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Use of Asymptotically Correct Wave Function for Three-Body Rayleigh-Ritz Calculations*

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A quickly converging expansion for three-body variational wave functions is obtained by adding to the usual Hylleraas wave-functions terms which express the correct asymptotic behavior. This modified expansion is applied to three problems: the H^- ground state; a search for a $He-e^+$ bound state; a search for a $H-e^+$ scattering resonance below the positronium threshold. The H^- calculation shows a marked improvement in convergence over using Hylleraas functions alone. It is also found that there is no $H-e^+$ bound state unless the mass of the positron is greater than 2.20 electron masses. Similarly, no positron scattering resonance below positronium threshold exists unless the mass of the positron is less than about 0.7 electron masses.

I. INTRODUCTION

For many calculations, especially those involving moments of the electron coordinates, it is important that wave functions derived from a variational principle have the correct asymptotic behavior, a feature to which variational principles are rather insensitive. In our attempts to incorporate the correct asymptotic behavior into trial wave functions, it was found that the effect upon the calculated ground-state energies was marked. Indeed, the terms added to the usual Hylleraas trial functions for H^- to incorporate the asymptotic behavior accounted for 98% of the total function's modulus; the Hylleraas part which is orthogonal to the asymptotic terms devotes only 2% to the regions closer to the origin.

Also of practical importance is the economy of terms necessary to achieve a given accuracy of the eigenvalue. In the next section we demonstrate this by comparing our results to Pekeris',[1,2] among others,[3-5] calculations in H^-. In Sec. II we seek (in vain) a bound state of the $H-e^+$ system, and finally, in Sec. III we look for the $H-e^+$ scattering resonance below positronium formation threshold.

In all calculations, atomic units are used, and it is assumed that the mass of the proton is infinite.

II. CALCULATIONS

A. Ground State of H^-

In this and subsequent examples we write the normalized variational wave function in two parts

$$\psi_V = \psi_H + \psi_T, \tag{1}$$

where ψ_H is the usual Hylleraas wave function

$$\psi_H = (A/\pi\sqrt{8})e^{-\frac{1}{2}Qs}\sum a_i s^{n_i} t^{2l_i} u^{m_i} \tag{2}$$

with $s=r_1+r_2$, $t=r_1-r_2$, and $u=r_{12}$. The a_i and Q are variational parameters. The constant A is what is later referred to as the "tail coefficient." In Eq. (1) ψ_T is the "tail" function which asymptotically approaches the exact wave function:

$$\psi_T=(A/2\pi)\times\left(e^{-r_1}\frac{e^{-\alpha r_2}-e^{-\beta r_2}}{r_2}+e^{-r_2}\frac{e^{-\alpha r_1}-e^{-\beta r_1}}{r_1}\right), \tag{3}$$

where $\alpha=(2E_b)^{1/2}=-(E+0.5\text{ a.u.})^{1/2}$, and $\beta>\alpha$. The energies E and E_b are the total and binding energies, respectively. The terms containing β are there to avoid a singularity when either r_1 or r_2 approach zero, and do not affect the asymptotic behavior.

Equation (1) was used to minimize the expectation value of the Hamiltonian for H^-

$$\mathcal{H}=-\frac{1}{2}\left(\frac{\partial^2}{\partial r_1^2}+\frac{2}{r_1}\frac{\partial}{\partial r_1}+\frac{\partial^2}{\partial r_2^2}+\frac{2}{r_2}\frac{\partial}{\partial r_2}+2\frac{\partial^2}{\partial r_{12}^2}+\frac{4}{r_{12}}\frac{\partial}{\partial r_{12}}+\frac{r_1^2-r_2^2+r_{12}^2}{r_1 r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}+\frac{r_2^2-r_1^2+r_{12}^2}{r_2 r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}\right)-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}}. \tag{4}$$

Restrictions on the Hylleraas part of the variational function [Eq. (2)] were as follows:

$$n_i+2l_i+m_i\leq N \text{ and } m_i\leq 3.$$

The reason for the last restriction is that it was noticed that results were virtually independent of $m_i>3$. To demonstrate, let

$$\psi_V^M\equiv\psi_T+\sum_{k=0}^{M}u^k f_k(s,t). \tag{5}$$

This amounts only to a rearrangement of terms in Eq. (2). In addition, let E^M be the corresponding best result from the Rayleigh-Ritz principle using (5). It was then found that E^M converged very quickly as a function of M:

$$E^0=-0.514\,46,\quad E^1=-0.527\,736,$$
$$E^2=-0.527\,750\,7,\quad E^3=-0.527\,750\,9.$$

In Table I we summarize the results for the calculations of H^- with $N=1,2,\ldots,7$ [for $N=7$, computer limitations allowed us to use only 55 terms in Eq. (2) rather than the full 57]. We also list the values of the amplitude of the tail, A [Eq. (3)]. The amplitude A converges to the value calculated by Ohmura and Ohmura[6] from a 203 term function of Pekeris.

Comparison of the energy values shown in Table I with those of other authors[7] points out how important the tail function is. Our 5 parameter energy is lower than Henrich's[3] 11 parameter value, our 15 parameter energy is lower than Hart and Herzberg's[4] 21 parameter value, the 23 parameter energy is better than the 34 parameter energy of Chung and Hurst,[5] and finally, with 45 parameters, we calculate a lower energy than

TABLE I. Energy values and tail coefficients for H^- ground state. A was extrapolated from the odd N values; the absolute values of the differences $|A(N=1)-A(N=3|$, $|A(N=3)-A(N=5)|$, $|A(N=5)-A(N=7)|$ converge to 0 very rapidly, and the next difference should not exceed 0.0001. This result is in good agreement with the value of Ohmura and Ohmura (Ref. 6): 0.790 89.

N	No. of Parameters	E	A
1	5	−0.527 621	0.761
2	9	−0.527 648	0.737
3	15	−0.527 734 66	0.804 7
4	23	−0.527 746 95	0.770 8
5	33	−0.527 749 90	0.791 81
6	45	−0.527 750 71	0.790 47
7	57	−0.527 750 882	0.790 89
extrapolated			0.790 84 ± 0.000 05

TABLE II. Average values of various operators using H^- trial functions. The last two operators are defined in Sec. II-A.

	5 Parameters	15 Parameters	33 Parameters	Pekeris
$\langle r_1+r_2\rangle$	5.415	5.4230	5.420 22	5.420 36
$\langle r_1^2+r_2^2\rangle$	23.69	23.876	23.825 6	23.827 4
$\langle r_1^3+r_2^3\rangle$	150.	152.8	152.03	
$\langle r_1^4+r_2^4\rangle$	1 254.	1 303.	1 290.	
$\langle r_1^5+r_2^5\rangle$	13 140.	13 908.	13 697.	
M_{tot}^2	7.454	7.508	7.485 1	7.484 26
I_1-I_2	−10.536	−10.715	−10.665	

does Pekeris[1] with 125 or Frankowski and Pekeris[2] with 59 parameters.

In Table II are listed the first five moments of (r_1+r_2) using our 5, 15, and 33 parameter functions. In addition we list the more complicated function estimated by Inokuti and Kim[8]:

$$I_1 - I_2 = \int_1^\infty S_{\rm inc}(k)k^{-4}d(k^2) - \int_0^1 [M_{\rm tot} - k^{-2}S_{\rm inc}(k)]k^{-2}d(k^2),$$

where $M_{\rm tot} = \langle |\vec{r}_1 + \vec{r}_2|^2 \rangle$

and $$S_{\rm inc}(k) = \left\langle \left| e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2} \right|^2 \right\rangle - \left\langle e^{i\vec{k}\cdot\vec{r}_1} + e^{i\vec{k}\cdot\vec{r}_2} \right\rangle^2 .$$

In Table III we list the coefficients for the 5, 15, and 33 parameter functions. In all cases, $\alpha = (0.027\,751\,016)^{1/2}$, the exact value of Frankowski and Pekeris.[2]

B. Search for a Bound State of the $H-e^+$ System

The search, using the Rayleigh-Ritz principle, for a bound state whose existence is in doubt[9] is a precarious business, since, when the state is not found, one is always plagued with the fear of having been caught in a local minimum, or of not having a trial function of high enough accuracy. It is much more satisfying to change a parameter (such as a mass) so that binding is achieved and then, after calculating the binding energy as a function of this mass, extrapolating it back to its physical value. We have followed such a procedure in an attempt to find a bound state of the $H-e^+$ system, the variable mass being that of the positron.

We first develop an extrapolation formula. Let m_0 be the mass of the positron at which binding is just achieved. Then for m slightly greater than m_0, the positron is bound at a distance which is great compared to a_0, the Bohr radius. Asymptotically the positron is in a static potential $V=-b/r^4$, $b>0$. Near the origin the potential is $V=1/r$. Thus for $m>m_0$, and $r\gg a_0$, the wave function for bound positron satisfies

$$y'' - 2mVy = 2mE_b y \tag{6}$$

with the boundary conditions

$$y(0)=0;$$
$$y \to \exp[-(2mE_b)^{1/2}r], \quad r \gg (E_b/b)^{-1/4}. \tag{7}$$

At the critical mass m_0

$$y_0'' - 2m_0 V y_0 = 0 \tag{8}$$

with

$$y_0(0)=0; \quad y \to 1, \quad r \gg (E_b/b)^{-1/4}. \tag{9}$$

TABLE III. Coefficients for H^- variational functions nonlinear coefficients of ψ_H and ψ_T.

N	α	β	Q	A
1	0.235 588 692	0.85	1.572 259 77	0.760 817 91
3	0.235 588 692	0.9	1.757 910 254	0.804 755 14
5	0.235 588 692	1.712	1.860 807 68	0.791 974 00

Linear Coefficients of ψ_H

No.	n	$2l$	m	$N=5$	$N=3$	$N=1$
1	0	0	0	−3.372 829 3	−1.088 300 8	−0.888 544 58
2	1	0	0	0.209 337 49	−0.228 819 26	−0.112 566 00
3	0	0	1	0.345 179 26	0.321 579 91	0.263 528 05
4	2	0	0	−0.069 809 807	0.002 169 692 3	
5	0	2	0	−0.008 715 223 6	0.014 431 692	
6	1	0	1	0.039 682 831	0.018 278 886	
7	0	0	2	−0.054 118 628	−0.029 438 149	
8	3	0	0	0.000 575 042 16	−0.002 601 913 6	
9	1	2	0	0.010 181 674	−0.003 398 556 0	
10	2	0	1	−0.002 901 029 4	0.001 278 131 1	
11	0	2	1	−0.015 308 818	−0.001 565 627 4	
12	1	0	2	0.010 788 827	0.003 822 738 2	
13	0	0	3	0.005 860 731 8	0.000 141 911 11	
14	4	0	0	−0.000 053 162 557		
15	2	2	0	−0.000 890 865 34		
16	0	4	0	0.000 353 575 43		
17	3	0	1	0.000 816 928 36		
18	1	2	1	0.000 411 234 53		
19	2	0	2	−0.000 461 313 05		
20	0	2	2	0.001 050 822 8		
21	1	0	3	−0.001 535 963 6		
22	5	0	0	−0.000 022 246 859		
23	3	2	0	−0.000 175 094 39		
24	1	4	0	−0.000 041 184 624		
25	4	0	1	0.000 005 049 451 6		
26	2	2	1	0.000 365 759 60		
27	0	4	1	−0.000 010 615 391		
28	3	0	2	−0.000 014 877 062		
29	1	2	2	−0.000 242 625 04		
30	2	0	3	0.000 095 995 793		
31	0	2	3	0.000 029 620 107		

From Eqs. (6)–(7) it is found that it is the asymptotic contribution which is energy dependent. By multiplying Eqs. (6), (8) by y_0 and y, respectively, subtracting and integrating over r one obtains

$$(mE_b)^{1/2} = C(m - m_0) \tag{10}$$

correct to first order in $(m - m_0)$.[10]

In order to implement Eq. (10) the following Hamiltonian was minimized

$$\mathcal{H} = -\frac{1}{2}\left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \mu\left(\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2}\right)\right.$$
$$+ (1+\mu)\left(\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right)$$
$$+ \frac{r_1^2 - r_2^2 + r_{12}^2}{r_1 r_{12}}\frac{\partial^2}{\partial r_1 \partial r_{12}}$$
$$\left. + \mu\frac{r_2^2 - r_1^2 + r_{12}^2}{r_2 r_{12}}\frac{\partial^2}{\partial r_2 \partial r_{12}}\right] - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}, \tag{11}$$

where r_1 and r_2 are the electron and positron coordinates, respectively, and $\mu = 1/m$, m being the mass of the positron. The variational wave function takes the form $\psi_V = \psi_T + \psi_H$, where

$$\psi_T = \frac{D}{2\pi} e^{-r_1}\frac{e^{-\alpha r_2} - e^{-\beta r_2}}{r_2}, \quad \beta > \alpha \tag{12}$$

$$\alpha = (2E_b/\mu)^{1/2}, \quad E_b = -(E + 0.25) \text{ a.u.}$$

and

$$\psi_H = (D/\pi\sqrt{8})\exp(-A_1 r_1 - A_2 r_2 - A_{12} r_{12})$$
$$\times \sum a_i r_1^{n_i} r_2^{l_i} r_{12}^{m_i}, \tag{13}$$

where $n_i + l_i + m_i \leq N$.

Note that the symmetry restriction has been lifted from Eqs. (12) and (13). The binding energy was calculated for $\mu = 0.40, 0.41, \ldots, 0.45$ with $N = 4, 5, 6$. The energy for $N = \infty$ was estimated by assuming geometric convergence as a function of N. The results are summarized in Table IV. Figure 1 contains the plot of $(\mu E_b)^{1/2}$ against μ. The graph is a precise straight line and extrapolates to $\mu = 0.454$, or $m_0 = 2.20$, which corroborates other[11] theoretical evidence that there is no $H - e^+$ bound state.

C. Search for a Scattering Resonance of the $H - e^+$ System

The method used in searching for a bound state of the $H - e^+$ system is also applied to the search for a scattering resonance below the threshold

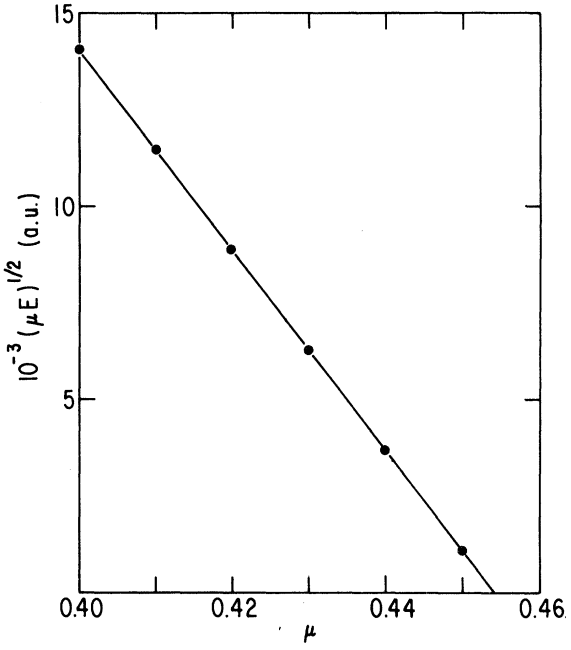

FIG. 1. Binding energy of the positron in the $H - e^+$ system as a function of inverse positron mass. The points show the computed values; the straight line is given by Eq. (10). The line extrapolates to $\mu_0 = 0.454$ or $m_0 = 2.20$ electron masses for zero binding. The data are taken from Table IV.

TABLE IV. Binding energy of the positron in the H-e^+ system as a function of positron mass. The values in the last column were used in Fig. 1.

$\mu (=1/m)$	E_b $N=4$	E_b $N=5$	E_b $N=6$	E_b Extrapolated	$10^3(\mu E_b)^{1/2}$
0.40	0.000 480 8	0.000 491 5	0.000 494 5	0.000 496	14.10
0.41	0.000 308 2	0.000 317 7	0.000 320 5	0.000 322	11.45
0.42	0.000 177 0	0.000 183 1	0.000 186 5	0.000 191	8.95
0.43	0.000 083 7	0.000 088 6	0.000 090 5	0.000 092	6.30
0.44	0.000 023 5	0.000 028 6	0.000 030 0	0.000 031	3.7
0.45	0.000 001 15	0.000 001 93	0.000 002 35	0.000 002 8	1.1

for positronium formation.[12] The resonance problem is converted to a bound state problem by projecting out the ground state of hydrogen from the trial function. A method for accomplishing the projection numerically is described in the Appendix.

For very small binding energy, the variational function describes positronium bound to an infinitely massive proton. That is, instead of using the form of Eq. (12) for the tail function, we use

$$\psi_T = B \exp\left(-\frac{r_{12}}{1+\mu}\right) \frac{e^{-\alpha r_2} - e^{-\beta r_2}}{r_2}, \qquad (14)$$

where r_2 is the positron-proton distance. We use r_2 instead of $\frac{1}{2}|\vec{r}_1 + \vec{r}_2|$ for convenience.

Relation (10) should roughly hold in this case also, with two restrictions: (1) The potential depends strongly on m and this dependence causes the binding to occur for $m < m_0$. The constant C also becomes strongly m dependent. (2) In the range of μ, where the binding energy could be calculated ($\mu > 1.6$), r_{12} is of the same order of magnitude as $\frac{1}{2}|\vec{r}_1 + \vec{r}_2|$, and, therefore, Eq. (10) need not be valid. Nevertheless, empirically we found that

$$\sqrt{E_b} = C'(m_0^{-1} - m^{-1}), \quad 0.5 < m < 0.6. \qquad (15)$$

The binding energy is calculated for $\mu = 1.7$, 1.8, ..., 2.0. Convergence as a function of N is not as strong as in the previous case, especially near μ_0; nevertheless, extrapolation of the data to $E_b = 0$ gives $\mu_0 \simeq 1.45$. Table V and Fig. 2 summarize the results. While we cannot rigorously rule out the existence of a resonance below the positronium threshold, we cannot see any reasonable change in Fig. 2 which will bring μ_0 near 1.

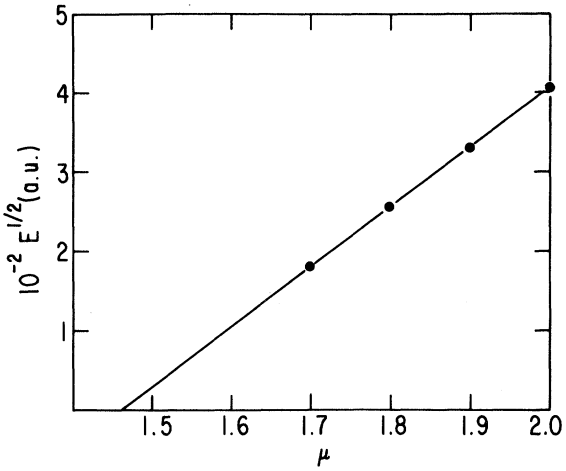

FIG. 2. Binding energy of a positron in the auto-ionizing level below positronium threshold as a function of inverse positron mass. The points show the computed values; the straight line is given by Eq. (15). The line extrapolates to $\mu_0 = 1.47$ or $m_0 = 0.68$ electron masses. All reasonable estimates of the errors in the computed binding energies give values of $1.4 < \mu_0 < 1.5$, or $m_0 = 0.7 \pm 0.03$ electron masses. The data are taken from Table V.

APPENDIX

In this Appendix,[13] an approximate, but arbitrarily accurate method for calculating the projection operator Q in variational calculations is given.

TABLE V. Auto-ionization levels in the H-e^+ system below positronium threshold using 4th, 5th, and 6th order wave functions, as a function of positron mass. (Because of storage limitations only 70 terms of ψ_H were used for $N = 6$ instead of the 84.) The values of the last column are used in Fig. 2.

$\mu = \frac{1}{m}$	E_b $N=4$	E_b $N=5$	E_b $N=6$	$10^2 E_b^{1/2}$ $(N=6)$
1.7	0.000 17	0.000 275	0.000 32	1.80
1.8	0.000 50	0.000 62	0.000 65	2.55
1.9	0.000 91	0.001 08	0.001 10	3.30
2.0	0.001 51	0.001 64	0.001 65	4.05

We suppose the unprojected variational function is composed from a basis $\{\varphi_i\}$

$$\psi_V = \sum_{i=1}^{K} a_i \varphi_i(r_1, r_2, r_{12}). \qquad (A1)$$

Then a typical term in $Q\psi_V$ is

$$Q\varphi = \varphi - u_0 \int_0^\infty \varphi u_0 r_1^2 dr_1 \equiv \varphi - u_0 F(r_2). \qquad (A2)$$

We assume that the integral in (A2) can be expressed as a Laguerre series either exactly, or to arbitrary accuracy,

$$F(r_2) \simeq F_M(p; r_2) \equiv e^{-pr_2} \sum_{j=0}^{M} b_j r_2^j. \qquad (A3)$$

The corresponding approximation to Q will be determined by

$$\int Q_M(p; r_1, r_2, r_{12}) \varphi(r_1, r_2, r_{12}) u_0(r_1) \times e^{-pr_2} r_2^k r_1 r_2 r_{12} dr_1 dr_2 dr_{12} = 0$$
$$\text{for } k = 0, 1, 2, \ldots, M. \qquad (A4)$$

We now proceed to find the eigenvalues of $Q_M H Q_M$ without actually realizing Q_M itself.

(a) Construct the two $(K+M+1)$ order matrices H and N:

$$H_{\lambda\mu} = \langle v_\lambda | \mathcal{H} | v_\mu \rangle; \quad N_{\lambda\mu} = \langle v_\lambda | v_\mu \rangle, \qquad (A5)$$

where

$$v_\lambda = u_0(r_1) r_2^\lambda e^{-pr_2}, \quad \text{for } \lambda = 0, 1, \ldots, M \tag{A6}$$

and

$$v_\lambda = \varphi_{\lambda - M}(r_1, r_2, r_{12}), \quad \text{for } \lambda = M+1, M+2, \ldots, M+K. \tag{A7}$$

(b) Invert N using the standard Gauss elimination process

$$N^{-1} = SRR^T S^T$$

$$R = R^{M+K} R^{M+K-1} \cdots R^1$$

$$R_{\mu\nu}^{\ \lambda} = \delta_{\mu\nu}, \quad \text{for } \mu \neq \lambda, \text{ or } \mu = \lambda \text{ and } \nu \geq \lambda$$

$$= -N_{\lambda\nu}^{\lambda-1} / N_{\nu\nu}^{\lambda-1}, \quad \text{for } \mu = \lambda, \ \nu < \lambda$$

$$N^0 = N, \quad N^\lambda = R^\lambda N^{\lambda-1} (R^\lambda)^T,$$

$$S_{\mu\nu} = (N_{\mu\mu}^{M+N})^{-1/2} \delta_{\mu\nu}$$

and apply the same process to H

$$\bar{H} = SRHR^T S^T . \tag{A8}$$

(c) The K eigenvalues of $\hat{H}_{i,j} \equiv \bar{H}_{i+M, j+M}$, $(i, j = 1, 2, \ldots, K)$ are the eigenvalues of $Q_M H Q_M$ which we are seeking.

The matrix $\bar{H}$ of Eq. (A8) is identical to the matrix one would obtain by applying the Gramm-Schmidt orthogonalization process to the set $\{v_0, \ldots, v_M, v_{M+1}, \ldots, v_{M+K}\}$ to obtain $\{w_0, \ldots, w_M, w_{M+1}, \ldots, w_{M+K}\}$,

where

$$\bar{w}_0 = v_0, \quad w_0 = \bar{w}_0 / \langle \bar{w}_0 | \bar{w}_0 \rangle^{1/2};$$

$$\bar{w}_1 = v_1 - \langle w_0 | v_1 \rangle w_0, \quad w_1 = \bar{w}_1 / \langle \bar{w}_1 | \bar{w}_1 \rangle^{1/2}, \text{ etc};$$

$$\bar{H}_{\lambda\mu} = \langle w_\lambda | \mathcal{H} | w_\mu \rangle .$$

Not only are the w_λ mutually orthogonal, but the Gramm-Schmidt process has the property of leaving the w_λ orthogonal to all the v_μ such as the $\mu < \lambda$. Therefore the subset $W \equiv \{w_{M+1}, \ldots, w_{M+K}\}$ is orthogonal to the subset $V \equiv \{v_0, \ldots, v_M\}$. The subset V forms the basis for the ground state, therefore W must span $\{Q_M \varphi_1, Q_M \varphi_2, \ldots, Q_M \varphi_K\}$.

In Table VI are shown the lowest eigenvalues of H as a function of M, for $\mu = 1.7$, $K = 36$. At $M = 6$ all the spurious levels below the resonance disappear, and the eigenvalue is correct to five significant digits. At $M = 9$, the energy is correct to seven significant digits. Since the ground state of positronium for $\mu = 1.7$ is $-0.185\,185$ a.u., $M = 6$ yields a binding of $-0.000\,17$ a.u.

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TABLE VI. Lowest eigenvalues of $\hat{H}$ as functions of M with $\mu = 1.7, K = 36$, $N = 4$, $P = 0.5$. The first eigenvalue in each row corresponds to the resonance energy in a.u. and converges to $-0.185\,3557$. The other eigenvalues are spurious and disappear as M increases. (The positronium ground state is $-0.185\,185\,185$.)

M	Lowest eigenvalues				
0	−0.185 057	−0.187 534	−0.325 283	−0.411 351	−0.465 034
1	−0.185 062	−0.225 642	−0.361 905	−0.445 492	
2	−0.185 186	−0.298 356	−0.421 187		
3	−0.185 298	−0.201 617	−0.386 016		
4	−0.185 332	−0.334 191			
5	−0.185 347	−0.255 474			
6	−0.185 3533				
7	−0.185 3545				
8	−0.185 3556				
9	−0.185 3557				

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[13]The material presented in this Appendix will also appear in a Ph. D. thesis by N. Minsky, Department of Physics, The Hebrew University, Jerusalem, Israel.

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Elastic Scattering of 145-, 279-, 412-, and 662-keV γ Rays from Lead*

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The differential cross section for elastic scattering of 145-, 279-, 412-, and 662-keV γ rays from lead has been measured in the angle interval 30 to 150° using a lithium-drifted germanium detector. The experimental results are in general agreement with the theory of Brown *et al.* Approximative formulas for the differential cross section of Rayleigh scattering are discussed.

I. INTRODUCTION

The good energy resolution of lithium-drifted germanium detectors lead to an enormous increase in the accuracy of many experiments in γ-ray spectrometry. One of these experiments is the determination of the differential cross section for elastic scattering of γ rays which requires the separation of the elastic- and inelastic-scattering components. The elastic scattering is composed of four different processes: Rayleigh scattering, nuclear Thomson scattering, nuclear-resonance scattering, and Delbrück scattering. Of these four processes the Delbrück scattering is by far the most interesting one since it yields in addition to the Lamb shift an information about the vacuum polarization. Unfortunately this process is also the weakest one, so that its contribution to the cross section can only be detected when the competing processes are very well known. This is one reason for being interested in an accurate determination of the differential cross section for Rayleigh scattering.

An exact calculation of the differential cross section for Rayleigh scattering has been carried out by Brown *et al.*[1–4] for the K electrons of mercury and the γ-ray energies 163, 327, 654, and 1308 keV. The main purpose of the present work was to check these calculated cross sections experimentally. For this reason the ex-