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Accuracy of the optimal subset approximation

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The accuracy of the optimal subset approximation, which reduces the number of coupled equations in the hyperspherical harmonic method, is checked theoretically and numerically. The critical parameter that determines the error of the method is shown to be proportional to the product of potential matrix elements connecting the $K=0$ state to states with $K>0$, and the matrix elements between $K>0$ states. In particular this means that the accuracy is largely independent of the degree of excitation of the system. The numerical precision of the optimal subset method in calculating energies and expectation values of Coulomb-bound three-body systems is checked by comparison of optimal subset results with exact results for fixed maximum global angular momentum $K_{\max}$. Errors range from less than one percent for the helium atom ground state energy to 100 percent or more for certain positronium ion expectation values. This precision is consistent with the theoretically determined error parameters.

I. INTRODUCTION

The hyperspherical method of solution of the N-body Schrödinger equation was introduced nearly simultaneously, in slightly different forms, by several authors in the early sixties.[1-6] Since then it has been used successfully in a wide variety of atomic[8-14] and nuclear[15-34] physics calculations. Among the advantages of this method one can count, besides its natural elegance and generality, are the possibility of analytic calculation of hyperspherical harmonic (HH) potential matrix elements,[35] the knowledge of the analytical structure of radial solutions[14] and convergence properties.[29,33,36,37]

The method consists of the expansion of the N-body wave function into a series of products of so-called hyperspherical harmonics (which are solutions of Laplace's equation on the $3N$-3 dimensional sphere), and radial wave functions (depending only on the radius of this sphere). The subsequent substitution of this series into the Schrödinger equation gives an infinite system of coupled radial second-order differential equations, which after truncation, can be solved numerically. Also, when the wave function is represented by the HH series, containing a complete set of basis functions, one is assured that the wave function and the corresponding energy and expectation values converge to the correct values, an advantage which is not present with *ad hoc* variational wave functions.

The convergence of the hyperspherical expansion is explained by the fact that each hyperspherical function is characterized by a global angular momentum K, which determines the height of the potential barrier. Therefore, the probability of particle interactions and with it the contribution of the hyperspherical harmonics, decreases with K. Thus hypersphericals with large K can be neglected, which results in truncating the number of radial coupled equations. Unfortunately, because of the enormous degeneracy of the hyperspherical harmonics, the number of coupled equations is still prohibitively large, which prevents, at least for $N\geq 4$, taking into account the complete basis in practical calculations. To overcome this difficulty it was suggested by Fabre de la Ripelle[34] that for each particular problem one has to select a so-called "optimal subset;" that is, to use only a part of the complete HH basis especially appropriate for a chosen problem. This subset was shown[33] to contain specific linear combinations of hyperspherical functions. The enormous advantage of working with the optimal subset (OS) basis is that it removes all the degeneracies, resulting in a dramatic reduction of the number of coupled equations. For example, in the case of fully symmetric S-state systems, one equation results for every global momentum K. The application of the OS method made possible not only nuclear three-body calculations, with realistic nuclear potentials,[26] but also allowed the extension of hyperspherical calculations to systems of four and even larger number of particles. (See, for example, Ref. 33 and the references therein.)

The main assumption of the OS method is that the basis functions outside the "optimal" subset contribute insignificantly to the energy as well as to the wave function, and thus also to expectation values. Indeed, the first atomic[10] and nuclear[19,29] computations carried out with the OS method have shown very satisfactory agreement with other methods. Even more delicate features, such as the numerically calculated convergence trends of energies with maximal global momentum, $K_{\max}$, were proven to be in agreement with analytical, theoretical predictions.[36,37] More extensive comparison, made by Erens *et al.*,[17] led to the same conclusions. This last work demonstrated that, in the case of a simple triton model, the inclusion of nonpotential harmonics, orthogonal to the optimal subset, changes the binding energy at most by 0.0001 MeV (i.e., about 0.001 percent). In these calculations it has been shown that the norm of the partial waves not corresponding to the optimal subset did not exceed 10^{-7}, even for potentials with unreasonably high repulsive cores, which are, of course, especially difficult to treat by the hyperspherical method. These results seem so convincing that since then practically all three- and N-body hyperspherical calculations were done using the optimal subset basis.[33]

The proof that the OS method leads to a good solution cannot as of yet be considered complete. Indeed, the overwhelming majority of optimal subset calculations are compared with those done by variational or some other method, so that the effect of the neglect of harmonics outside the OS is mixed with those caused by the neglect of harmonics with larger K. Only Erens *et al.*[17] studied exclusively OS error by considering the solutions in which some harmonics not belonging to the OS were included. In this investigation comparisons with the full set of coupled equations for a given $K_{\max}$ occur only up to $K_{\max}=8$, and then only for a symmetric system where only four coupled equations are involved. Furthermore, in their test case, over 98% of the wave function is $K=0$, so there was not much room in their test for nonoptimal subset contributions to begin with. Also, only the influence of contributions on energy levels and wave function norms was studied, while their neglect of expectation values was never explored. Besides, the question of the applicability of the OS method for excited states was also left unanswered.

Recently, the results of very precise hyperspherical computations of energies, wave functions, and expectation values of ground and excited states of systems of three Coulomb bound particles, which used the complete set of hyperspherical harmonics, for a given maximal global quantum number $K_{\max}$, have become available.[11,14] Comparison of these calculations with those with the same $K_{\max}$ using only the optimal subset would provide an accurate estimate of nonoptimal subset harmonic contributions to different physical quantities. In the present work we report the results of just such a comparison. The Coulomb potentials considered have the same type of $(1/r)$ singularity at the origin as most nuclear potentials (e.g., Yukawa), and it is this behavior that ultimately determines the convergence of the hyperspherical and optimal subset expansions. Of course, we would expect both types of expansions to work better for smoother (e.g., Gaussian, Morse) potentials.

Our investigation is ordered as follows: In Sec. II we give a short description of the optimal subset method and our notation. Section III is devoted to the results of actual comparisons of full HH calculations with those of the OS method, while the conclusions are summed up in Sec. IV. Our main conclusion is that the accuracy of the OS method is determined by the product of parameters $\varepsilon\delta$, where ε is a measure of the matrix element ratio $V_{00,K\nu}/V_{00,00}$ $(K,\nu>0)$ and δ of the ratio $V_{K\nu,K'\nu'}/V_{00,00}(K,\nu,K',\nu'>0)$. The error of the OS method ranges from a fraction of a percent for the ground state energy of the He atom, to order one for correlation integrals of the positronium ion (P_s^-).

II. THE OPTIMAL SUBSET METHOD AND ITS ERRORS

The notion of an "optimal" subset of basis functions spanning the most "important" part of the considered solution space is a perfectly general concept. However, the choice of the OS basis is not unique. In what follows below we adopt the particular choice of Refs. 10 and 17 because, to date, this choice has been employed in most OS calculations of atomic and nuclear systems. This choice also leads to the greatest reduction of number of coupled equations (one for each K).

In this section and throughout the paper we will use the notation of our previous work.[14] Consider the Green's function bound state equation

$$|\Psi\rangle = GV|\Psi\rangle \;, \tag{2.1}$$

which in the hyperspherical basis will be written as

$$\Psi_{K\nu}(\rho)=\sum_{K'\nu'}\int d\rho' G_K(\rho,\rho')V_{K\nu,K'\nu'}(\rho')\Psi_{K'\nu'}(\rho') \;. \tag{2.2}$$

We have restricted ourselves to three-body systems of zero angular momentum so the hyperspherical basis $|K\nu\rangle$ is characterized by two indices only. In this case the partial hyperspherical Green's function can be written explicitly[7] and we will use the usual notation $\Psi_{K\nu}(\rho)=\langle K\nu|\Psi\rangle$ and

$$V_{K\nu,K'\nu'}(\rho)=\langle K\nu|V|K'\nu'\rangle \;.$$

Let us assume now that of the matrix elements of the potential, the element $V_{00,00}$ is dominant, while the elements $V_{K\nu,00}=V_{00,K\nu}$ and $V_{K\nu,K'\nu'}(K,\nu,K',\nu'>0)$ are of order ε and δ, respectively. In this case one can proceed using perturbation theory. Clearly the zero-order wave function is the following:

$$\begin{aligned}\Psi^{(0)}_{00}(\rho)&=\int d\rho' G_0(\rho,\rho')V_{00,00}(\rho')\Psi^{(0)}_{00}(\rho') \;,\\ \Psi^{(0)}_{K\nu}(\rho)&=0,\quad K>0 \;.\end{aligned} \tag{2.3}$$

In first-order the terms of order ε will enter:

$$\begin{aligned}\Psi^{(1)}_{00}(\rho)&=0 \;,\\ \Psi^{(1)}_{K\nu}(\rho)&=\int d\rho' G_K(\rho,\rho')V_{K\nu,00}(\rho')\Psi^{(0)}_{00}(\rho'),\quad K,\nu>0 \;.\end{aligned} \tag{2.4}$$

The next corrections will be

$$\begin{aligned}\Psi^{(2)}_{00}(\rho)&=\sum_{K'\nu'>0}\int d\rho' G_0(\rho,\rho')V_{00,K'\nu'}(\rho')\Psi^{(1)}_{K'\nu'}(\rho') \;,\\ \Psi^{(2)}_{K\nu}(\rho)&=\sum_{K'\nu'>0}\int d\rho' G_K(\rho,\rho')V_{K\nu,K'\nu'}(\rho')\Psi^{(1)}_{K'\nu'}(\rho') \;,\end{aligned} \tag{2.5}$$

which are of order ε^2 and $\varepsilon\delta$, respectively.

If we confine ourselves to the first-order approximation (2.4), the full wave function

$$|\Psi\rangle=\sum_{K\nu}|K\nu\rangle\langle K\nu|\Psi\rangle \tag{2.6}$$

will be given by

$$|\Psi\rangle = |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle ,$$

where

$$|\Psi^{(0)}\rangle = |00\rangle \Psi_{00}^{(0)}(\rho)$$

and

$$|\Psi^{(1)}\rangle = \sum_{K,\nu>0} \int d\rho' G_K(\rho,\rho') |B_K(\rho')\rangle \Psi_{00}^{(0)}(\rho') , \tag{2.7}$$

where we introduce a new ρ-dependent orthogonal basis

$$|B_K(\rho)\rangle = \sum_{\nu} |K\nu\rangle V_{K\nu,00}(\rho), \quad (K>0) . \tag{2.8}$$

Since $|00\rangle$ is a constant vector, $V_{K\nu,00} \neq 0$ only for those (so-called potential) harmonics that enter the expansion of the potential V. The $|B_K(\rho)\rangle$ thus is a certain linear combination of the potential harmonics which form the so-called "optimal" subset. We see that for a description of the wave function $|\Psi\rangle$, up to an error of order ε^2 and $\varepsilon\delta$ in the small parameters ε,δ, we need only the optimal subset. Since all the calculations with orthogonal basis functions are necessarily variational, the error in the binding energy will be governed by the parameters ε^4, ε^2, δ^2, and $\varepsilon^3\delta$.

We will show that the optimal subset basis contains all powers of ε even if we are calculating $\Psi_{K\nu}$ nonperturbatively in parameter ε, that is, if we take into account all powers of $V_{K\nu,00}$.

Assuming $\delta=0$ (i.e., $V_{K\nu,K'\nu'}=0$ for $K,\nu,K',\nu'>0$) then (2.2) yields

$$\Psi_{00}(\rho) = \sum_{K'\nu'} \int d\rho' G_0(\rho,\rho') V_{00,K'\nu'}(\rho') \Psi_{K',\nu'}(\rho') \tag{2.9}$$

and for $K,\nu>0$

$$\Psi_{K\nu}(\rho) = \int d\rho' G_K(\rho,\rho') V_{K\nu,00}(\rho') \Psi_{00}(\rho') . \tag{2.10}$$

Substitution of (2.10) into (2.9) yields an integral equation for $\Psi_{00}(\rho)$ that takes into account all powers of ε

$$\Psi_{00}(\rho) = \int d\rho' d\rho'' G_0(\rho,\rho') U(\rho',\rho'') \Psi_{00}(\rho'') , \tag{2.11}$$

where the effective nonlocal potential $U(\rho',\rho'')$ is given by

$$U(\rho',\rho'') = V_{00,00}(\rho')\delta(\rho'-\rho'') + \sum_{K'\nu'>0} V_{00,K'\nu'}(\rho') G_{K'}(\rho',\rho'') V_{K'\nu',00}(\rho'') . \tag{2.12}$$

The substitution of a solution of (2.11) into (2.10) will yield $\Psi_{K\nu}$ with $K,\nu>0$, which will be of order ε smaller than Ψ_{00}, but precise in all orders of ε.

Using the optimal subset definition (2.8) we can rewrite Eqs. (2.10) and (2.12) in somewhat different form

$$|\Psi_K\rangle = \int d\rho' G_K(\rho,\rho') |B_K(\rho')\rangle \Psi_{00}(\rho'), \quad (K>0) , \tag{2.13}$$

$$U(\rho,\rho') = V_{00,00}(\rho')\delta(\rho-\rho') + \sum_{K'>0} G_{K'}(\rho,\rho') \langle B_{K'}(\rho) | B_{K'}(\rho') \rangle . \tag{2.14}$$

The full wave function thus will be given by

$$|\Psi\rangle = \sum_K |\Psi_K\rangle \tag{2.15}$$

where

$$|\Psi_0\rangle = |00\rangle \Psi_{00} .$$

We see that for $\delta=0$ the optimal subset approximation yields, in fact, the exact result; for small δ the error in $\Psi_{K\nu}(K,\nu>0)$ will be of order $\varepsilon\delta$ [see Eq. (2.2)]. That means that if all the coupling between $K=0$ and other hyperspherical harmonics is zero ($\varepsilon=0$), or if all coupling between hypersphericals $K\nu$ and $K'\nu'$ ($K,\nu,K',\nu'>0$) vanishes ($\delta=0$), the optimal subset formulation is exact. The error in the full wave function thus is also of order $\varepsilon\delta$, i.e., it is determined by the product of matrix elements $V_{K\nu,00}$ and $V_{K\nu,K'\nu'}$. The energy error, since calculations that are carried out with a truncated orthogonal basis are necessarily variational, will be of order $\varepsilon^2\delta^2$. Note that while the quality of the 0S method is determined by $\varepsilon\delta$, the state probabilities (for $K>0$) are determined by ε^2. Thus, for small δ and rather large ε, values of state probabilities for $K>0$ do not give a direct indication of the precision of the OS approximation.

Another way of deriving the OS prescription makes use of matrix considerations. Let us split the space spanned by the hypersphericals for $K \le K_{\max}$ into three subspaces: (1) the "0" space, consisting of $K=0$ only, (2) the "P" space, consisting of an "optimal" subset, to be determined, and (3) the "Q" space, being the remainder which is neglected in OS calculations. We assume that kinetic energy T and the matrix element $V_{00,00}$ are the dominant parts of the Hamiltonian H, with the remaining matrix elements $V_{K\nu,00}=V_{00,K\nu}$ and $V_{K\nu,K'\nu'}$ being described, as earlier, by small parameters ε,δ, respectively. The matrix equation in the eigenvalue problem will look like

$$\begin{bmatrix} T+V_{00}-E & V_{0P} & V_{0Q} \\ V_{0P} & T+V_{PP}-E & V_{PQ} \\ V_{0Q} & V_{PQ} & T+V_{QQ}-E \end{bmatrix} \begin{bmatrix} \Psi_0 \\ \Psi_P \\ \Psi_Q \end{bmatrix} = 0 . \tag{2.16}$$

Clearly, V_{0P}, V_{0Q}, V_{PQ}, and V_{QQ} are all of first order in the smallness parameters ε,δ. The third equation generated by (2.16) implies that Ψ_Q is of first order in these parameters, while the second equation implies that Ψ_P is also of first order. However, if V_{0Q} vanishes, then

$$(T+V_{QQ}-E)\Psi_Q = -V_{PQ}\Psi_P . \tag{2.17}$$

The right-hand side of (2.17) is of second order in this case, and therefore Ψ_Q is of second order, and eigenvalue errors are of fourth order with the neglect of Ψ_Q. So the condition

$$V_{0Q}=0 \tag{2.18}$$

is the prescription of the "optimal" subset.

Let, for each K, the "P" vector be described by $|B_K\rangle$ such that

$$|B_K\rangle = \sum_{\nu} a_{K\nu} |K\nu\rangle \tag{2.19a}$$

and the Q vectors by

$$|Q_K^i\rangle=\sum_\nu q_{K\nu}^i|K\nu\rangle,\quad i=1\cdots\left[\left[\frac{K}{2}\right]-1\right]. \qquad (2.19b)$$

Orthogonality requires, assuming that all vectors are real

$$\begin{aligned}&\sum_\nu a_{K\nu}q_{K\nu}^i=0\,,\\&\sum_\nu q_{K\nu}^i q_{K\nu}^j=\delta_{ij}\,,\\&\sum_\nu a_{K\nu}a_{K\nu}=1\,.\end{aligned} \qquad (2.20)$$

The requirement $V_{0Q}=0$ yields

$$\left\langle 00\left|V\sum_\nu q_{K\nu}^i\right|K\nu\right\rangle=0$$

or

$$\sum_\nu q_{K\nu}^i V_{00,K\nu}=\sum_\nu q_{K\nu}^i V_{K\nu,00}=0\,. \qquad (2.21)$$

Obviously, in view of (2.20), (2.21) is satisfied if we choose

$$a_{K\nu}\sim V_{00,K\nu} \qquad (2.22a)$$

and, for orthonormality

$$a_{K\nu}=V_{00,K\nu}\Bigg/\left[\sum_{\nu'}V_{00,K\nu'}^2\right]^{1/2}. \qquad (2.22b)$$

(Note, since $a_{K\nu}$ is of order one, it is reasonable to assume that the $q_{K\nu}^i$ are also of order one.)

Now we evaluate matrix elements of different types:

$$\begin{aligned}&V_{0P}\sim\left\langle 00\left|V\sum_\nu a_{K\nu}\right|K\nu\right\rangle\sim\varepsilon\,,\\&V_{0Q}=0\,,\\&V_{PQ}\sim\sum_\nu a_{K\nu}\left\langle K\nu\left|V\sum_{\nu'}q_{K'\nu'}^i\right|K'\nu'\right\rangle\sim\delta\,.\end{aligned} \qquad (2.23)$$

Likewise V_{QQ} is of order δ. Therefore, by the third equation of (2.16), when $V_{0Q}=0$, $\Psi_Q\sim V_{PQ}\Psi_P\sim\delta\varepsilon$. [The second equation of (2.16) implies $\Psi_P\sim\varepsilon\Psi_0$.] Thus, again the wave function error by including only the "optimal" subset is $\sim\varepsilon\delta$ and the energy error, by the variational principle, is $\sim\varepsilon^2\delta^2$. In reality, ε,δ are determined not only by the ratios with $V_{00,00}$, but also with the kinetic energy T (and the total energy E). So this will vary somewhat for different states of the system. One can also see that the energy correction is of order $\varepsilon^2\delta^2$ directly from considering perturbation theory up to fourth order.[33]

As might often be the case, the diagonal elements $V_{K\nu,K\nu}$, not $V_{K\nu,00}$, may actually be the dominant matrix element of the $V_{K\nu,K'\nu'}$ for a given K,ν. Then the matrix elements in the PQ sector are given by

$$V_{PQ}=\sum_{\nu\nu'}V_{K\nu,K'\nu'}V_{K\nu,00}q_{K'\nu'}^i\Bigg/\left[\sum_{\nu'}V_{K\nu',00}^2\right]^{1/2}. \qquad (2.24)$$

For $K=K'$, only small nondiagonal terms of order δ are involved. For $K=K'$ the contribution from (large) diagonal matrix elements to the right-hand side of (2.24) is

$$\begin{aligned}V_{PQ}&\approx\frac{\sum_\nu V_{K\nu,K\nu}V_{K\nu,00}q_{K\nu}^i}{\left[\sum_{\nu''}V_{K\nu'',00}^2\right]^{1/2}}\\&=\frac{\overline{V}_{K\nu}\sum_\nu V_{K\nu,00}q_{K\nu}^i+\delta\sum_\nu V_{K\nu,00}q_{K\nu}^i\upsilon_{K\nu}}{\left[\sum_{\nu''}V_{K\nu'',00}^2\right]^{1/2}}\,,\end{aligned} \qquad (2.25)$$

where we have set $V_{K\nu,K\nu}=\overline{V}_K+\delta\upsilon_{K\nu}$, and $\overline{V}_K$ is the average value of $V_{K\nu',K\nu'}$ over all possible ν' values for a given K. In view of (2.21) the first term on the right-hand side of (2.25) vanishes, and thus, for $K=K'$, the diagonal contribution to V_{PQ} in (2.24) gives

V_{PQ}(diagonal contribution)

$$=\delta\sum_\nu\upsilon_{K\nu}V_{K\nu,00}q_{K\nu}^i\Bigg/\left[\sum_{\nu''}V_{K\nu'',00}^2\right]^{1/2}. \qquad (2.26)$$

Therefore, according to the definition of $\overline{V}_K,\upsilon_{K\nu}$, it is the departure of $V_{K\nu,K\nu}$ from the average over ν that determines δ, so δ may actually be small even if the diagonal matrix elements are large.

III. RESULTS

We now discuss the results of optimal subset calculations of energies and correlation integrals for the Coulomb-bound three-body systems of the H^- ion, positronium ion (P_s^- or $e^+e^-e^-$) and the ground and excited states of the helium atom (He, He*, respectively). We compare our present results with our previous complete set (CS) hyperspherical calculations,[14] where all the hypersphericals up to $K=K_{\max}$ were taken into account. Generally $K_{\max}$ is taken to be 12, but for the ground state of He the case of $K_{\max}=10$ is also considered to enable direct comparison with the previous OS atomic calculations of Ballot and Navarro.[10] The present calculations were carried out with the same version of the computer program used earlier for CS calculations,[14] so all the values in our CS and OS calculations were computed exactly the same way.

Let us consider Table I, where the results of our CS and OS calculations for the ground and excited states of the He atom are presented along with the OS calculations of Ballot and Navarro.[10] One can see that for the ground state the OS method gives excellent results for the binding energy and rather good results for most of the correlation integrals and state probabilities. Only the state probabilities and correlation integrals sensitive to the electron-electron repulsion, such as P_2, P_6, P_{10},[29] and r_3^p ($p=\pm1,\pm2$), $\delta(r_3)$ show unsatisfactory agreement with CS calculations. Table I also shows that the use of the power series method of Ref. 14 with the OS method improves the agreement between the OS numerical calculations and the exact CS calculations. The improvement over Ballot-Navarro is small, except for P_2. The important point, however, is that our present OS calculations give 0.2% too little binding in comparison with the CS computa-

TABLE I. Comparison of complete set (CS) and optimal subset (OS) helium calculations. (All quantities are in atomic units.) See Ref. 14 for notation of type.

Atom	He			He		He*	
Calculation type	CS	OS[a]	OS[b]	CS	OS[a]	CS	OS[a]
$K_{\max}$	10	10	10	12	12	12	12
E_B	2.850 38	2.845 60	2.857	2.876 01	2.869 65	1.878 53	1.844 98
P_0	0.942 91	0.945 53	0.942	0.935 36	0.939 09	0.537 81	0.573 12
P_2	0.004 202	0.003 865	0.006 32	0.004 066	0.003 708	0.001 933	0.001 154
P_4	0.048 51	0.046 52	0.0479	0.053 91	0.051 15	0.345 18	0.332 52
P_6	0.000 036 40	0.000 010 30	0.000 007 52	0.000 033 83	0.000 008 772	0.001 506	0.000 105 6
P_8	0.004 375	0.004 090	0.004 14	0.005 651	0.005 176	0.085 72	0.076 44
P_{10}	0.000 004 972	0.000 002 487	0.000 001 89	0.000 003 735	0.000 001 595	0.000 012 54	0.000 010 65
P_{12}				0.000 966 0	0.000 871 1	0.019 18	0.016 57
r_2^{-2}	5.431 67	5.403 82		5.632 92	5.595 39	2.724 41	2.660 94
r_2^{-1}	1.667 86	1.665 30		1.678 18	1.674 09	1.047 16	1.031 83
r_2	0.907 49	0.906 10		0.914 71	0.912 35	2.025 96	2.015 95
r_2^2	1.108 83	1.102 12		1.136 94	1.126 19	6.275 27	6.131 50
r_3^{-2}	1.543 49	1.884 38		1.510 67	1.836 27	0.411 85	0.499 69
r_3^{-1}	0.970 84	1.053 99		0.961 20	1.042 36	0.419 11	0.446 04
r_3	1.378 41	1.291 13		1.393 34	1.306 11	3.334 18	3.220 26
r_3^2	2.351 27	2.083 30		2.404 93	2.134 72	12.829 58	12.083 81
$\delta(r_2)$	1.164 484	1.154 425		1.292	1.276 374	0.491 869	0.484 564
$\delta(r_3)$	0.123 759	0.187 403		0.1173	0.175 710	0.032 576	0.049 631

[a] This work.

[b] Reference 29.

TABLE II. Comparison of complete set (CS) and optimal subset (OS) hydrogen and positronium ion calculations.

Ion	P_s^-		H^-	
Calculation type	CS	OS	CS	OS
$K_{\max}$	12	12	12	12
E_B	0.250 40	0.221 01	0.512 61	0.501 35
P_0	0.694 62	0.825 05	0.858 05	0.895 34
P_2	0.198 32	0.154 19	0.014 60	0.012 36
P_4	0.054 26	0.011 57	0.109 02	0.081 52
P_6	0.032 90	0.007 282	0.000 186 1	0.000 071 34
P_8	0.004 962	0.001 160	0.015 27	0.009 141
P_{10}	0.004 121	0.000 516 8	0.000 014 70	0.000 006 486
P_{12}	0.002 111	0.000 292 6	0.002 863	0.001 592
r_2^{-2}	0.239 01	0.090 65	0.988 94	0.952 45
r_2^{-1}	0.341 89	0.238 94	0.686 17	0.680 90
r_2	4.650 48	5.527 38	2.373 93	2.306 53
r_2^2	29.989 65	37.605 58	7.997 79	7.313 67
r_3^{-2}	0.047 39	0.199 60	0.187 01	0.281 74
r_3^{-1}	0.182 23	0.340 56	0.347 02	0.412 18
r_3	6.890 10	4.057 85	3.777 12	3.281 63
r_3^2	56.385 53	20.891 43	17.449 02	13.440 17
$\delta(r_2)$	0.011 08	0.001 621	0.0983	0.092 418
$\delta(r_3)$	0.000 305	0.006 553	0.003 97	0.009 845

tions. This result is consistent with the variational principle, since OS calculations use a restricted subset of a full hyperspherical basis. The previous numerical estimates of Ballot and Navarro[10] resulted in 0.2% too much binding energy, in contradiction with the Ritz principle, as was recently pointed out.[13,38] Note also that this discrepancy could not be attributed to center-of-mass effects connected with different prescriptions[10,14] for the nuclear mass. Indeed, the change of the mass of the He atom from infinity to the correct value of $7349.12 m_e$ decreases the ground state binding in the OS power series calculations from 2.845 60 to 2.845 17 for $K_{\max}=10$, that is, by less than 0.02%.

The agreement of the OS and CS calculations is only slightly worse for the excited helium atom than for the ground state. This result seems surprising in view of the fact that the He* wave function extends much further from the nucleus and has to be described by a much larger number of hypersphericals. However, as we conclude in Sec. II, the quality of the OS method is governed by the product of the parameters ε and δ which characterize smallness of different nondiagonal potential matrix elements.

Since potential matrix elements are the same for ground and excited states, we expect that the quality of the OS method should not change for excited states. This idea is indeed supported by our present numerical results for the excited states of helium, for which the maximum values of δ and ε are of the order 0.3, so $\varepsilon\delta < 0.09$. We can expect also reasonably good agreement between the OS and CS calculations for the H^- ion, since (see Table III) there $\varepsilon_{\max}=0.44$ and $\delta_{\max}=0.51$, so εδ is less than 0.22. That is indeed confirmed by the results of our numerical calculations in Tables I and II. The OS method, however, should be and is consistently poor for P_s^-, where $\varepsilon_{\max}=0.8$ and $\delta_{\max}=0.98$, so εδ is of order one and much larger than for H^-, He, or He*.

We stress that, as we mentioned in Sec. II, the size of the $K>0$ state probabilities are determined by the smallness parameter ε^2, while the quality of the OS approximation by εδ. Therefore, the value of P_K ($K>0$) does not by itself give the correct indication of how the OS method will fare. In view of this remark, it should not be surprising, for example, that though the $K=4$ state probabilities for excited helium contributes about 33% of the norm (compared to a 53% contribution for $K=0$) the quality of the method is still quite satisfactory, since, as we saw in Table III, εδ is reasonably small. On the contrary, in the

TABLE III. Matrix elements $V_{K\nu,K'\nu'}/V_{00,00}$.

K	ν	K'	ν'	He	H^-	P_s^-
0	0	2	1	0.086	0.219	0.800
0	0	4	0	−0.148	−0.148	−0.148
0	0	4	2	−0.300	−0.460	−0.420
0	0	6	1	−0.029	−0.074	−0.269
0	0	6	3	0.029	0.074	−0.135
2	1	2	1	0.841	0.727	0.743
2	1	4	0	−0.073	−0.186	−0.682
2	1	4	2	0.104	0.264	0.614
2	1	6	1	0.014	0.097	0.086
2	1	6	3	−0.205	−0.340	−0.58
4	0	4	0	1.061	1.061	1.061
4	0	4	2	0.352	0.515	0.492
4	0	6	1	0.087	0.221	0.807
4	0	6	3	−0.039	−0.099	−0.181
4	2	4	2	1.235	1.235	0.962
4	2	6	1	−0.072	−0.183	−0.341
4	2	6	3	0.106	0.269	0.985
6	1	6	1	0.825	0.711	0.727
6	1	6	3	0.160	0.277	0.534
6	3	6	3	1.100	1.059	1.249

TABLE IV. Matrix element products $V_{K\nu,00}(V_{K\nu,K\nu}-\bar{V}_K)/V^2_{00,00}$.

K	ν	He	H^-	P_s^-
0	0	0.0	0.0	0.0
2	1	0.0	0.0	0.0
4	0	0.013	0.013	−0.007
4	2	−0.026	−0.038	0.021
6	1	0.004	0.013	0.070
6	3	0.004	0.013	−0.035

case of P_s^- where $K=0$ contributes about 70% of the norm (and $K=2$ contributes about 20%) the agreement between the OS and CS calculations is much worse, due to a large $\varepsilon\delta$. Also, as we pointed out in the end of Sec. II, for diagonal matrix elements it is only the departure $V_{K\nu,K\nu}$ from the average over ν that determines δ. We tabulate the contribution of diagonal elements to $\varepsilon\delta$ in Table IV. The comparison of Tables III and IV shows that though the diagonal elements are rather large, their contributions to V_{PQ} [Eq. (2.26)] are quite small for all the systems studied.

IV. CONCLUSIONS

We have presented the first comprehensive tests of the OS method, which were made by direct comparison between the CS and OS calculations with the same global quantum number $K_{\max}$ for different systems of three Coulomb-bound particles. We have found the critical parameters which govern the convergence of the method. We have checked our analytical conclusions numerically using systems that have very large (up to 47%) contributions to the norm from states with $K>0$. (Previous tests[17,29] were carried out only for systems where $P_K \approx 98\%$ for $K>0$.) In this paper we have shown analytically and numerically that, if the OS method works for the ground state, it will also work for excited states, even in cases of large nonzero hyperspherical contributions to the norm. Also, our tests include, unlike all the previous tests, comparisons of not only binding energies, but also correlation integrals.

Our main conclusion is that the OS method works reasonably well if the dimensionless product of matrix $V_{00,K\nu}V_{K\nu,K'\nu'}/V^2_{00,00}$ is small. Since the pair Coulomb potentials are singular when any of the interparticle distances approach zero, the convergence of the hyperspherical expansion is much slower than for smooth potentials, and close, qualitatively, to those of nuclear potentials with strong repulsive cores. In such cases one can expect that the serious restriction of the number of basis states, as in the OS method, could reflect itself quite unfavorably on the results of calculations. Nevertheless, we have shown numerically that this does not happen if $\varepsilon\delta$ is small, in agreement with our theoretical estimates. Thus the resulting precision should be generally rather good even for singular nuclear potentials. In nuclear calculations, where OS methods are usually used, and where a few percent agreement is usually good enough, the OS method should be quite satisfactory. However, the OS method cannot be recommended for the precise demands of atomic calculations.

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