)_{r'} .$$

Since the convergence of the iteration in $G_W(V-V_W)$ depends on the smallness of the difference between the true eigenvalues k of K and the guessed eigenvalue $k^{(W)}$, the M method described above which makes use of the expansion in terms of the states ϕ_j seems to be more systematic, and hence preferable. The present quasiparticle method now consists in writing Eq. (4.1) in the form

$$(H_0+V_M-E)f=-(V-V_M)f \tag{6.17}$$

and obtaining the exact solution iteratively

$$f=f_M+G_M(V-V_M)f_M +[G_M(V-V_M)]^2f_M+\cdots . \tag{6.18}$$

The smallness of the terms in this series depends on how closely the $\Gamma^{(M)}$'s approximate the true eigenvectors Γ of the operator K, as discussed in Appendix B. For the two numerical examples discussed in Sec. IV, the eigenvalues $k_s^{(M)}$ rapidly approach the origin as s increases. This is illustrated in Fig. 6. One sees that only two eigenvalues k_s lie near or outside the unit circle.

In the next section the first term $G_M(V-V_M)f_M$ is evaluated numerically for the example of Sec. IV.

VII. NUMERICAL EVALUATION OF $G_M(V-V_M)f_M$

As is shown in Sec. V, the error $\Delta S_M^{(0)}$ in the scattering matrix S_M decreases only slowly with M, and thus inclusion of one or more iterations in

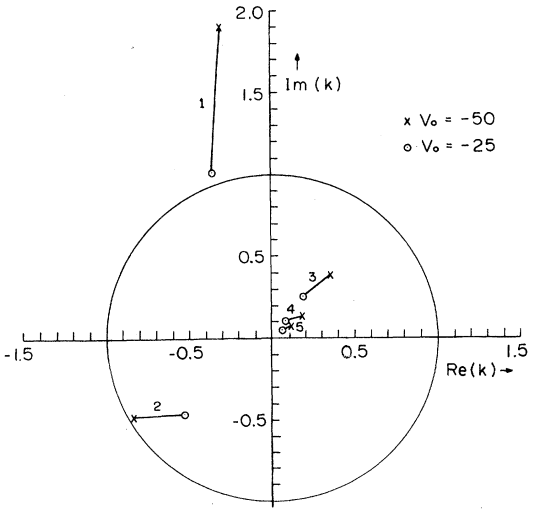

FIG. 6. Argand plot of the eigenvalues k_s of G_0V, obtained by solving Eq. (6.7). The open circles and crosses correspond to cases 1 and 2 of the numerical example described in Table III. The value of M was taken equal to 14; the difference between the exact eigenvalues and $k_s^{(M)}$ should be very small. The numbers next to each set of points denote the value of s.

$G_M(V-V_M)$, Eq. (6.18), becomes desirable. The first such iteration is described in the present section. Depending on the size of V, reduction of the error by factors of 20 or more are achieved, as will be seen.

By using for G_M the expression (6.16), for f_M Eq. (6.10), for V_M Eqs. (6.12) and (6.13), and by using Eqs. (6.14)–(6.16) one obtains

$$G_M(V-V_M)f_M=\langle G_0Vf_0\rangle_r-\sum_{s=1}^{M}\Gamma_s^{(M)}(r)k_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle$$
$$+\sum_{s=1}^{M}k_s^{(M)}R_s^{(M)}\{[\Phi_s^{(M)}(r)-\Gamma_s^{(M)}(r)]\langle\Gamma_s^{(M)}(r)Vf_0\rangle$$
$$+\Gamma_s^{(M)}(r)\langle(\Phi_s^{(M)}-\Gamma_s^{(M)})Vf_0\rangle\}$$
$$+\sum_{s,s'=1}^{M}\Gamma_s^{(M)}(r)R_s^{(M)}[\langle\Gamma_s^{(M)}V\Phi_{s'}^{(M)}\rangle-\delta_{ss'}]k_{s'}^{(M)}R_{s'}^{(M)}\langle\Gamma_{s'}^{(M)}Vf_0\rangle\ , \tag{7.1}$$

$$\Phi_s^{(M)}(r)=\langle G_0V\Gamma_s^{(M)}\rangle_r/k_s^{(M)}\ . \tag{7.2}$$

The quantities in each of the lines above tend to cancel each other the more so the larger the value of M, and since $k_sR_s\approx k_s^2$, the three last lines should be small for s large.

To first order in $G_M(V-V_M)$, one obtains for f_M the result

$$f_M^{(1)}(r)=f_0(r)+\psi_M(r)+\sum_{s=1}^{M}\Gamma_s^{(M)}R_s^{(M)}[\langle\Gamma_s^{(M)}V\psi_M\rangle-R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle]\ , \tag{7.3}$$

where

$$\psi_M(r)=\langle G_0Vf_M\rangle_r\ . \tag{7.4}$$

This result is more suitable for numerical calculations than Eq. (7.1) but it does not exhibit the decrease with M. However, in the limit of large M, the square bracket in the sum in the second line in Eq. (7.3) goes to zero.

Taking asymptotic values in Eq. (7.3), and defining the asymptotic value of $\Gamma_s^{(M)}$ as

$$\gamma_s^{(M)}=[\Gamma_s^{(M)}(r)/H^{(+)}(r)]_{r\to\infty}$$
$$=\sum_{j=1}^{M}e_{js}^{(M)}\beta_j\ , \tag{7.5}$$

one obtains for the S matrix element the result

$$S_M^{(1)}=S_0-2i(\hbar^2/2mk)\int_0^\infty f_0Vf_Mdr+\sum_s 2i\gamma_s^{(M)}R_s^{(M)}[\langle\Gamma_s^{(M)}V\psi_M\rangle-R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle]\ . \tag{7.6}$$

In the above, k is the wave number. By comparison, for the zero'th order expression for S_M, which results from Eq. (6.10), one obtains

$$S_M^{(0)}=S_0+2i\sum_{s=1}^{M}\gamma_s^{(M)}R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle\ , \tag{7.7}$$

which is the same as Eq. (4.8) or (4.11).

For the numerical examples described in Sec. IV, the values of the first order s-matrix elements $S_M^{(1)}$ have been calculated. The results are shown by means of Argand diagrams in Figs. 7 and 8, for cases 1 and 2, respectively. The parameters for the potentials V_0, $\bar{V}$, and V are given in Table III for the two cases. One sees from Fig. 7 that the values of $S_M^{(1)}$ approach the exact value of S much more rapidly than $S_M^{(0)}$, as a function of M. The absolute value of the error $\Delta S_M^{(1)}=S_M^{(1)}-S$ is compared with $\Delta S_M^{(0)}$ in Fig. 4. One sees that already for five auxiliary Weinberg states ϕ_j, the error in $S^{(1)}$ is ≈ 0.02 which, compared to the error of ≈ 0.4 in $S_M^{(0)}$ represents an improvement by a factor of ≈ 18. For $M=8$, the improvement is by a factor ~ 48.

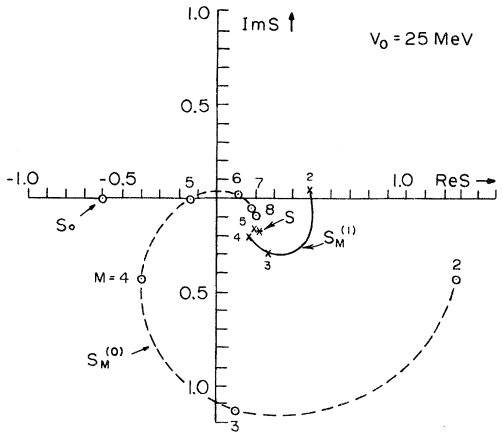

FIG. 7. Argand diagram of the S matrix elements for the numerical examples of case 1. The result corresponding to scattering from potential V_0 is denoted as S_0, the exact result S obtained in the presence of V_0+V is denoted by *, the M approximant $S_M^{(0)}$ to S is shown by the open circles, with the number M of Weinberg states written next to each point. The value of $S_M^{(0)}$ corrected by the first order iteration $G_M(V-V_M)f_M$ is denoted by $S_M^{(1)}$ and is represented by crosses. Expressions for $S_M^{(0)}$ and $S_M^{(1)}$ are given by Eqs. (4.11) or (7.7) and (7.6), respectively.

For the second case ($V\sim 50$ MeV), the convergence with M of the $S_M^{(1)}$ values toward S is not as good as for the first case. The corresponding eigenvalues of G_0V, illustrated in Fig. 6, are much larger than for case 1, one of them lying substantially outside the unit circle. As a result, the straightforward iteration in G_0V should not converge at all. For $M=5$ the value of $\Delta S_M^{(1)}$ is now smaller than $\Delta S_M^{(0)}$ by only a factor of 9, and for $M=8$ the reduction is only a factor of 17. Here a second iteration in $G_M(V-V_M)$ may probably be preferable to increasing M.

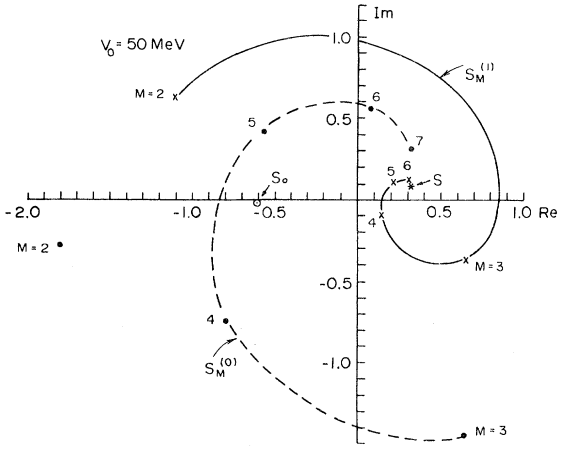

FIG. 8. Same as Fig. 7, but with the potential of case 2.

In spite of the fact that some of the eigenvalues of G_0V are so large, the values of the terms in the second line of Eq. (7.6) are quite small. These values, scaled by 10^3, are displayed in Table IV.

The contributions to $S_M^{(0)}$ from the individual "channels" Γ_s comes mainly from the first few s values. This is shown in Table V, which lists the absolute value of the terms in the sum over s in Eq. (7.7).

One sees from Table V that the first five s values provide most of the contribution. The conclusion is that even for this unusually large value of the potential V, five Weinberg states ϕ should suffice to construct five s channels Γ_s. Two iterations involving $G_M(V-V_M)$ should then suffice to obtain a reliable value of the S matrix element.

VIII. SUMMARY AND CONCLUSIONS

The present paper gives a numerical method of calculating positive energy Weinberg states in the presence of local diagonal potentials, and provides an example for a simple Woods-Saxon case. Such Weinberg states are then used as a basis set for obtaining the scattering solution in the presence of a complicated potential V, which, either because it is nonlocal or because it provides coupling between a large number of channels, is difficult to treat by the usual techniques. Also approximations to the eigenvectors and eigenvalues of the operator G_0V are obtained by the present method in a systematic way. Knowledge of the latter is important in order to assess[12] the convergence of the distorted wave Born series in G_0V and to construct a separable approximation of finite rank of the potential V in the quasiparticle (QP) method.[2,13]

The present method is somewhat different from the QP method. It leads to algebraic matrix equations which can be manipulated formally, thus giving new insights into the scattering formalism, especially in connection to the reduction of the number of channels for a large system of coupled equations.[14] It is thus quite possible that the Weinberg formalism is akin to a Feshbach projection formalism, in that it should enable one to represent a large number of physical channels by means of a small number of separable terms. This question needs to be examined in further detail.

From the numerical point of view the present

TABLE IV. Value[a] of the terms in the second line of Eq. (7.6)

$$|\gamma_s^{(M)}R_s^{(M)}[\langle\Gamma_s^{(M)}V\psi_M\rangle - R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle]| \times 10^3 .$$

M/s	1	2	3	4	5	6	7	8	9
2	16.65	281.68							
3	2.48	118.47	152.53						
4	38.78	0.64	112.73	18.04					
5	13.70	0.15	78.30	48.72	3.42				
6	4.98	0.05	15.40	24.57	4.42	0.84			
7	1.62	0.03	4.99	4.99	4.96	13.05	0.85	0.22	
8	0.52	0.03	1.12	1.34	3.44	0.59	0.17	0.06	
9	0.58	0.03	0.16	0.48	0.18	1.04	0.09	0.03	0.01
10	0.61	0.03	0.25	0.28	0.19	0.06	0.47	0.03	0.01

[a]The numerical example corresponds to case 2, described in Table III and in the text. A scaling factor of 10^3 has been introduced for the purposes of this table.

method, as it now stands, is expected to be advantageous over the conventional method of solving N coupled equations N times, when the number of channels N is larger than 30 or 40. The computing time for the conventional method increases as N^3, while most of the computing time of the present method is spent in obtaining $N^2 \times M^2$ matrix elements, where M, the number of auxiliary Weinberg states in each channel, is expected to be of order 5 or 6, according to the simple examples given in Secs. IV and VII. Whether the present method is numerically advantageous over other methods which also involve expansions over sets of basis functions[8,9] or which proceed iteratively[10,11,15] will not be clear until further work is done.

In summary, the positive energy Weinberg basis enables one to reformulate scattering theory in terms of channels Γ_s which are similar to the normal modes in a system of coupled oscillators. It is shown here that this formulation, although known for many years,[2,3] can actually be used for numerical applications without much difficulty and may be more economical than the conventional method for solving a large system of coupled equations.

TABLE V. $|\gamma_s^{(M)}R_s^{(M)}\langle\Gamma_s^{(M)}Vf_0\rangle|$ for the numerical case 2.[a]

s	1	2	3	4	5	6	7	8	9
$M=2$	0.020	1.204							
3	0.005	0.895	0.334						
4	0.773	0.006	0.821	0.027					
5	0.832	0.005	0.790	0.192	0.007				
6	0.861	0.005	0.371	0.359	0.012	0.003			
7	0.865	0.005	0.420	0.035	0.329	0.004	0.001		
8	0.862	0.005	0.454	0.070	0.198	0.004	0.002	0.0006	
9	0.859	0.005	0.464	0.109	0.004	0.150	0.002	0.001	0.0004
10	0.858	0.005	0.465	0.122	0.026	0.001	0.112	0.001	0.0005
14	0.859	0.005	0.460	0.122	0.053	0.019	0.024	0.001	0.045
14[b]	0.634	0.011	0.215	0.025	0.015	0.002	0.012	0.000	0.022

[a]These are the contributions to $S_M^{(0)}$ from each channel s, according to Eq. (7.7).
[b]These results correspond to case 1, i.e., $V=25$ MeV.

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APPENDIX A

The conditions under which the operator

$$K_{1/2}(r,r')=[V(r)]^{1/2}G_0(r,r')[V(r')]^{1/2} \tag{A1}$$

is completely continuous will be discussed below. From the complete continuity it will follow that the spectrum of eigenvalues of $K_{1/2}$ is discrete, with an accumulation point at zero, and that $K_{1/2}$ can be approximated uniformly by a sequence of operators of finite rank. Furthermore, the eigenvectors of $K_{1/2}$ form a complete set in the region of space where $V\neq 0$. The properties of completely continuous operators are reviewed in the articles by Coester,[3] Meetz,[3] and Tani[3] and a mathematical discussion can be found in the book by Ringrose.[16]

The proof of complete continuity of $K_{1/2}$, given by Coester and Meetz, consists in showing that the trace of $K_{1/2}$ is finite

$$\int d\vec{r}\int |K_{1/2}(\vec{r},\vec{r}')|^2 d\vec{r}'<\infty\ . \tag{A2}$$

However, the function G_0 used by these authors is the free Green's function $\alpha \exp ik\rho/\rho$, where $\rho=|\vec{r}-\vec{r}'|$ and k is the asymptotic wave number. For spherically symmetric potentials $V(r)$ the boundedness of the trace implies that

$$\int_0^\infty r\,|V(r)|\,dr<\infty\ , \tag{A3}$$

which does rule out the presence of Coulomb potentials.

The present argument also consists in showing that the trace of $K_{1/2}$ is finite, but G_0 in this case is a partial wave distorted Green's function

$$G_0(r,r')=-Mf_0(r_<)h_0(r_>)\ , \tag{A4}$$

where f_0 and h_0 are the regular and (outgoing) irregular solutions of Eq. (2.2), in which V_0, in addition to the $L(L+1)/r^2$ term, also may contain complex optical potentials as well as a Coulomb potential. In Eq. (A4) as well as in subsequent equations the angular momentum number L will not be explicitly indicated. M is the constant $(2m/\hbar^2k)$ and the functions f_0 and h_0 are normalized such that asymptotically they approach

$$\begin{aligned} f_0&\rightarrow \sin\phi\ ,\\ h_0&\rightarrow \exp(i\phi) \end{aligned} \tag{A5}$$

with

$$\phi=kr-\eta\ln(2kr)-L\pi/2+\sigma_L+K_L\ ,$$

where σ_L and K_L are the Coulomb and the (complex) nuclear phase shifts, respectively, and η is the usual Coulomb parameter.

The trace of $K_{1/2}$ can be written as

$$\mathrm{Tr}=\int_0^\infty I(r)\,dr \tag{A6}$$

with

$$\begin{aligned} I(r)&=\int_0^\infty |K_{1/2}(r,r')|^2 dr'\\ &\leq M^2|V(r)|\left\{|h_0(r)|^2\int_0^r |f_0(r')|^2|V(r')|\,dr'+|f_0(r)|^2\int_r^\infty |h_0(r')|^2|v(r')|\,dr'\right\}. \end{aligned} \tag{A7}$$

The turning point r_t is now defined such that

$$\left.\begin{aligned} |f_0|^2 &\lesssim c_f r^{2L+2} \\ |h_0|^2 &\lesssim c_h r^{-2L} \end{aligned}\right\} r < r_t \ , \tag{A8}$$

where c_f and c_h are positive constants. It is further assumed that $V(r)$ is not singular, such that an upper bound θ_0 exists, i.e.,

$$|V(r)| < \theta_0 \ . \tag{A9}$$

It will further be assumed that the integral θ_1

$$\theta_1 = \int_0^\infty |V(r')| \, dr' \tag{A10}$$

exists and is finite. Under these conditions the trace of $K_{1/2}$ will now be shown to be finite. From Eqs. (A7)—(A10) one can show that for $r < r_t$

$$I(r) \lesssim M^2 |V(r)| \{ r^3 c_h c_f \theta_0 (4L+2)/(2L+3)(2L-1) + c_f r^{2L+2} [c_h r_t^{-2L+1}/(1-2L) + H_t] \} \ , \tag{A11}$$

where

$$H_t = \int_{r_t}^\infty |h_0(r')|^2 |V(r')| \, dr' \ . \tag{A12}$$

Since $|h_0|^2$ is of order unity for $r > r_t$, the above integral is finite if θ_1 is finite, and $I(r)$ is a bounded nonsingular function of r for $r < r_t$.

For $r > r_t$, one can obtain an upper bound for $I(r)$ by noting that for all values of r the absolute value of f_0 is of the same order of magnitude or less than the magnitude of its asymptotic value, and that for $r > r_t$ the asymptotic value of the product $|h_0 f_0|^2$ is of order unity. Hence for $r > r_t$

$$|h_0(r)|^2 \int_0^r |f_0|^2 |V| \, dr' \lesssim \int_0^\infty |V| \, dr' = \theta_1$$

$$|f_0(r)|^2 \int_r^\infty |^2 |V| \, dr' \approx \int_r^\infty |V| \, dr' < \theta_1$$

and hence

$$I(r) \lesssim M^2 |V(r)| \theta_1, \quad r > r_t \ . \tag{A13}$$

From Eqs. (A11) and (A13) one can see that if $|V(r)|$ is bounded, and if the integral θ_1 [Eq. (A10)] exists and is finite, then the trace of $K_{1/2}$ is bounded and $K_{1/2}$ is in the Hilbert-Schmidt class.

The eigenvalues of the operator $K_{1/2}$ are the same as those of the operator K. If Γ_s is an eigenvector of K

$$\int G_0(r,r') V(r') \Gamma_s(r') dr = k_s \Gamma_s(r) \tag{A14}$$

then it also follows that

$$V^{1/2}(r) \int G_0(r,r') V^{1/2}(r') V^{1/2}(r') \Gamma_s(r') \, dr' = k_s V^{1/2}(r) \Gamma_s(r) \tag{A15}$$

provided that the branch for the square root of V is chosen such that $V^{1/2} \times V^{1/2} = V$.

The eigenvector of $K_{1/2}$ which corresponds to the same eigenvalue is

$$\eta_s(r) = V^{1/2}(r) \Gamma_s(r) \ . \tag{A16}$$

The functions η_s are L^2 integrable if $\theta_1 < \infty$ and if $\Gamma_s(r)$ is bounded,

$$|\Gamma_s(r)| < \gamma \tag{A17}$$

since

$$\int_0^\infty |V^{1/2}(r) \Gamma_s(r)|^2 dr < \gamma^2 \int_0^\infty |V(r)| \, dr \ .$$

Asymptotically, the Γ's are proportional to h_0, which is bounded, and at small distances the Γ's are regular, and thus are also bounded. However, the integral

$$\int_0^\infty \Gamma_s(r) V(r) \Gamma_s(r) dr$$

can accidentally vanish and hence, the normalization condition of Eq. (6.3) cannot be satisfied. In this case Γ_s may not be bounded.

The arguments made above for $K_{1/2}$ also hold for the operator $\bar{K}_{1/2}$

$$\bar{K}_{1/2}(r,r') = \bar{V}^{1/2} G_0 \bar{V}^{1/2} \ ,$$

where $\bar{V}(r)$ is the auxiliary potential in terms of which the auxiliary Weinberg states ϕ_j are defined [Eq. (2.1)], provided that $\int_0^\infty |\bar{V}| \, dr$ exists and is finite, and that $\bar{V}$ has no singularities. In this case the eigenvectors $\bar{\eta}_j$ of $\bar{K}_{1/2}$ form a complete set, and they are given in terms of the ϕ_j according to

$$\bar{\eta}_j(r) = [\alpha_j \bar{V}(r)]^{1/2} \phi_j(r) \ . \tag{A18}$$

Hence $(\bar{V})^{1/2}$ times the eigenfunctions Γ_s of the operator K can be expanded in the complete set of $\bar{\eta}$'s

$$\bar{V}^{1/2}(r)\Gamma_s(r)=\sum_{j=1}^{\infty}\bar{\eta}_j(r)e_{js}\alpha_j^{-1/2}\ . \tag{A19}$$

If the sum is truncated at $j\geq M$ and if e_{js} is replaced by $e_{js}^{(M)}$, then after replacing the $\bar{\eta}$'s by the ϕ_j's according to Eq. (A18), and dividing both sides by $V^{1/2}$, one obtains the M-approximant $\Gamma_s^{(M)}$ to Γ_s, given by Eq. (6.6). In Appendix B it will be shown that the $\Gamma^{(M)}$'s should converge to the Γ's as $M\to\infty$.

APPENDIX B

The diagonalizability of the matrix $\underline{V}$, whose elements are defined in Eq. (4.6), as well as the convergence of $\Gamma_s^{(M)}$ to Γ_s as $M\to\infty$, will be discussed below.

Since the operator $K_{1/2}$ is assumed to be completely continuous there exists a sequence of finite rank operators $\tilde{K}_M$ which converge to $K_{1/2}$ as $M\to\infty$. The operators $\tilde{K}_M$ will be constructed and it will be shown that their eigenvectors are $V^{1/2}\Gamma_s^{(M)}$, and the eigenvalues are $k_s^{(M)}$, $s=1,2...M$. Since the $\tilde{K}_M$'s approach $K_{1/2}$ as $M\to\infty$, the $\Gamma_s^{(M)}$ must converge to the Γ_s as $M\to\infty$, which completes the proof. The operators are defined as

$$\tilde{K}_M(r,r')=[V(r)]^{1/2}\int_0^{\infty}G_0(r,r'')\tilde{V}_M(r'',r')dr'' \tag{B1}$$

with

$$\tilde{V}_M(r'',r')=\bar{V}(r'')\sum_{j=1}^{M}\phi_j(r'')\alpha_j\phi_j(r')[V(r')]^{1/2}\ . \tag{B2}$$

In view of Eq. (2.8), $\tilde{K}_M$ can also be written as

$$\tilde{K}_M(r,r')=\sum_{j=1}^{M}[V(r)]^{1/2}\phi_j(r)\phi_j(r')[V(r')]^{1/2}\ , \tag{B3}$$

which shows that $\tilde{K}_M$ is symmetric in r and r', and is of rank M. It can be shown that the trace of $\tilde{K}_M$ remains finite as $M\to\infty$, provided that the integral in Eq. (A10) is finite. Since

$$\tilde{V}_M(r,r')V^{1/2}(r')=V_M(r,r') \tag{B4}$$

as can be seen from the definition of V_M, Eq. (5.3), it follows from Eq. (6.14) that $V^{1/2}\Gamma_s^{(M)}$ is an eigenvector of $\tilde{K}_M$

$$\tilde{K}_M V^{1/2}\Gamma_s^{(M)}=k_s^{(M)}V^{1/2}\Gamma_s^{(M)}\ . \tag{B5}$$

What will be shown next is that

$$\lim_{m\to\infty}\tilde{K}_M=K_{1/2}\ . \tag{B6}$$

The proof consists in showing that

$$\lim_{m\to\infty}\tilde{V}_M(r'',r')=\delta(r''-r')[V(r')]^{1/2}\ . \tag{B7}$$

This property follows from the completeness of the ϕ's, which gives

$$\delta(r'-r'')=\sum_{j=1}^{\infty}\phi_j(r')\alpha_j\phi_j(r'')\bar{V}(r'')\ . \tag{B8}$$

One can see Eq. (B8) by expanding a function $\psi(r)$ in terms of the ϕ's

$$\psi(r)=\sum_{j'=1}^{\infty}c_{j'}\alpha_{j'}\phi_{j'}(r)\ . \tag{B9}$$

Upon multiplying both sides of Eq. (B9) with $\phi_j(r)\bar{V}(r)$ integrating over r, and using the orthonormality between the ϕ's, Eq. (2.4), one obtains

$$\psi(r)=\sum_j\phi_j(r)\alpha_j\langle\phi_j\bar{V}\psi\rangle \tag{B10}$$

from which Eq. (B8) follows. In Eq. (B1) the variable of integration is r'', and hence Eq. (B6) follows from Eq. (B1) and (B7).

The eigenfunctions of the operators $\tilde{K}_M$ are given in terms of the $\bar{\eta}_j$'s by

$$V^{1/2}\Gamma_s^{(M)}=\sum_{j=1}^{M}(V/\alpha_j\bar{V})^{1/2}\bar{\eta}_j e_{js}^{(M)}\ , \tag{B11}$$

where, according to Eq. (6.7), the $e_{js}^{(M)}$'s are the eigenvectors of the matrix $\underline{V}$, defined by Eq. (4.6). If $\underline{V}$ could not be diagonalized, then the eigenfunctions of $\tilde{K}_M$, $V^{1/2}\Gamma_s^M$, would not all exist. This is unlikely since in the limit $M\to\infty$ the eigenfunctions $V^{1/2}\Gamma_s$ of $K_{1/2}$ do exist. It will now be shown that iterations in the operator $G_M(V-V_M)$ should converge faster the larger the value of M. Here G_M is defined in Eq. (6.16), and the iterations occur in Eq. (6.18).

One can consider $G_M(V-V_M)$ acting on a function ψ, and expand the result in the complete set of eigenstates of K [similar to the expansion (B10)]

$$\langle G_M(V-V_M)\psi\rangle_r=\sum_i\langle G_M(V-V_M)\Gamma_i\rangle_r \times\langle\Gamma_i V\psi\rangle\ . \tag{B12}$$

By making use of Eqs. (6.11), (6.16), (6.15), and (6.2) one obtains for each coefficient of $\langle\Gamma_i V\psi\rangle$ the result

$$\langle G_M(V-V_M)\Gamma_i\rangle_r=\Gamma_i(r)k_i-\sum_{s=1}^{M}\Gamma_s^{(M)}(r)k_s^{(M)}\langle\Gamma_s^{(M)}V\Gamma_i\rangle$$
$$+\sum_{s=1}^{M}\Gamma_s^{(M)}(r)k_s^{(M)}(k_i-k_s^{(M)})\langle\Gamma_s^{(M)}V\Gamma_i\rangle/(1-k_s^{(M)})\ . \tag{B13}$$

As M increases, $\Gamma_s^{(M)}$ and $k_s^{(M)}$ should approach Γ_s and k_s, respectively. Hence, the terms in the first line on the right hand side of Eq. (B13) should nearly cancel, and so should the terms in the second line, in view of the fact that

$$\lim_{M\to\infty}\langle\Gamma_s^{(M)}V\Gamma_j\rangle=\delta_{sj}\ .$$

It can also be shown that[17]

$$\langle G_M(V-V_M)\psi\rangle_r=\langle G_0V\psi\rangle_r+\sum_{s=1}^{M}R_s^{(M)}\Gamma_s^{(M)}(r)\{\langle\Gamma_s^{(M)}VG_0V\psi\rangle-\langle\Gamma_s^{(M)}V\psi\rangle\}\ . \tag{B14}$$

Although the above expression is useful for numerical evaluations, it does not show the various cancellations explicitly. However, if ψ is replaced by f_M, then Eq. (7.1) follows. In view of the fact that $\Phi_s^{(M)}$, defined in Eq. (7.2), should approach Γ_s as M increases, inspection of Eq. (7.1) shows that the terms in each line should nearly cancel each other. In order for the quasiparticle method of Weinberg to be useful, it is sufficient that all the eigenvalues of the operator $G_M(V-V_M)$ lie inside the unit circle.

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