

Improvement to wave functions and energy values of the ground state of helium

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(Received 27 January 1975; revised manuscript received 30 April 1975)

Nonrelativistic wave functions and energy values for the ground state of helium are calculated accurately by using the conventional Rayleigh-Ritz technique. However, the trial wave functions used are more general than those used by Hylleraas and others. They contain interelectronic separation coordinates in the exponential function beside the variational parameters. Groups of three- and four-parameter wave functions are obtained with comparatively smaller energies. Also, improved wave functions and energies have been obtained by solving determinants of orders 7, 13, 22, 34, 50, 70, 95, and 125, using a simple model. The last determinant yields an energy value of $-2.903\,724\,371$ a.u., as compared with $-2.903\,724\,370$ a.u. obtained by Pekeris by solving a determinant of order 715. The first determinant (ten parameters) yields an energy value of $-2.903\,425\,858$ a.u., as compared with the recent value of -2.9022 a.u. computed by Tweed with the use of a 41-parameter wave function.

I. INTRODUCTION

The principle given by Coolidge and James¹ on the convergence of Hylleraas functions, or any function, even if no formal solution of the wave equation exists, has been extended by several authors to obtain the ground state of different complex atoms. The necessity of improving the accuracy of theoretical prediction for the ground-state energy of helium was pointed out by Chandrasekhar, Elbert, and Herzberg.² They used a ten-parameter trial wave function with the Ritz variation method to obtain more accurate energy. In order to identify the source of discrepancy between theory and experiment, Chandrasekhar and Herzberg³ computed the nonrelativistic energy up to 18 parameters, and they pointed out that the discrepancy originates mostly from the poor convergence of the variational calculation. Kinoshita⁴ used more general Hylleraas wave functions, up to 39 terms, to remove most of the discrepancy stated before. Pekeris^{5,6} has considered the interelectronic separation coordinate terms for two-electron atoms and ions. He achieved rapid convergence and was able to calculate measurable quantities within the limits of the experimental results.

Recently, Tweed⁷ used trial wave functions up to 41 terms, taking fully into account the correlation term of the Hamiltonian, to calculate wave functions for the helium atom. Thomas and Hummerston⁸ used the Rayleigh-Ritz principle to generate a series of systematic helium ground-state wave functions up to 50 terms.

The use of simple wave functions (few parameters) to predict results of scattering experiments introduces large errors due to inaccuracies in these simple wave functions. Peterkop and Rabik⁹

discussed these difficulties for the position-hydrogen scattering length. Houston¹⁰ extended Peterkop and Rabik's work to calculate the positron-helium scattering length. The scattering of slow and zero-energy positrons by helium atoms were discussed by Houston and Drachman,¹¹ and Moussa and Radi.¹²⁻¹⁵ These authors concluded that the use of inexact target wave functions affect the scattering results. Drachman⁶ presented the method of models to overcome these difficulties. He suggested that by using a sequence of improved forms of the model wave function one can obtain improved scattering results, provided that the model wave functions describe well the essentials of the target state. This has generated renewed interest in obtaining simple, but more accurate wave functions.

Though the measurement and theory have reached such a high precision, it is necessary to improve the accuracy further, but with a small number of terms in the trial wave functions. This is carried out in this paper by choosing a more general trial function and treating it variationally to obtain the minimum energy.

II. COMPUTATIONAL METHOD

The most exact results for eigenvalues and eigenfunctions of the ground state of helium may be obtained by means of the Rayleigh-Ritz variational method. In stationary-state problems the evaluation of eigenenergies E_η and eigenfunctions ψ_η of a Hamiltonian H is obtained from the Schrödinger wave equation, assuming an infinitely heavy nucleus,

$$\left[-\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - 2/r_1 - 2/r_2 + 1/r_{12} \right] \psi_\eta = E_\eta \psi_\eta, \quad (1)$$

where r_1 and r_2 are the distances of the electrons

from the nucleus, r_{12} is the interelectronic separation, ∇_1^2 and ∇_2^2 are the Laplacian operators with respect to the coordinates of the two electrons, and lengths and energies are expressed in atomic units.

An arbitrary, quadratically integrable, bounded trial function Ψ can be expanded in terms of the eigenfunction ψ_η ($\Psi = \sum_\eta a_\eta \psi_\eta$). So, the upper bounds of the ground-state energy satisfy

$$E_0 \leq E(\Psi), \quad (2)$$

where

$$E(\Psi) = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle. \quad (3)$$

In Eq. (3) we now substitute a suitable trial function Ψ which depends on a number of variable parameters c_μ ($\mu = 1, 2, \dots, n$), chosen in such a way that E is a minimum. This is accomplished by solving the n equations $\partial E(\Psi) / \partial c_\mu = 0$. The minimum energy determined by this method will be near to the true ground-state-energy value, if Ψ has a form closely resembling the ground-state eigenfunction ψ_0 . Thus $E(\Psi) \rightarrow E_0$ as $\Psi \rightarrow \psi_0$.

Often, a given atomic structure is represented by a wave function consisting of a linear combination of basis function χ_μ as

$$\Psi = N_\eta \sum_{\mu=1}^n c_\mu^\eta \chi_\mu, \quad (4)$$

where the real variable parameter c_μ^η is the μ th amplitude factor for η th eigenvalue, and N_η is the normalization constant defined for that eigenvalue. Using the above method, after substituting Eq. (4) into Eq. (3), one can obtain the set of n equations

$$\sum_{\mu=1}^n H_{\mu\nu} c_\mu^\eta = \sum_{\mu=1}^n S_{\mu\nu} c_\mu^\eta E_\eta \quad (\nu = 1, \dots, n), \quad (5)$$

where

$$H_{\mu\nu} = \langle \chi_\mu | H | \chi_\nu \rangle \text{ and } S_{\mu\nu} = \langle \chi_\mu | \chi_\nu \rangle. \quad (6)$$

Equation (5) may be written in the usual matrix notation form as

$$\tilde{H}\tilde{C} = \tilde{S}\tilde{C}\tilde{E}, \quad (7)$$

where both \tilde{H} and \tilde{S} are real symmetric matrices and \tilde{E} is diagonal.

One has to solve Eq. (7) to obtain the eigenenergies E_η ($\eta = 1, \dots, n$), and then pick out the minimum eigenenergy E_λ and its corresponding coefficients c_μ^λ ($\mu = 1, \dots, n$). The procedure is then to calculate the eigenvalues and the matrix of eigenvectors for the symmetric matrix \tilde{S} .¹⁷ The reciprocal of the square root of each eigenvalue is formed. The matrix $\tilde{S}^{-1/2}$ is also formed. The symmetric matrix $\tilde{H}' = (\tilde{S}^{-1/2})' \tilde{H} (\tilde{S}^{-1/2})$ is then formed and the eigenvalues E_η and the matrix of

eigenvectors \tilde{M} are calculated. Following that, the matrix $\tilde{S}^{-1/2}\tilde{M}$ is formed and its vectors can be normalized to form the eigenvectors of \tilde{C} by the equation

$$c_\nu^\eta = (\tilde{S}^{-1/2}\tilde{M})_{\eta\nu} / \left(\sum_{\epsilon=1}^n (\tilde{S}^{-1/2}\tilde{M})_{\epsilon\eta}^2 \right)^{1/2}.$$

In this work, double-precision arithmetic computation was used throughout the calculations.

III. CHOICE OF BASIS FUNCTIONS

Since the Coulomb interaction between the two electrons plays an important role in the behavior of the helium atom, the basis function chosen will contain interelectronic separation coordinates in the exponential function. (The magnetic interaction due to the spin of the electrons is very small and will be neglected in the present work.) It will be written in the form

$$\chi_\mu = (4\pi)^{-1} [1 + P_{12}] r_1^{j_\mu} r_2^{k_\mu} r_{12}^{l_\mu} \exp[-(\alpha r_1 + \beta r_2 + \gamma r_{12})], \quad (8)$$

where j_μ , k_μ , and l_μ are non-negative integer values; α , β , and γ are non-negative variational parameters; and P_{12} is an operator to exchange the labels of r_1 and r_2 . The sum in Eq. (4), after substituting with Eq. (8), becomes over all the values of j_μ , k_μ , and l_μ , such that $j_\mu + k_\mu + l_\mu \leq M$, and M takes integer values from 1 to 9 giving rise to determinants of orders 3, 7, 13, 22, 34, 50, 70, 95, and 125, respectively, in the case of $\alpha = \beta$. Generally, the variational parameters α , β , and γ are varied to ensure the maximum value of the energy E_λ obtained from the solution of Eq. (7).

IV. SOLUTION OF INTEGRALS

The Hamiltonian of the system is

$$H = T + V, \quad (9)$$

where

$$T = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) \text{ and } V = -2/r_1 - 2/r_2 + 1/r_{12}.$$

Then, the Hamiltonian integral $H_{\mu\nu}$ defined by Eq. (6) can be divided into two parts, the kinetic-energy integral $T_{\mu\nu}$ and the potential-energy integral $V_{\mu\nu}$. These integrals (including the overlap integral $S_{\mu\nu}$) must be evaluated in analytic form to maintain the required accuracy of the energy obtained successively until $n = 125$. The kinetic-energy integral is given by

$$T_{\mu\nu} = \langle \chi_\mu | T | \chi_\nu \rangle = \int \int d\tau_1 d\tau_2 [\xi_\mu(12)T\xi_\nu(12) + \xi_\mu(12)T\xi_\nu(21) + \xi_\mu(21)T\xi_\nu(12) + \xi_\mu(21)T\xi_\nu(21)], \quad (10)$$

where

$$\xi_\mu(12) = (4\pi)^{-1} r_1^{j_\mu} r_2^{k_\mu} r_{12}^{l_\mu} \exp[-(\alpha r_1 + \beta r_2 + \gamma r_{12})]. \quad (11)$$

Since the operator T is symmetric with respect to the exchange of the labels 1 and 2, then $T_{\mu\nu}$ can take the form

$$T_{\mu\nu} = 2 \int \int d\tau_1 d\tau_2 \{ \xi_\mu(12)T[\xi_\nu(12) + \xi_\nu(21)] \}. \quad (12)$$

The operator $\nabla_1^2 + \nabla_2^2$ has been given by Hylleraas¹⁸ as

$$\begin{aligned} \nabla_1^2 + \nabla_2^2 = (1 + P_{12}) & \left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} + \frac{r_1^2 - r_2^2 + r_{12}^2}{r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_{12}} \right) \\ & + 2 \frac{\partial^2}{\partial r_{12}^2} + \frac{4}{r_{12}} \frac{\partial}{\partial r_{12}}. \end{aligned} \quad (13)$$

Substituting this expression for $\nabla_1^2 + \nabla_2^2$ in Eq. (12), exchanging the labels of some integrals to reduce their numbers, and using some rules of differentiation and algebraic manipulation, the kinetic-energy integral will take the form

$$T_{\mu\nu} = \sum_{\epsilon=1}^{23} g_\epsilon [\mathcal{L}(2\alpha, 2\beta, 2\gamma/j_\mu + j_\nu + a_\epsilon, k_\mu + k_\nu + b_\epsilon, l_\mu + l_\nu + c_\epsilon) + \mathcal{L}(\alpha + \beta, \alpha + \beta, 2\gamma/k_\mu + j_\nu + a_\epsilon, j_\mu + k_\nu + b_\epsilon, l_\mu + l_\nu + c_\epsilon)], \quad (14)$$

where the values of g_ϵ , a_ϵ , b_ϵ , and c_ϵ ($\epsilon = 1, \dots, 23$) for definite values of α , β , γ , j_μ , k_μ , l_μ , j_ν , k_ν , and l_ν are given in Table I. The function \mathcal{L} is defined by

$$\mathcal{L}(\rho, \sigma, \omega/j, k, l) = (4\pi)^{-1} \int \int d\tau_1 d\tau_2 \exp[-(\rho r_1 + \sigma r_2 + \omega r_{12})] r_1^j r_2^k r_{12}^l. \quad (15)$$

This integral is evaluated analytically in the Appendix.

The potential energy integral and the overlap integral can now be easily evaluated to take the following forms:

$$V_{\mu\nu} = \sum_{\epsilon=1}^3 h_\epsilon [\mathcal{L}(2\alpha, 2\beta, 2\gamma/j_\mu + j_\nu + a_\epsilon, k_\mu + k_\nu + b_\epsilon, l_\mu + l_\nu + c_\epsilon) + \mathcal{L}(\alpha + \beta, \alpha + \beta, 2\gamma/j_\mu + k_\nu + a_\epsilon, k_\mu + j_\nu + b_\epsilon, l_\mu + l_\nu + c_\epsilon)] \quad (16)$$

and

$$S_{\mu\nu} = 2\mathcal{L}(2\alpha, 2\beta, 2\gamma/j_\mu + j_\nu, k_\mu + k_\nu, l_\mu + l_\nu) + 2\mathcal{L}(\alpha + \beta, \alpha + \beta, 2\gamma/j_\mu + k_\nu, k_\mu + j_\nu, l_\mu + l_\nu), \quad (17)$$

where the values of h_ϵ , a_ϵ , b_ϵ , and c_ϵ ($\epsilon = 1, \dots, 3$) in Eq. (16) are given in Table II.

V. RESULTS AND DISCUSSIONS

As was discussed earlier, the inexactness of the ground-state helium wave function affects the computed value of the scattering length,^{9,15,16} as well as the phase shifts. So, different models with simple (but more accurate) wave functions and their corresponding energies are presented to be used in the scattering problems. In these models, the variational parameters α , β , and γ that appear in the basis function given by Eq. (8) are varied to obtain a minimum value of E_0 . The variation of these parameters is very important in decreasing

the eigenvalue of the Rayleigh-Ritz calculation. However, Pekeris *et al.*,¹⁹ in carrying out similar work past 1000 parameters, have not tried to vary these parameters in the most simple case when $\alpha = \beta$ and $\gamma = 0$ to reduce the numerical computations. At the outset of our program we decided to adopt Pekeris's approach, but we were led back to varying α , β , and γ . For this reason, it must be pointed out that the program is written in such a way that a great deal of calculation is unnecessarily repeated to save computing time.

The final forms of the five models as determined by this calculation are

TABLE I. Values of g_ϵ , a_ϵ , b_ϵ , and c_ϵ ($\epsilon=1, \dots, 23$) in formula (14).

ϵ	g_ϵ	a_ϵ	b_ϵ	c_ϵ
1	$-(\alpha^2 + \beta^2 + 2\gamma^2)$	0	0	0
2	$-l_\nu(j_\nu + k_\nu + 2l_\nu + 2)$	0	0	-2
3	$+\alpha(2j_\nu + l_\nu + 2)$	-1	0	0
4	$+\beta(2k_\nu + l_\nu + 2)$	0	-1	0
5	$-j_\nu(j_\nu + l_\nu + 1)$	-2	0	0
6	$-k_\nu(k_\nu + l_\nu + 1)$	0	-2	0
7	$+j_\nu l_\nu$	-2	2	-2
8	$+k_\nu l_\nu$	2	-2	-2
9	$+\alpha l_\nu$	1	0	-2
10	$+\beta l_\nu$	0	1	-2
11	$-\alpha l_\nu$	-1	2	-2
12	$-\beta l_\nu$	2	-1	-2
13	$+\gamma(j_\nu + k_\nu + 4l_\nu + 4)$	0	0	-1
14	$-j_\nu \gamma$	-2	2	-1
15	$-k_\nu \gamma$	2	-2	-1
16	$+j_\nu \gamma$	-2	0	1
17	$+k_\nu \gamma$	0	-2	1
18	$-\alpha \gamma$	1	0	-1
19	$-\beta \gamma$	0	1	-1
20	$+\alpha \gamma$	-1	2	-1
21	$+\beta \gamma$	2	-1	-1
22	$-\alpha \gamma$	-1	0	1
23	$-\beta \gamma$	0	-1	1

Model I: $\Psi = N[c_1 + c_2(r_1 + r_2) + c_3 r_{12}] \times \exp[-\alpha(r_1 + r_2)],$ (18a)

Model II: $\Psi = N[c_1 + c_2(r_1 + r_2) + c_3 r_{12}] \times \exp[-\alpha(r_1 + r_2) - \gamma r_{12}],$ (18b)

Model III: $\Psi = N(1 + p_{12})(c_1 + c_2 r_1 + c_3 r_{12}) \times \exp[-(\alpha r_1 + \beta r_2)],$ (18c)

Model IV: $\Psi = N(1 + P_{12})(c_1 + c_2 r_1 + c_3 r_2 + c_4 r_{12}) \times \exp[-(\alpha r_1 + \beta r_2)],$ (18d)

Model V: $\Psi = N(1 + P_{12})(c_1 + c_2 r_1 + c_3 r_2 + c_4 r_{12}) \times \exp[-(\alpha r_1 + \beta r_2 + \gamma r_{12})],$ (18e)

where values of the parameters of these wave functions and their corresponding energies are listed in Table III.

TABLE II. Values of h_ϵ , a_ϵ , b_ϵ , and c_ϵ ($\epsilon=1, \dots, 3$) in formula (16).

ϵ	h_ϵ	a_ϵ	b_ϵ	c_ϵ
1	-4	-1	0	0
2	-4	0	-1	0
3	2	0	0	-1

TABLE III. Values of the parameters in the wave function Ψ for the five models [Eqs. 18(a)–18(e)].

Model	E (a.u.)	N	α	β	γ	c_1	c_2	c_3	c_4
I	-2.891232377	0.752621421	1.8135			1.884741868	-0.095826600	0.641106186	
II	-2.891512055	0.797820324	1.7442		0.092	1.776479122	-0.229225527	0.796206358	
III	-2.901495456	0.696487729	1.479	2.214		0.953268283	0.073224085	0.293117407	
IV	-2.902473533	435.119758341	1.79520	1.78574		0.001548006	0.707059316	-0.707152415	0.000434366
V	-2.903271263	25.081449033	1.694	1.704	0.1341	0.026770072	0.703032785	-0.710555186	0.011815017

In Table IV the wave functions were checked for agreement with the virial theorem, which predicts $-\langle T \rangle / \langle V \rangle = 0.5$, where $\langle T \rangle$ and $\langle V \rangle$ are the expectation values of the kinetic- and potential-energy operators, respectively. Also expectation values of various powers of electronic and interelectronic separation coordinates are listed in Table IV.

In the second investigation we aimed at achieving an accuracy in the nonrelativistic energy values with a comparatively smaller number of terms. This could be achieved by choosing a suitable basis function, similar to the one given by Eq. (8), and varying α , β , and γ in the trial function for different values of n . This procedure is very complicated, especially for a great number of terms. As a result of that, we simplify the basis function by taking $\alpha = \beta$ and $\gamma = 0$, and apply the previous procedure with an increasing number of terms similar to the method discussed at the end of Sec. III. The general form of the wave function based on this method is

$$\Psi = N \sum_{\mu=1}^n c_{\mu} (r_1^{j_{\mu}} r_2^{k_{\mu}} + r_1^{k_{\mu}} r_2^{j_{\mu}}) r_{12}^{l_{\mu}} \exp[-\alpha(r_1 + r_2)], \quad (19)$$

where the energy values corresponding to different values of n are listed in Table V. [All the coefficients involved in Eq. (19) are available upon request from the author.] In this table we have energy values, for fixed number of parameters, less than other energy values obtained by different authors.^{7,8,19} This effect comes out from the variation of the parameter α . The expectation values of various functions for Eq. (19), for different values of n , are also listed in Table VI.

The maximum value used for n was 125, corre-

sponding to the relation $j_{\mu} + k_{\mu} + l_{\mu} \leq 9$. This was due to memory limitation for the IBM 370 computer system used. But from the convergence of the energy values of Table V, we can conclude that if we increase n , we can get more accurate energies with a comparatively smaller number of terms.

Nevertheless, the value $-2.903\,724\,371$ a.u. obtained by solving determinant of order 125 is very near to the value $-2.903\,724\,375$ a.u. obtained by Pekeris *et al.*,¹⁹ by solving determinant of the order of 1078. Thus, we can conclude that the present work, with the Rayleigh-Ritz method, yields reliable results.

One has to note that the energy value of Model I and the energy value for $n=7$ in Table V are more accurate than those obtained by Moussa and Radi.^{12,14} The reason is the variation of the parameter α and the use of the double-precision arithmetic computation in every statement in the computer program.

ACKNOWLEDGMENTS

I would like to thank Professor A. H. Moussa for all his great help and discussion. Also, I am very grateful for the staff of the IBM 370 computer center, Planning Board, Kuwait, for allowing me to use the computer extensively.

APPENDIX

The general form of the integral evaluated here is

$$\mathcal{L}(\rho, \sigma, \omega/j, k, l) = (4\pi)^{-2} \iint d\tau_1 d\tau_2 \exp[-(\rho r_1 + \sigma r_2 + \omega r_{12})] r_1^j r_2^k r_{12}^l. \quad (A1)$$

TABLE IV. Expectation values of various operators for the five different models of the ground state of helium. Values of $-\langle T \rangle / \langle V \rangle$ are included to indicate the degree of agreement with the virial theorem.

	I	II	Model III	IV	V
$\langle T \rangle$	2.891 221 293	2.891 498 960	2.901 726 610	2.902 461 973	2.903 272 716
$\langle V \rangle$	-5.782 453 670	-5.783 011 015	-5.803 222 066	-5.804 935 506	-5.806 543 980
$-\langle T \rangle / \langle V \rangle$	0.499 999 042	0.499 998 868	0.500 019 916	0.499 999 004	0.500 000 125
$\langle 1/r_1 \rangle$	1.689 008 278	1.689 187 110	1.688 157 894	1.689 190 076	1.688 283 375
$\langle 1/r_{12} \rangle$	0.973 579 512	0.973 738 533	0.949 410 562	0.957 223 984	0.946 575 538
$\langle r_1 \rangle$	0.898 707 202	0.898 000 822	0.925 252 288	0.927 917 570	0.926 243 473
$\langle r_{12} \rangle$	1.377 095 806	1.373 478 122	1.420 338 007	1.421 157 412	1.417 651 569
$\langle r_1^2 \rangle$	1.083 360 485	1.080 963 845	1.181 142 249	1.211 443 425	1.180 654 250
$\langle r_{12}^2 \rangle$	2.347 941 846	2.331 982 726	2.511 267 313	2.475 737 316	2.490 200 607
$\langle 1/r_1 r_{12} \rangle$	1.989 643 768	1.989 922 173	1.920 833 814	1.919 051 822	1.918 078 772
$\langle 1/r_1 r_2 \rangle$	2.791 906 287	2.793 575 451	2.700 163 818	2.694 687 666	2.700 742 108

Since the integrand of (A1) depends only on the electronic distances r_1 , r_2 , and r_{12} , then we can transform the usual element of volume to take the form²⁰

$$d\tau_1 d\tau_2 = 8\pi^2 r_1 r_2 r_{12} dr_1 dr_2 dr_{12},$$

where the limit of r_1 and r_2 is from 0 to ∞ , and the limit of r_{12} is from $|r_1 - r_2|$ to $|r_1 + r_2|$. Thus, after some manipulation, the value of the integral \mathcal{L} will be given by

$$\mathcal{L}(\rho, \sigma, \omega/j, k, l)$$

$$= -\frac{(l+1)!}{2\omega^{l+2}} \sum_{\epsilon=0}^{l+1} \sum_{\kappa=0}^{\epsilon} \frac{\omega^{\epsilon}}{\epsilon!} \binom{\epsilon}{\kappa} [(-1)^{\kappa+1} I(\sigma - \omega, \rho + \omega/K, J) + (-1)^{\epsilon+\kappa+1} I(\rho - \omega, \sigma + \omega/J, K) + G(\rho + \omega/J)G(\sigma + \omega/K)]$$

for $\omega > 0$, $l \geq -1$

and

$$\mathcal{L}(\rho, \sigma, \omega/j, k, l) = \frac{1}{2(l+2)} \sum_{\kappa=0}^{l+2} \binom{l+2}{\kappa} \{ [1 - (-1)^{\kappa}] I(\sigma, \rho/K, N) + [1 - (-1)^{\kappa+l}] I(\rho, \sigma/N, K) \} \text{ for } \omega = 0, l \geq -2,$$

where $J = j + 1 + \epsilon - \kappa$, $K = k + \kappa + 1$, and $N = j + 3 + l - \kappa$. The formulas G and I used in the above expressions are

$$G(\alpha/j) = j! / \alpha^{j+1} \quad (\alpha > 0, j \geq 0)$$

and

$$\begin{aligned} I(\alpha, \beta/j, k) &= \int_0^{\infty} \exp(-\alpha x) x^j dx \int_x^{\infty} \exp(-\beta y) y^k dy \\ &= \frac{k!}{\beta^{k+1}} \sum_{\epsilon=0}^k \frac{\beta^{\epsilon}}{\epsilon!} G(\alpha + \beta/j + \epsilon) \text{ if } j, k \geq 0 \\ &= \frac{(j+k+1)!}{\alpha^{j+1}} \sum_{\nu=1}^j (-1)^{\nu} \binom{j}{\nu} \beta^{\nu} [F_{(k+\nu+2)}(\alpha + \beta) - F_{(k+\nu+2)}(\beta)] \text{ if } j \geq 0, k < 0, \text{ and } j+k+1 \geq 0, \end{aligned}$$

where

$$F_l(x) = \begin{cases} \log(x) & \text{if } l=1 \\ x^{(1-l)/(1-l)} & \text{if } l \neq 1. \end{cases}$$

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