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Variational Methods in a Harmonic Oscillator Basis

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The advantages of using variational methods for solving the Schrödinger equation to obtain the binding energy, well depth, wavefunction, and the potential times the wavefunction for the excited as well as the ground states of a potential are discussed. To illustrate the variational techniques the problem of a particle bound in a Woods–Saxon well is solved using a Harmonic Oscillator basis. Upper and lower bounds for both the eigenvalue and the overlap of the approximate eigenfunction with the true eigenfunction are determined.

1. INTRODUCTION

For most potentials, the three-dimensional Schrödinger equation can be reduced to a one-dimensional linear differential equation which must be solved numerically. Of the two most common methods of solution, variational methods and numerical integration, the variational methods are far superior. In the linear variational method the wavefunction is expanded in a convenient basis and the coefficients of the expansion determined by the solution of a set of linear equations. The approximate eigenfunction is thus found in a simple manner and its eigenvalue is determined to a great precision. Furthermore, one of many sets of basis functions may be used for the expansion of the approximate eigenfunction; hence, the set most useful for further calculations may be chosen. The resulting wavefunction is determined in closed form and is represented by a small number of expansion coefficients. In addition, the accuracy of the results may be assessed using one of the many expressions for bounds on both the eigenvalues, and the overlap of the approximate eigenfunction with the true solution. Bounds may even be obtained on the matrix element of an arbitrary operator calculated with the approximate wavefunction.

Numerical integration [1], while straightforward and easy to use, yields an approximate eigenfunction and eigenvalue whose accuracies are difficult to determine. Also, the wavefunction is obtained in tabular form on the particular grid of

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points appropriate to the numerical quadrature employed; thus the wavefunction is inconvenient to store and awkward to use in further calculations.

For instance, in nuclear physics, approximate wavefunctions are often used as the input to the complicated calculations necessary to describe stripping and transfer reactions [2], and the structure of the nucleus [3]. In this paper we demonstrate the advantages of the variational method when used with the basis set typically chosen for nuclear calculations, i.e., the three-dimensional Harmonic Oscillator (HO) eigenfunctions. These functions not only have several additional properties which simplify subsequent calculations [4] but also enable the initial eigenfunction calculation to be done in an extremely efficient way. With this basis set the eigenvalues and approximate eigenfunctions of the Schrödinger equation can be found quickly and easily using the Rayleigh–Ritz (RR) variational principle. While this is well known for the ground state [3, 5], it is also true for the excited states [6]. The properties of the HO functions can be used to considerably simplify the calculations for the excited states. Since in many scattering calculations the potential times the wavefunction must be used as input, we show how the Schwinger variational principle, as modified by Schwartz [7], can be used to directly obtain this expansion in the HO basis.

To demonstrate the use of these methods, we find the discrete solutions of the Schrödinger equation for a Woods–Saxon potential for the following cases: (1) Given the potential, find the binding energy and wavefunction for the k-th state; (2) Given the binding energy of the k-th state and the form of the potential, find the strength (i.e., coupling constant) of the potential which produces that state and find the wavefunction; and (3) Given the binding energy of the k-th state and the form of the potential, find the coupling constant and the expansion of the potential times the wavefunction.

2. METHODS

A. *Binding Energy and Wavefunction*

In theory, the variational principle provides a method for the exact solution of the Schrödinger equation;

$$E[\Phi] = \langle \Phi \mid H \mid \Phi \rangle / \langle \Phi \mid \Phi \rangle \tag{2.1}$$

is an extremum if and only if Φ is equal to an eigenfunction of the Hamiltonian H. In practice, one cannot consider all possible variations of Φ; instead, one chooses a restricted set of trial functions and determines the functions Φ_k for which E_k is stationary for variations within the restricted basis. This is known as the variational method or variational approximation.

Here we use the method of linear variational parameters which is most commonly known as the Rayleigh–Ritz variational principle [8]. The trial function for the k-th level is written as

$$\Phi_k = \sum_{n=1}^{N} a_{kn}\varphi_n , \tag{2.2}$$

where the φ_n is a set of linearly independent functions and the a_{kn} are parameters to be determined from the condition

$$\delta\langle\Phi_k \mid (H - E) \mid \Phi_k\rangle = 0 \tag{2.3}$$

where the variation is with respect to the parameters. From (2.3) one obtains the linear equations

$$\sum_{n=1}^{N} \langle\varphi_m \mid (H - E) \mid \varphi_n\rangle\, a_{kn} = 0, \qquad m = 1, 2,\ldots, N. \tag{2.4}$$

Therefore, given the matrix elements $\langle\varphi_m \mid (H - E) \mid \varphi_n\rangle$, this set of equations has nontrivial solutions only for those values of E for which

$$\det |\langle\varphi_m \mid (H - E) \mid \varphi_n\rangle| = 0. \tag{2.5}$$

The N roots, $\mathscr{E}_k$, of this equation are upper bounds [6] to the N lowest eigenvalues of H. If one is interested in a particular eigenvalue and its corresponding eigenstate, Eq. (2.4) can be readily solved for that $\mathscr{E}_k$ and Φ_k by an iteration procedure [8]. In this method one uses $\langle\varphi_k \mid H \mid \varphi_k\rangle$ as an initial guess, $\mathscr{E}_k^{(0)}$, to solve (2.4) for a first approximation, $\Phi_k^{(0)}$. This $\Phi_k^{(0)}$ is used to generate the next guess for $\mathscr{E}_k^{(1)} = \langle\Phi_k^{(0)} \mid H \mid \Phi_k^{(0)}\rangle$, and the process is iterated until the change in $\mathscr{E}_k^{(i)}$ is less than the desired accuracy. This process will work only if the k-th trial function φ_k, which is used to start the iteration, is similar to the final eigenstate, i.e., $\mathscr{E}_k^{(0)}$ is closer to $\mathscr{E}_k$ than to any other eigenvalue. The harmonic oscillator functions are well suited to this iteration procedure since the k-th HO state has the correct number of nodes to represent the true function. In practice a few iterations (less than six) are required for most cases.

A good lower bound to the energy is derived in Appendix A. This bound is similar to that obtained by Stevenson and Crawford [9], i.e.,

$$E_k \geqslant \alpha - \langle\chi \mid (H - \alpha)^2 \mid \chi\rangle^{1/2} = \epsilon_k \tag{2.6}$$

where α is a real number nearer to E_k than to any other eigenvalue, and χ is an arbitrary function. Once the upper and lower bounds to the binding energy are known, bounds on the overlap integral

$$S_k = \langle\Phi_k \mid \Psi_k\rangle / [\langle\Phi_k \mid \Phi_k\rangle\langle\Psi_k \mid \Psi_k\rangle]^{1/2} \tag{2.7}$$

can be determined. The Ψ_k are the true eigenfunctions and Φ_k are the approximate wavefunction. An easy bound to evaluate [10] is found from

$$S_k^2 \geqslant \frac{\epsilon_{k+1} - \mathscr{E}_k}{\epsilon_{k+1} - \epsilon_k}\left[1 - \frac{(\mathscr{E}_k - \epsilon_k)(\mathscr{E}_{k-1} - \epsilon_1)}{(\mathscr{E}_k - \mathscr{E}_{k-1})(\epsilon_k - \epsilon_1)}\right] \quad \text{for} \quad k > 1$$

and

$$S_1^2 \geqslant (\epsilon_2 - \mathscr{E}_1)/(\epsilon_2 - \epsilon_1). \tag{2.8}$$

In practice one usually chooses for χ_k the variational wavefunction found from solving Eq. (2.4).

B. *Coupling Constant and Wavefunction*

The variational principle for the coupling constant (or well depth) can be developed in a manner analogous to that for the binding energy. One writes the Hamiltonian in the form:

$$H = H_0 + Vf(r) \tag{2.9}$$

where V is the coupling constant which is to be determined and H_0 is the kinetic energy plus any other potential whose strength is already known (e.g., the Coulomb potential). Thus, the problem is to find a value of V such that

$$(H_0 - E)\Psi_k = Vf(r)\Psi_k \tag{2.10}$$

where Ψ_k has the appropriate boundary conditions. The variational form of Eq. (2.10) is

$$V[\Phi] = \langle\Phi \mid (H_0 - E) \mid \Phi\rangle/\langle\Phi \mid f \mid \Phi\rangle. \tag{2.11}$$

Using the Rayleigh–Ritz variational method and the trial function given in Eq. (2.2), one finds

$$\sum_{n=1}^{N} \langle\varphi_m \mid [(H_0 - E) - Vf(r)] \mid \varphi_n\rangle\, a_{kn} = 0, \qquad m = 1, 2, \ldots, N. \tag{2.12}$$

This set of linear equations has nontrivial solutions only for those values of V for which

$$\det |\langle\varphi_m \mid [(H_0 - E) - Vf(r)] \mid \varphi_n\rangle| = 0 \tag{2.13}$$

and it is a straightforward generalization of MacDonald's proof for the energy [6] to show that for $f(r)$ everywhere nonnegative, the N roots, Λ_k, of this equation are upper bounds to the N lowest eigenvalues of Eq. (2.10). Any potential can be expressed as a sum of two terms, one of which is nonnegative. This part is chosen to be $Vf(r)$ and the remainder of the potential, which must have fixed depth, is included in H_0. If one is interested in a particular state, Eq. (2.12) can be solved in an iterative method analogous to that described for the energy bounds. It is shown in Appendix A that

$$V_k \geqslant \alpha - \langle \chi \mid (H_0 - E - \alpha f) f^{-1} (H_0 - E - \alpha f) \mid \chi \rangle^{1/2} = \lambda_k \qquad (2.14)$$

where α is a real number whose value is nearer to V_k than to any other eigenvalue, and once again the function χ is arbitrary.

Given the upper and lower bounds on V_k, bounds on the overlap integral

$$S_k = \langle \Phi_k \mid f \mid \Psi_k \rangle / [\langle \Phi_k \mid f \mid \Phi_k \rangle \langle \Psi_k \mid f \mid \Psi_k \rangle]^{1/2} \qquad (2.15)$$

can be determined. A good lower bound for the overlap is given by [11]

$$S_k^2 \geqslant \frac{\lambda_{k+1} - \Lambda_k}{\lambda_{k+1} - \lambda_k} \left[1 - \frac{(\Lambda_k - \lambda_k)(\Lambda_{k-1} - \lambda_1)}{(\Lambda_k - \Lambda_{k-1})(\lambda_k - \lambda_1)} \right] \quad \text{for} \quad k > 1$$

and

$$S_1^2 \geqslant (\lambda_2 - \Lambda_1)/(\lambda_2 - \lambda_1). \qquad (2.16)$$

C. *Coupling Constant and $f\Psi$*

In nuclear transfer reaction calculations it is necessary to obtain $f\Psi$ rather than Ψ itself. In this type of calculation the problem is: given the form of the potential, $Vf(r)$, the energy of the k-th excited state of angular momentum l, find the value V_k which produces a bound state at this energy, and find an expansion for $f\Psi$ in a convenient basis. Here we use an approach which directly yields an expansion of $f\Psi$. This method has the following advantages: (1) it yields the expansion of $f\Psi$ directly in the desired set of functions; (2) it yields a highly accurate (variational) result for V; (3) the integrals involved may be done analytically (at least for the Woods–Saxon, Coulomb, Yukawa, Eckhart and other smooth analytic potentials). This method is the well-known Schwinger variational principle (SVP) which Schwartz [7] showed could be made into a useful tool for the calculation of binding energies and scattering amplitudes.

The Schrödinger equation for a bound state may be written as

$$\Psi = G_0 V f \Psi \qquad (2.17)$$

where G_0 is the free particle Green's function. Multiplying both sides of this equation by f, we have

$$f\Psi = f G_0 V f \Psi. \qquad (2.18)$$

The stationary expression for V is obtained by taking the inner product of Eq. (2.18) with Ψ, i.e.,

$$\langle \Psi \mid f \mid \Psi \rangle = V \langle \Psi \mid f G_0 f \mid \Psi \rangle. \qquad (2.19)$$

Thus the stationary SVP expression for V is

$$V[\Phi] = \langle \Phi \,|\, f \,|\, \Phi \rangle / \langle \Phi \,|\, f G_0 f \,|\, \Phi \rangle. \tag{2.20}$$

Following Schwartz, we use $f\Phi$ rather than Φ itself as the function to be varied. With $U = f\Phi$ the variational expression for V and U is

$$V[U] = \langle U \,|\, f^{-1} \,|\, U \rangle / \langle U \,|\, G_0 \,|\, U \rangle. \tag{2.21}$$

Here f^{-1} is the inverse of the radial potential $f(r)$ which, we assume for convenience, does not equal zero for any finite value of r. The generalization to include the case where $f(r)$ can equal zero is straightforward and has been discussed by Kaufman [12]. Since $U = f\Phi$, the integrals in Eq. (2.21) are all convergent despite the (exponential) growth at large r of $f^{-1}(r)$.

It is now an easy matter to use Eq. (2.21) to obtain an upper bound for V and a good representation of $f\Psi$. In general we would pick a set of convenient trial functions to represent U, which should incorporate as many of the features of the correct wavefunction as possible.

The trial function for the k-th level is written as

$$U_k = \sum_{n=1}^{N} a_{kn} \varphi_n \tag{2.22}$$

where the φ_n is a set of linearly independent functions and the a_{kn} parameters to be determined from the variational principle in Eq. (2.21). Forming a matrix representation of Eq. (2.21) in the basis given in Eq. (2.21) and varying the parameters a_{kn} yields

$$\sum_{n=1}^{N} \langle \varphi_m \,|(G_0 - [Vf]^{-1})|\, \varphi_n \rangle \, a_{kn} = 0, \qquad m = 1, 2, \ldots, N. \tag{2.23}$$

These equations are solved by the methods described above for V_k and $f\Phi_k$.

3. APPLICATIONS

We demonstrate the use of the variational method to find eigenvalues and eigenvectors for the Schrödinger equation using for the basis states the three-dimensional Harmonic Oscillator functions. An expansion of the eigenfunction in this basis is particularly advantageous for many reasons. Most important, the transformation properties of the HO functions can considerably simplify further calculations. Furthermore, since the k-th HO function has the correct number of nodes, it is a good first approximation to the eigenfunction. Finally, many of the matrix elements required for the evaluation of the upper and lower bounds can be done quite simply in this basis set. Even though these states have the wrong asymptotic behavior, we show that a small number of them can provide very accurate approximations to the true state.

The specific problem we solve is a particle of mass 1 amu bound in a Woods–Saxon (WS) well of the form

$$f(r) = \{1 + \exp[(r - R_0)/a]\}^{-1}. \tag{3.1}$$

The HO states are specified by the parameters b and n, where

$$b = (\hbar/M\omega)^{1/2} \tag{3.2}$$

and the energy of the n-th state with orbital angular momentum l is

$$E_{nl} = (2n + l - 1/2)\,\hbar\omega. \tag{3.3}$$

A. *Upper Bounds*

To obtain the upper bounds for both the energy and coupling constants, it is necessary to evaluate the matrix elements of the kinetic energy and the potential. The matrix elements of the kinetic energy can be done analytically and are given in Appendix B. For the Woods–Saxon potential, $2N$ of the N^2 required matrix elements of f must be obtained by numerical integration, and the remainder are obtained using the recursion relations given in Appendix B. The matrix elements of G_0 and f^{-1} are obtained analytically by the methods described in Appendix B.

TABLE I

Upper Bound to the Binding Energy of the Ground State ($k = 1$, $l = 0$) of a Woods–Saxon Well With a Depth $V = 59.325619$ MeV, Radius $R_0 = 3.0$ F, and a Diffuseness $a = 0.65$ F. N is the Number of HO States Used as a Basis Set and b is the HO Parameter

$b \backslash N$	5	10	20
0.5	19.245128	32.413744	35.809366
1.0	35.925377	36.030516	36.031721
1.5	36.031511	36.031723	36.031723
2.0	36.025924	36.031682	36.031723
2.5	36.005617	36.029762	36.031702
3.0	35.602998	36.027841	36.031631
3.5	34.395894	35.991046	36.029895
4.0	32.425732	35.736178	36.028205
4.5	29.953928	35.090119	36.023581
5.0	27.247978	34.015972	35.969519
5.5	24.513146	32.575679	35.787150
6.0	21.885201	30.868528	35.412436

TABLE II

Same as Table I for the Upper Bound to the Binding Energy of the First Excited State ($k = 2, l = 0$)

N b	5	10	20
1.00	−0.346314	4.259564	4.945702
1.25	3.652250	4.865612	4.994286
1.50	4.660154	4.974407	4.999391
1.75	4.901074	4.994856	4.999934
2.00	4.927064	4.997833	4.999994
2.25	4.749687	4.996706	4.999982
2.50	4.221878	4.997043	4.999970
2.75	3.383561	4.977435	4.999606
3.00	2.420734	4.865865	4.998356
3.25	1.512757	4.586636	4.997546
3.50	0.768114	4.119745	4.996896

TABLE III

Coefficients a_{kn} and Bounds Calculated with $b = 2\text{F}$ for the State Given in Table I

N n	5	10	20
1	0.963800	0.963811	0.963811
2	0.255490	0.255476	0.255476
3	0.074895	0.074698	0.074695
4	0.013932	0.012798	0.012794
5	−0.003350	−0.002678	−0.002682
6		−0.005252	−0.005255
7		−0.003969	−0.003967
8		−0.002344	−0.002338
9		−0.001109	−0.001095
10		−0.000365	−0.000352
11			0.000031
12			0.000185
13			0.000216
14			0.000190
15			0.000145
16			0.000100
17			0.000062
18			0.000035
19			0.000017
20			0.000005
$\mathscr{E}$	36.025924	36.031682	36.031723
ϵ	36.049959	36.032035	36.031725
S_1	0.999595	0.999995	0.999999

In Tables I and II we give the upper bounds for the binding energy of the ground and first excited states evaluated with 5, 10, and 20 basis states for various values of the HO parameter b. The depth of the well was chosen by the methods in Section 2 to give the first excited state a binding energy of 5 MeV.

In Tables III and IV we give the expansion coefficients a_{kn}, the upper and lower bounds to the binding energy, and the bound for the overlap, S_k. These values all were calculated with $b = 2F$. From these tables one can see that an accurate expansion of the ground or excited states can be obtained by the variational method.

As an illustration of variational method of Eq. (2.11) to determine the upper bound to the coupling constant and the eigenfunction, we use a Woods–Saxon well of the form given in (2.1) to bind a particle with a mass of 1 amu by 5 MeV. The results for the upper bound to the magnitude of the depth are given in Tables V through VII for various values of b and for 5, 10, and 20 basis states. Only those values of b for which the iteration method converged are given in the tables. In

TABLE IV

Coefficient a_{kn} and Bounds Calculated with $b = 2$ F for the State Given in Table II

$n \diagdown N$	5	10	20
1	−0.260434	−0.258409	−0.258300
2	0.936548	0.932350	0.932026
3	0.120426	0.109958	0.109592
4	0.200011	0.221007	0.221545
5	0.023369	−0.006058	−0.007014
6		0.049095	0.050485
7		−0.019166	−0.021285
8		0.010087	0.012851
9		−0.009889	−0.013934
10		−0.000139	0.004991
11			−0.007106
12			0.003021
13			−0.003324
14			0.002056
15			−0.001533
16			0.001318
17			−0.000710
18			0.000737
19			−0.000286
20			0.000290
$\mathscr{E}$	4.927064	4.997833	4.999994
ϵ	5.786371	5.039774	5.000081
S_2	0.922757	0.995830	0.999991

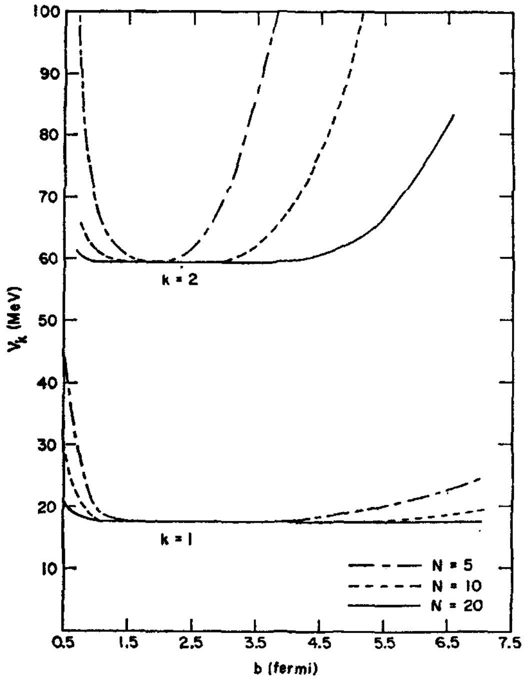

FIG. 1. V_k versus b for the ground and first excited s-states of a particle with mass 1 amu bound by 5 MeV in a Woods–Saxon well with $R_0 = 3$ F, $a = 0.65$ F.

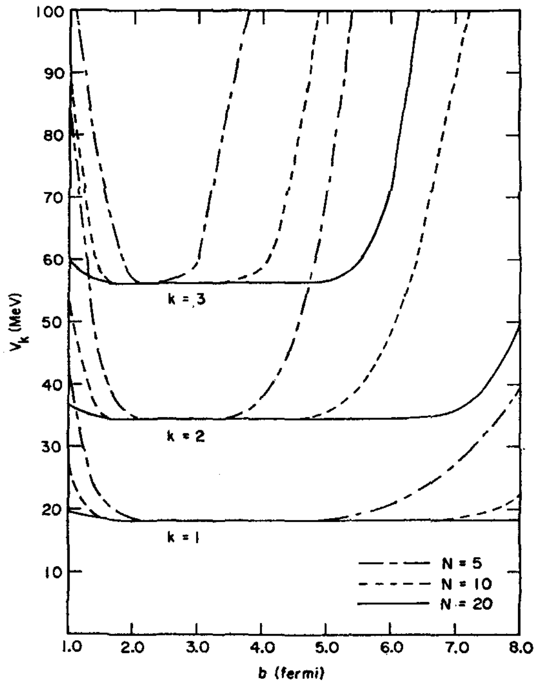

FIG. 2. V_k versus b for the first three f-states of a particle with mass 1 amu bound by 5 MeV in a Woods–Saxon well with $R_0 = 8$ F and $a = 0.65$ F.

Fig. 1 and 2 we plot the coupling constant for a wider range of b, these values were obtained by solving for all the eigenvalues, i.e., all the zeros of the determinant of Eq. (2.13). From these results one can see that the range of b for which good bounds are obtained depends upon the state being considered. From Tables V through VII it is clear that accurate upper bounds to the coupling constant can be obtained for widely varying well parameters.

In Tables VIII and IX we show two examples of the upper bound to the coupling constant calculated using the SVP of Eq. (2.21). These claculations were performed for the same binding energy and well as for the RR calculation of Tables V and VI. This comparison shows that fewer basis states are required in the SVP to obtain the same accuracy as the RR variational principle. In addition we list in Tables X and XI the coefficients for the expansion of $Vf\Psi$ calculated with $b = 1.3F$.

B. *Lower Bounds*

A lower bound to the binding energy is given by Eq. (2.6). While the function χ in this expression is arbitrary, it must be judiciously chosen to obtain an adequate

TABLE V

Rayleigh–Ritz Upper Bound to the Coupling Constant for a Woods–Saxon Well with a Radius $R_0 = 3$F and Diffuseness $a = 0.65$ F Whose Ground State ($k = 1$, $l = 0$) Has a Binding Energy of 5 MeV. N is the Number of Basis States and b is the HO Parameter

b \ N	5	10	20
0.6	33.341145	22.975758	18.789944
0.8	23.509460	19.073948	17.790319
1.0	19.873585	17.999737	17.621356
1.2	18.478912	17.701327	17.592929
1.4	17.931997	17.618656	17.588158
1.6	17.719732	17.595835	17.587359
1.8	17.639958	17.589605	17.587225
2.0	17.610479	17.587908	17.587202
2.2	17.599522	17.587416	17.587199
2.4	17.594990	17.587252	17.587198
2.5	17.593452	17.587240	17.587199
3.0	17.592342	17.588394	17.587213
3.5	17.657287	17.589692	17.587250
4.0	17.887074	17.591492	17.587890
4.5	18.344404	17.617035	17.589144
5.0	19.051678	17.705570	17.489513
5.5	20.012000	17.891194	17.590883
6.0	21.222966	18.194457	17.602356
6.5	22.682479	18.624684	17.638048
7.0	24.390595	19.184656	17.712399

TABLE VI

Same as Table V for the First Excited State ($k = 2, l = 0, E = 5$ MeV) of the Well

N b	5	10	20
0.8	82.045040	64.988940	60.107963
0.9	73.275983	62.319850	59.647288
1.0	67.984255	60.907771	59.457613
1.1	64.751923	60.160170	59.379716
1.2	62.733251	59.765258	59.347773
1.3	61.442991	59.556857	59.334686
1.4	60.613225	59.446676	59.329326
1.5	60.093111	59.388498	59.327134
1.6	59.785146	59.358202	59.326239
1.7	59.614850	59.342843	59.325874
1.8	59.526356	59.335291	59.325723
1.9	59.489704	59.331876	59.325659
2.0	59.505205	59.331009	59.325635
2.1	59.598460	59.331853	59.325435
2.2	59.809283	59.333310	59.325654
2.3	60.180928	59.333980	59.325672
2.4	60.753300	59.333252	59.325676
2.5	61.560240	59.332985	59.325693
2.6	62.629459	59.338887	59.325828
2.7	63.983689	59.360964	59.326242

TABLE VII

Rayleigh–Ritz Upper Bound to the Coupling Constant for a Woods–Saxon Well with a Radius $R_0 = 8$ F and Diffuseness $a = 0.65$ F Whose Third f-state ($k = 3, l = 3$) has a Binding Energy of 5 MeV. N is the Number of Basis States and b the HO Parameter

N b	5	10	20
1.8	58.747078	56.294287	56.193952
1.9	57.183830	56.245885	56.193355
2.0	56.679946	56.223086	56.193122
2.1	56.592274	56.206454	56.193056
2.2	56.586934	56.196995	56.193041
2.3	56.698622	56.198000	56.193031
2.4	56.902485	56.200163	56.193029
2.5	56.994163	56.200611	56.193083
2.6	56.861967	56.208852	56.193090
2.7	56.659549	56.223405	56.193180
2.8	56.681764	56.229106	56.193424

TABLE VIII

Schwinger Upper Bound to the Coupling Constant for a Woods–Saxon Well with a Radius $R_0 = 3$ F and Diffuseness $a = 0.65$ F Whose Ground State ($k = 1, l = 0$) has a Binding Energy of 5 MeV. N is the Number of Basis State and b the HO Parameter

b \ N	5	8	10
.5	24.466072	20.165664	18.971937
1.0	17.612024	17.588510	17.587442
1.1	17.593442	17.587430	17.587234
1.2	17.588265	17.587224	17.587204
1.3	17.587402	17.587208	17.587197
1.4	17.588421	17.587213	17.587204
1.5	17.588643	17.587312	17.587207
1.6	17.589115	17.587752	17.587243
1.7	17.596243	17.588161	17.587504
1.8	17.613867	17.588098	17.587922
1.9	17.635322	17.589219	17.588032
2.0	17.647371	17.595305	17.588197
2.5	18.174913	17.638021	17.635042
3.0	26.130532	18.939539	17.948930

TABLE IX

Same as Table VIII for the First Excited State ($k = 2, l = 0, E = 5$ MeV)

b \ N	5	8	10
1.0	59.626813	59.342356	59.328716
1.1	59.419811	59.328798	59.326093
1.2	59.348370	59.325893	59.325723
1.3	59.332607	59.326612	59.325636
1.4	59.396950	59.327623	59.326301
1.5	59.460581	59.329285	59.327211
1.6	59.441431	59.351679	59.327460
1.7	59.567610	59.396577	59.338322
1.8	60.398230	59.416683	59.371226
1.9	62.635469	59.415163	59.402931
2.0	67.045159	59.583807	59.403709
2.5	165.69059	79.713136	66.363299

lower bound. Obviously, the closer χ is to the true eigenfunction, the better the lower bound. We calculated the lower bounds to the ground and first excited state energies of a particle with a mass of 1 amu bound in a Woods–Saxon well with a radius $R_0 = 3F$ and a diffuseness $a = 0.65F$. These bounds are given in Tables I and II.

TABLE X

Coefficients a_{kn} for the Expansion of $Vf\Psi$ for the State in Table VIII ($b = 1.3$ F)

N	5	8	10
i	$\Lambda = 17.58740$	$\Lambda = 17.58721$	$\Lambda = 17.58719$
1	11.42108	11.32587	11.30992
2	−3.36691	−3.33989	−3.33523
3	0.02629	0.02622	0.02628
4	0.05273	0.06067	0.06091
5	0.07966	0.09575	0.09566
6		0.01295	0.01160
7		0.00035	−0.00296
8		−0.00339	−0.00772
9			−0.00327
10			−0.00113

TABLE XI

Coefficients a_{kn} for the Expansion of $Vf\psi$ for the State in Table IX ($b = 1.3$ F)

N	5	8	10
i	$\Lambda = 59.33261$	$\Lambda = 59.32661$	$\Lambda = 59.32563$
1	16.92442	16.55704	16.49640
2	27.10433	26.52106	26.42356
3	−2.01783	−1.98928	−1.98517
4	−1.61808	−1.67331	−1.67336
5	−0.75560	−0.85394	−0.84759
6		−0.02676	0.00349
7		0.07163	0.13248
8		0.04306	0.11229
9			0.04441
10			0.01155

The best bound found using Eq. (2.6) is obtained when α is as large as possible, subject to the restriction that α is closer to E_k than to any other eigenvalue. To maximize α, the calculation of the lower bound is done in two steps. First, rough lower bounds to both E_k and E_{k+1} are calculated. Next a value of α chosen to be halfway between the two rough lower bounds is used to obtain a more accurate lower bound to E_k. This new lower bound is used to find an even larger value of α halfway between the lower bounds. Then this new value of α is used to find a better bound to E_k. The process may be iterated until the bound no longer improves. This scheme is dependent upon obtaining the initial rough lower bounds to E_k and E_{k+1}. We obtained these bounds by using Eq. (2.6) with α equal to the upper bound to the eigenvalue. The rough lower bound calculated with this value of α is valid only if $\mathscr{E}_k$ is closer to E_k than to any other eigenvalue. For the Woods–Saxon potential and the HO basis set this is not a difficult requirement to meet. However, the validity of this choice must be reexamined when a different potential or basis set is considered. For the energy bounds given in Tables I and II, χ was chosen to be the variational wavefunction and no iterations in α were necessary.

Once accurate lower bounds are available, bounds on matrix elements can be evaluated. As an example we calculate the lower bound to the overlap of the RR variational function with the true wavefunction. The results are given in Tables III and IV.

Lower bounds for the coupling constant were calculated using Eq. (2.14) and an iteration method similar to that described for the energy bound. However, the matrix element in Eq. (2.14) is much more sensitive to the trial function χ than the matrix element appearing in the energy bounds, and accurate bounds could not be obtained using only HO functions. Since we are primarily interested in knowing the lower bound to the overlap of the variational wavefunction with the true eigenfunction, the function χ is used only to obtain a lower bound to the coupling constant, which is then used in Eq. (2.16). Consequently, χ can be expanded in any convenient basis and the expansion coefficients chosen such that λ_k is maximized for a fixed value of α. This is done by minimizing the matrix element

$$I(\alpha) = \langle \chi \mid (H_0 - E - \alpha f) f^{-1} (H_0 - E - \alpha f) \mid \chi \rangle$$

using the RR variational method. It was found that accurate bounds could be obtained only if χ had the correct asymptotic behavior. Thus, we chose for the basis set the HO functions plus the function

$$\varphi_0 = [1 - \exp(-r^2/b^2)]^{l+2}\, h_l^{(1)}(i\kappa r), \tag{3.4}$$

where b is the HO parameter, κ is the bound state wavenumber, and $h_l^{(1)}$ is a Hankel function of the first kind [13]. Using this procedure, lower bounds for the coupling constants V_1 and V_2 were calculated for the Woods–Saxon well with $R_0 = 3F$ and $a = 0.65F$ for a 1 amu particle bound by 5 MeV. (See Tables V and VI and Tables VIII and IX for the upper bounds to these coupling constants.) Using a basis set with 14 trial functions, we found after several iterations in α

$$\begin{aligned} \lambda_1 &= 17.5614 \text{ MeV}, \\ \lambda_2 &= 59.2431 \text{ MeV}. \end{aligned} \tag{3.5}$$

To calculate the lower bound to the overlap, we need the lower bound to V_3 which is found to be

$$\lambda_3 = 127.9503 \text{ MeV}. \tag{3.6}$$

Using these values we found

$$S_1 \geqslant 0.999691, \qquad S_2 \geqslant 0.999399, \tag{3.7}$$

where S_1 and S_2 are bounds for either

$$\langle \Phi_k \,|\, f \,|\, \Psi_k \rangle / [\langle \Phi_k \,|\, f \,|\, \Phi_k \rangle \langle \Psi_k \,|\, f \,|\, \Psi_k \rangle]^{1/2},$$

using 20 trial functions and $b = 2.0F$, or

$$\langle U_k \,|\, \Psi_k \rangle / [\langle U_k \,|\, f^{-1} \,|\, U_k \rangle \langle \Psi_k \,|\, f \,|\, \Psi_k \rangle]^{1/2},$$

using 10 trial functions and $b = 1.3F$.

From this it can be seen that an accurate expansion of $f\Psi$ requires fewer terms than an expansion of Ψ to the same accuracy. One reason for this is that the function $f\Psi$ is more localized in coordinate space than Ψ and consequently the expansion in HO states converges more rapidly. Both methods give very accurate expansions using relatively few terms.

Thus we have shown that variational techniques can be used to obtain accurate approximate solutions to the Schrödinger equation in a basis which is convenient for further calculations.

APPENDIX A

We derive the expression, Eq. (2.14), for the lower bound to the coupling constant. Consider the positive definite matrix element

$$I(\alpha) = \langle \chi \,|\, (H_0 - E - \alpha f) f^{-1} (H_0 - E - \alpha f) \,|\, \chi \rangle \tag{A.1}$$

where α is a real number and χ is arbitrary.

We use the solutions Ψ_l of

$$(H_0 - E)\Psi_l = V_l f(r) \Psi_l \tag{A.2}$$

as a basis set to write

$$f^{-1}(H_0 - E - \alpha f)\chi = \sum_l c_l \Psi_l$$

where c_l is found from the orthogonality of the Ψ_l, i.e., by using

$$\langle \Psi_k \,|\, f \,|\, \Psi_l \rangle = \delta_{kl}. \tag{A.3}$$

Using (A.3) and (A.2) one finds

$$c_l = \langle \Psi_l \mid (H_0 - E - \alpha f) \mid \chi \rangle = (V_l - \alpha) \langle \Psi_l \mid f \mid \chi \rangle. \tag{A.4}$$

Therefore, Eq. (A.1) can be written in the form

$$\begin{aligned} I(\alpha) &= \sum_l c_l \langle \chi \mid (H_0 - E - \alpha f) \mid \Psi_l \rangle \\ &= \sum_l c_l (V_l - \alpha) \langle \chi \mid f \mid \Psi_l \rangle \\ &= \sum_l (V_l - \alpha)^2 \langle \chi \mid f \mid \Psi_l \rangle \langle \Psi_l \mid f \mid \chi \rangle \\ &\geqslant (V_k - \alpha)^2 \sum_l \langle \chi \mid f \mid \Psi_l \rangle \langle \Psi_l \mid f \mid \chi \rangle \end{aligned} \tag{A.5}$$

if α is closer to V_k than to any other eigenvalue.

Expanding χ in the basis set Ψ_l, one obtains

$$\chi = \sum_l a_l \Psi_l \tag{A.6}$$

where

$$a_l = \langle \Psi_l \mid f \mid \chi \rangle. \tag{A.7}$$

Thus

$$\begin{aligned} \langle \chi \mid f \mid \chi \rangle &= \sum_l a_l \langle \chi \mid f \mid \Psi_l \rangle \\ & \sum_l \langle \chi \mid f \mid \Psi_l \rangle \langle \Psi_l \mid f \mid \chi \rangle. \end{aligned} \tag{A.8}$$

Therefore, Eq. (A.5) can be written in the form

$$I(\alpha) \geqslant (V_k - \alpha)^2 \langle \chi \mid f \mid \chi \rangle. \tag{A.9}$$

If the function χ is normalized such that

$$\langle \chi \mid f \mid \chi \rangle = 1, \tag{A.10}$$

it follows that

$$\langle \chi \mid (H_0 - E - \alpha f) f^{-1} (H_0 - E - \alpha f) \mid \chi \rangle^{1/2} \geqslant \alpha - V_k \tag{A.11}$$

where now α has the additional restriction that it is larger than V_k. Hence we find

$$V_k \geqslant \alpha - \langle \chi \mid (H_0 - E - \alpha f) f^{-1} (H_0 - E - \alpha f) \mid \chi \rangle^{1/2}. \tag{A.12}$$

The expression, Eq. (2.6), for the lower bound to the energy can be derived in an analogous manner. Starting with the positive definite matrix element

$$J(\alpha) = \langle \chi \mid (H - \alpha)^2 \mid \chi \rangle = \langle \chi \mid (H - \alpha)(H - \alpha) \mid \chi \rangle, \tag{A.13}$$

we use the completeness of the solutions of the equation

$$H\Psi_l = E_l \Psi_l \tag{A.14}$$

to write

$$\begin{aligned} J(\alpha) &= \sum_l \langle \chi \mid (H - \alpha) \mid \Psi_l \rangle \langle \Psi_l \mid (H - \alpha) \mid \chi \rangle \\ &= \sum_l (E_l - \alpha)^2 \langle \chi \mid \Psi_l \rangle \langle \Psi_l \mid \chi \rangle \\ &\geqslant (E_k - \alpha)^2 \sum_l \langle \chi \mid \Psi_l \rangle \langle \Psi_l \mid \chi \rangle \end{aligned} \tag{A.15}$$

if α is closer to E_k than to any other eigenvalue. Now using the completeness of the Ψ_l once again, one finds

$$\langle \chi \mid (H - \alpha)^2 \mid \chi \rangle \geqslant (E_k - \alpha)^2. \tag{A.16}$$

Using the additional restriction that α is larger than E_k, we find

$$\langle \chi \mid (H - \alpha)^2 \mid \chi \rangle^{1/2} \geqslant \alpha - E_k . \tag{A.17}$$

This can be rewritten in the form

$$E_k \geqslant \alpha - \langle \chi \mid (H - \alpha)^2 \mid \chi \rangle^{1/2} = \epsilon_k . \tag{A.18}$$

APPENDIX B

Here we derive the recursion relations for the matrix elements in a harmonic oscillator (HO) basis of the Green's function, the potential, and the inverse of the potential. Also, we give the expression for the matrix element of the kinetic energy.

The HO functions we use can be written in the form

$$\varphi_{nl}(r) = u_{nl}(r)/r$$

where

$$u_{nl}(r) = \left[\frac{2\Gamma(n)}{b\Gamma(n + l + 1/2)}\right]^{1/2} \left(\frac{r}{b}\right)^{l+1} \exp\left[-\frac{1}{2}\left(\frac{r}{b}\right)^2\right] L_{n-1}^{l+1/2}\left(\frac{r^2}{b^2}\right) \tag{B.1}$$

for $n = 1, 2, \ldots$, where $L_{l-1}^{l+1/2}(r^2/b^2)$ is the generalized Laguerre polynomial of Ref. [13].

The matrix element of the free particle Green's function can be written in the form

$$G_{nm}^l = \kappa \int_0^\infty dr \int_0^\infty dr'\, u_{nl}(r)\, rj_l(i\kappa r_<)\, r' h_l^{(1)}(i\kappa r_>)\, u_{ml}(r') \tag{B.2}$$

where $r_<(r_>)$ is the lesser (greater) of r and r', $j_l(i\kappa r)$ and $h_l^{(1)}(i\kappa r)$ are the spherical Bessel and Hankel functions, respectively. The bound state wave number, κ, is given by

$$\kappa = (2M \mid E \mid /\hbar^2)^{1/2}. \tag{B.3}$$

Equation (B.2) can be rewritten in the form

$$G_{nm}^l = \kappa(H_{nm}^l + H_{mn}^l) \tag{B.4}$$

where

$$H_{nm}^l = \int_0^\infty dr\, rj_l(i\kappa r)\, u_{nl}(r) \int_r^\infty dr'\, r' h_l^{(1)}(i\kappa r')\, u_{ml}(r') \tag{B.5}$$

This expression for H_{mn}^l can be integrated by parts using

$$(d/dr)[r^{-(l-1)} j_{l-1}(i\kappa r)] = -i\kappa r^{-(l-1)} j_l(i\kappa r), \tag{B.6}$$

$$(d/dr)[r^{-(l-1)} h_{l-1}^{(1)}(i\kappa r)] = -i\kappa r^{-(l-1)} h_l^{(1)}(i\kappa r), \tag{B.7}$$

and

$$r^{-l}(d/dr)[r^l u_{nl}(r)] = [(n + l - 1/2)^{1/2}\, u_{nl-1}(r) + n^{1/2} u_{m+1l+1}(r)]/b. \tag{B.8}$$

One finds

$$\begin{aligned} H_{nm}^l = & -[((n + l - 1/2)(m + l - 1/2))^{1/2} H_{nm}^{l-1} \\ & + ((n + l - 1/2)\, m)^{1/2} H_{nm+1}^{l-1} + (n(m + l - 1/2))^{1/2} H_{n+1m}^{l-1} \\ & + (nm)^{1/2} H_{n+1m+1}^{l-1}]/(\kappa b)^2 \\ & + (i\kappa)^{-1} \int_0^\infty dr\, u_{nl}(r)\, rj_l(i\kappa r)\, rh_{l-1}^{(1)}(i\kappa r)\, u_{ml}(r) \\ & + (\kappa^2 b)^{-1} \int_0^\infty dr\, u_{nl}(r)\, rj_{l-1}(i\kappa r)\, rh_{l-1}^{(1)}(i\kappa r) \\ & \times [(m + l - 1/2)^{1/2}\, u_{ml-1}(r) + m^{1/2} u_{m+1l-1}(r)] \end{aligned} \tag{B.9}$$

and

$$
\begin{aligned}
H^l_{mn} = &-[((m+l-1/2)(n+l-1/2)^{1/2}\,H^{l-1}_{mn} \\
&+((m+l-1/2)\,n)^{1/2}\,H^{l-1}_{mn+l}+(m(n+l-1/2))^{1/2}\,H^{l-1}_{m+1n} \\
&+(mn)^{1/2}\,H^{l-1}_{m+1n+1}]/(\kappa b)^2 \\
&-(i\kappa)^{-1}\int_0^\infty dr\,u_{ml}(r)\,rj_{l-1}(i\kappa r)\,rh^{(1)}_l(i\kappa r)\,u_{nl}(r) \\
&-(\kappa^2 b)^{-1}\int_0^\infty dr[(m+l-1/2)^{1/2}\,u_{ml-1}(r)+m^{1/2}u^{(r)}_{m+1l-1}] \\
&\times\, rj_{l-1}(i\kappa r)\,rh^{(1)}_{l-1}(i\kappa r)\,u_{nl}(r).
\end{aligned}
\tag{B.10}
$$

Equations (B.4), (B.9), and (B.10) give

$$
\begin{aligned}
G^l_{nm} = &-[((n+l-1/2)(m+l-1/2))^{1/2}\,G^{l-1}_{nm}+(nm)^{1/2}\,G^{l-1}_{n+1m+1} \\
&+(n(m+l-1/2))^{1/2}\,G^{l-1}_{n+1m}+((n+l-1/2)\,m)^{1/2}\,G^{l-1}_{nm+1}]/(\kappa b)^2-\delta_{nm}/\kappa^2.
\end{aligned}
\tag{B.11}
$$

Thus given G^0_{nm} for $n, m = 1, 2, \ldots, N + l$, one can use (B.11) to find G^l_{nm} for $n, m = 1, 2, \ldots, N$.

To obtain the recursion relation for G^0_{nm}, one writes

$$
\begin{aligned}
G^0_{nm} = &-(i\kappa)^{-1}\left[\int_0^\infty dr\,u_{n0}(r)\sin(i\kappa r)\int_r^\infty dr'\,e^{-\kappa r'}u_{m0}(r')\right. \\
&\left.+\int_0^\infty dr\,u_{m0}(r)\sin(i\kappa r)\int_r^\infty dr'\,e^{-\kappa r'}u_{n0}(r')\right]
\end{aligned}
\tag{B.12}
$$

and integrates by parts twice the integrations over u_{n0}. Then using

$$
\begin{aligned}
d^2u_{n0}/dr^2 = &-[(2n-1/2)\,u_{n0}+(n(n+1/2))^{1/2}\,u_{n+1\,0} \\
&+((n-1)(n-1/2))^{1/2}\,u_{n-1\,0}]/b^2
\end{aligned}
\tag{B.13}
$$

one finds

$$
\begin{aligned}
G^0_{n+1m} = &-\{b^2\delta_{nm}+[(\kappa b)^2+(2n-1/2)]\,G^0_{nm} \\
&+((n-1)(n-1/2))^{1/2}\,G^0_{n-1m}\}/(n(n+1/2))^{1/2}.
\end{aligned}
\tag{B.14}
$$

Thus, G^0_{11} can be used to generate all G^0_{mn}. Transforming to momentum space it is readily found that

$$
G^0_{11} = -2b^2\{\pi^{1/2}-\pi\kappa b\exp[(\kappa b)^2]\,erfc(\kappa b)\}/\pi^{1/2}.
\tag{B.15}
$$

The nonvanishing matrix elements of T^l_{mn} for the kinetic energy can be readily obtained by using Eq. (B.13). This gives

$$\begin{aligned} T^l_{nm} &= (2n + l - 1/2)\,\hbar\omega/2, \qquad m = n; \\ &= (n(n + l + 1/2))^{1/2}\,\hbar\omega/2, \qquad m = n + 1. \end{aligned} \tag{B.16}$$

A recursion relation for the matrix elements A^l_{nm}, of any function of the coordinates A, can be found by using

$$\begin{aligned} u_{nl}(r) = {} & [(r/b)^2\, u_{nl}(r) + (n(n + l + 1/2))^{1/2}\, u_{n+1l}(r) \\ & + ((n - 1)(n + l - 1/2))^{1/2}\, u_{n-1l}(r)]/(2n + l - 1/2). \end{aligned} \tag{B.17}$$

This yields

$$\begin{aligned} A^l_{n+1m} = {} & [2(n - m)\, A^l_{nm} - ((n - 1)(n + l - 1/2))^{1/2}\, A^l_{n-1m} \\ & + ((m - 1)(m + l - 1/2))^{1/2}\, A^l_{nm-1} \\ & + (m(m + l + 1/2))^{1/2}\, A^l_{nm+1}]/(n(n + l + 1/2))^{1/2}. \end{aligned} \tag{B.18}$$

Since $A^l_{nm} = A^l_{mn}$, this recursion relation can be used to generate A^l_{nm} for $n, m = 1, 2,\ldots, N$ if we have A^l_{1m} for $m = 1, 2,\ldots, 2N$.

For the matrix element of the potential these $2N$ matrix elements must be found by numerical integration. If the potential is a Woods–Saxon, the matrix elements of its inverse can be found by recursion relations. That is, for

$$f^{-1} = 1 + e^{(r-R_0)/a} \tag{B.19}$$

one finds

$$(f^{-1})_{nm} = \delta_{nm} + e^{-R_0/a} V^l_{nm} \tag{B.20}$$

where

$$V^l_{nm} = \langle u_{nl} \mid e^{r/a} \mid u_{ml} \rangle. \tag{B.21}$$

To obtain V_{1m}, write u_{nl} in the form

$$\begin{aligned} u_{nl}(r) = {} & \left[\frac{(2n + 2l - 1)\,!!\,2^{l-n+3}}{b\pi^{1/2}(n - 1)\,!}\right]^{1/2} \left(\frac{r}{b}\right)^{l+1} \\ & \cdot \exp\left[-\frac{1}{2}\left(\frac{r}{b}\right)^2\right] \sum_{k=0}^{n-1} (-2)^k \binom{n - 1}{k} \left(\frac{r}{b}\right)^{2k} \Big/ (2k + 2l + 1)\,!! \end{aligned} \tag{B.22}$$

Then

$$V^l_{1m} = K_{ml} \sum_{k=0}^{m-1} c_{km} h_k{}^l \tag{B.23}$$

where

$$K_{me} \left[\frac{(2m + 2l - 1)\,!!(m - 1)\,!}{2^{m-1}(2l + 1)\,!!}\right]^{1/2} \frac{2^{l+2}}{b\pi^{1/2}}, \tag{B.24}$$

$$c_{km} = (-2)^k/[(2k + 2l + 1)\,!!k\,!(m - k - 1)\,!], \tag{B.25}$$

$$h_k{}^l = \int_0^\infty dr \left\{\exp\left[-\frac{1}{2}\left(\frac{r}{b}\right)^2\right] \exp\left(\frac{r}{a}\right)\right\}\left(\frac{r}{b}\right)^{2(l+k+1)} = H(k + l + 1). \tag{B.26}$$

Integrating by parts one finds that for $p \geqslant 2$,

$$H(p + 1) = \left(\frac{b^2}{4a^2} + \frac{4p + 1}{2}\right) H(p) - \frac{p(2p - 1)}{2} H(p - 1). \tag{B.27}$$

Then using

$$H(0) = \pi^{1/2} b \exp[b^2/4a^2][1 + erf(b/2a)]/2 \tag{B.28}$$

and

$$H(1) = \left(\frac{b^2}{4a^2} + \frac{1}{2}\right) H(0) + \frac{b^2}{4a} \tag{B.29}$$

one can find the necessary $h_k{}^l$.

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