Lower bounds to the binding energies of $td\mu$

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We present lower bounds to the binding energies of the three-body Coulomb system, which were drawn from Rayleigh-Ritz variational upper bounds to the inverse of the Hamiltonian. The method is shown to generalize Temple's lower bound [Proc. R. Soc. London Ser. A **119**, 276 (1928)]. We applied the method to eigenvalues of the muonic molecular ion $td\mu^+$ where we reached accuracies of 10^{-5} natural atomic units or better.
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I. INTRODUCTION

The simple muonic molecular ions of the hydrogen isotopes are among the few true three-body Coulomb systems, which can be produced and studied experimentally. For the $dd\mu$ system, experiment was able to measure the binding energy of the first excited state of $dd\mu$, with angular momentum $J=1$, with an accuracy of 10^{-7} n.a.u. (natural atomic units $M^{-1}+m_\mu^{-1}=e^2=\hbar=1$, where M is the heaviest mass in the system and m_μ is the muon mass) [1]. Special attention has also been paid to the $td\mu$ system in the context of muon catalyzed fusion (for a recent review see Ref. [2]). In a major theoretical effort a few years ago accurate upper bounds were calculated for the binding energies of most states of all combinations of hydrogen isotopes in muonic molecules [3–11]. Where comparison is possible, agreement with experiment lies within the experimental error [1]. It was tempting to try to complete the solution of the three-body bound-state problem by calculating accurate lower bounds to the energies.

Unfortunately, as we will show, the powerful method of Bazley and Fox [12] and its generalizations are not applicable for true three-body systems. Therefore we resort to a Temple-like [13] variational principle for the lower bounds, which we derive in the following section. Section III discusses the technical complications involved in calculating matrix elements of H^2. Finally in Sec. IV we demonstrate the numerical power of the method by calculating bounds to the eigenvalues of $td\mu$.

II. LOWER BOUNDS TO EIGENVALUES

An efficient method to obtain lower bounds to heliumlike systems is the projection method (see, e.g., [14]), which generalizes the well-known bound by Bazley and Fox [12]. However, any of the nontrivial forms of this formula (e.g., [14–16]) requires that the Hamiltonian of the problem can be split in the form $H=H_0+H_1$ where H_0 is some comparison Hamiltonian and $H_1\geq 0$. A necessary condition for the calculation of a bound to the kth eigenvalue E_k of H is that H_0 have only a finite number of N eigenvalues below E_k. Since for this purpose the onset of the continuum counts as infinitely many eigenvalues, it follows that only eigenvalues below the continuum threshold of H_0 can be bounded by the projection method.

The full three-body Coulomb Hamiltonian after separation of the center-of-mass motion can be written in interparticle coordinates as

$$H=-\frac{1}{2\mu_1}(\nabla_{13})^2-\frac{1}{2\mu_2}(\nabla_{23})^2-\frac{1}{m_3}\nabla_{13}\cdot\nabla_{23}+\frac{Z_1Z_3}{r_{13}}+\frac{Z_2Z_3}{r_{23}}+\frac{Z_1Z_2}{r_{12}} \tag{1}$$

with the reduced masses $\mu_i^{-1}=m_i^{-1}+m_3^{-1}$, where m_i denotes the mass of the ith particle and Z_i are the respective charges. The coordinates $\mathbf{r}_{ij}$ connect the ith with the jth particle and ∇_{ij} are the corresponding derivatives.

For infinite "nuclear" mass m_3 and charges $Z_1=Z_2=-1$ and $Z_3=2$ ($\approx$ He), the obvious choice is $H_1=1/r_{12}$. Since in that case the continuum thresholds of H and H_0 coincide, any bound state of a system with infinite nuclear mass can in principle be bounded from below using the projection method.

For finite mass m_3 the mass polarization term can be expressed by $(\nabla_{13}+\nabla_{23})^2$ leading to

$$H_0=-\frac{1}{2m_1}(\nabla_{13})^2-\frac{1}{2m_2}(\nabla_{23})^2-\frac{2}{r_{13}}-\frac{2}{r_{23}}, \tag{2}$$

$$H_1=-\frac{1}{2m_3}(\nabla_{13}+\nabla_{23})^2+\frac{1}{r_{12}}\geq 0. \tag{3}$$

Here the continuum threshold of H_0 is reached, when the subsystem with the heavier mass, say m_1, is in the ground state, while the other one dissociates. This threshold lies $m_1/(2m_3)$ n.a.u. below the continuum threshold of the full Hamiltonian (1). Thus, with decreasing m_3 the projection method quickly becomes useless for lower bounding.

Assuming we know the number of eigenvalues of H below a given value E_s we may also choose the trivial splitting

$$H_0=H, \qquad H_1=0, \tag{4}$$

which leads to a generalization of Temple's lower bound.

We will give here a direct derivation of this particular bound, which elucidates the meaning of the conditions for its validity.

Suppose the Hamiltonian H has a finite number of eigenvalues N below 0 and for simplicity let us assume that 0 is not in the spectrum of H. Let E_k, $k = 1, \ldots, N$ denote the eigenvalues < 0 in ascending order. An upper bound U_k to the kth eigenvalue E_k can be readily obtained by the Rayleigh-Ritz variational method as the kth solution in ascending order of the finite-dimensional eigenvalue problem

$$\sum_{j=1}^{M}(\langle i|H|j\rangle - U_k\langle i|j\rangle)c_{j;k} = 0, \tag{5}$$

where $\{|i\rangle\} \subset D(H)$ is a linearly independent, but otherwise arbitrary set of basis functions from the domain of H. The inverse of the Hamiltonian H^{-1} will have exactly N eigenvalues $(E_k)^{-1}, k = 1, \ldots, N$ below 0. Again using the Rayleigh-Ritz method we can compute upper bounds $(L_k)^{-1} \geq (E_k)^{-1}$ by solving

$$\sum_{j=1}^{M}[(i|H^{-1}|j) - (L_k)^{-1}(i|j)]c_{j;k} = 0. \tag{6}$$

Since for arbitrary functions $|i)$ it will be quite difficult to calculate the matrix elements $(i|H^{-1}|j)$, we make the special choice $|i) = H|i\rangle$, with $\{|i\rangle\}$ the same as in Eq. (5). As we assumed that 0 is not in the spectrum of H, these $|i)$ will form a linearly independent set of functions and clearly $H^{-1}|i) = H^{-1}H|i\rangle = |i\rangle$ holds, which shows that the $|i)$ are from $D(H^{-1})$. Now Eq. (6) reads

$$\sum_{j=1}^{M}[\langle i|H|j\rangle - (L_k)^{-1}\langle i|H^2|j\rangle]c_{j;k} = 0. \tag{7}$$

Clearly, the upper bound $(L_k)^{-1}$ to the $(N+1-k)$-highest eigenvalue of H^{-1} turns into a lower bound L_k of the kth eigenvalue of H, provided $L_k \leq 0$ (Fig. 1), and we have bounds to the kth eigenvalue of H,

$$L_k \leq E_k \leq U_k. \tag{8}$$

The condition that the Hamiltonian have only a finite number of eigenvalues below 0 can be fulfilled in a trivial way by shifting the H by

$$H \rightarrow H - E_s,$$

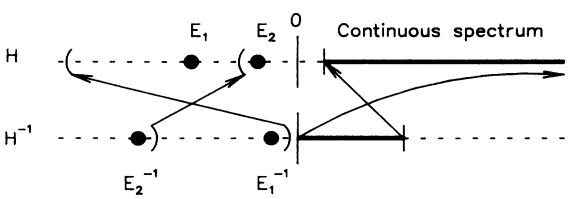

FIG. 1. Scheme of the correspondence of the spectrum of H^{-1} to the spectrum of H. Upper bounds to eigenvalues of H^{-1} turn into lower bounds for H.

where E_s is below the continuum threshold and possible accumulation points of the spectrum of H. With the substitution $L_k \rightarrow L_k - E_s$, Eq. (7) turns into

$$\sum_{j=1}^{M}[\langle i|H-E_s|j\rangle-(L_k-E_s)^{-1}\langle i|(H-E_s)^2|j\rangle]c_{j;k} = 0. \tag{9}$$

Temple's original bound results when we choose

$$E_k < E_s < E_{k+1} \tag{10}$$

and $M = 1$. Then Eq. (9) gives an upper bound to the lowest eigenvalue of $(H - E_s)^{-1}$, or a lower bound to the highest eigenvalue $< E_s$ of H of the form

$$E_{k+1} > E_s > E_k \geq L_k = \langle H\rangle - \frac{\langle H^2\rangle - \langle H\rangle^2}{E_s - \langle H\rangle}. \tag{11}$$

As to the choice of E_s, one sees by multiplying Eq. (9) by $c_{i;k}$, summing over i and differentiating that

$$\frac{dL_k}{dE_s} = \frac{\langle H\rangle - L_k}{E_s - \langle H\rangle} \geq 0, \tag{12}$$

where the expectation values are taken with the normalized function $\Psi_k = \sum_i c_{i;k}|i\rangle$, $||\Psi_k|| = 1$ belonging to L_k. Therefore one will try to choose for E_s a value as high as possible. However, the number of roots $L_k < E_s$ in Eq. (9) should be equal to N, the number of eigenvalues $E_k < E_s$. If this condition is not met, i.e., one has only $N' < N$ roots with $L_k < E_s$, the lower bounds to the N' highest eigenvalues $E_k < E_s$ will usually have trivial values close to some lower eigenvalues of H, unless one uses very good guesses for the basis functions $\{|i\rangle\}$.

Equation (9) optimizes Temple's inequality in the sense that it gives the best upper bound to the kth eigenvalue of $(H - E_s)^{-1}$ and therefore the best lower bound to the corresponding eigenvalue of $H - E_s$ with a given basis $\{|i\rangle\}$ and E_s fixed. Further improvement is achieved, because Eq. (9) is not subject to condition (10) and we can always choose the highest value E_s which allows N solutions $L_k < E_s < E_{N+1}$.

III. BASIS FUNCTIONS AND MATRIX ELEMENTS

We use a generalized Hylleraas basis of the form

$$|i\rangle = G_{J,j_i}\, r_{13}^{l_i} r_{23}^{m_i} r_{12}^{n_i} e^{-\alpha_i r_{13} - \beta_i r_{23} - \gamma_i r_{12}}. \tag{13}$$

Here the polynomials G_{J,j_i}, $j_i \in \{1, \ldots, J+1\}$ determine the angular symmetry of the basis. For $J=0$ and $J=1$ they were chosen as $G_{1,1} \equiv 1$ and $G_{1,j} = \cos(\theta_j) r_{j3}$, respectively, where θ_j is the angle of $\mathbf{r}_{j3}$ with the z axis. For $J=2$ the we use

$$G_{2,1} = r_{13}^2(3\cos^2\theta_1 - 1),$$
$$G_{2,2} = r_{23}^2(3\cos^2\theta_2 - 1),$$
$$G_{2,3} = r_{13}r_{23}(3\cos\theta_1\cos\theta_2 - \cos\theta_{12}),$$

with θ_{12} the angle between $\mathbf{r}_{13}$ and $\mathbf{r}_{23}$. Since $|i\rangle \in D(H)$, we require $l_i, m_i, n_i \geq 0$.

Applying (1) to (13) gives a sum of terms like (13), but with powers $l_i, m_i, n_i \geq -1$. Calculation of the matrix elements $(\langle j|H)H|i\rangle$ after angular integration leads to integrals of the general form

$$\int_0^\infty dr_{13} \int_0^\infty dr_{23} \int_{|r_{13}-r_{23}|}^{r_{13}+r_{23}} dr_{12}\, r_{13}^l\, r_{23}^m\, r_{12}^n \times e^{-\lambda r_{13}-\mu r_{23}-\nu r_{12}} \quad (14)$$

with one or two of the powers equal to -1. (Clearly, $\lambda = \alpha_i + \alpha_j$, $\mu = \beta_i + \beta_j$, and $\nu = \gamma_i + \gamma_j$.) If two powers are equal to -1, the integral cannot be expressed in terms of known functions. If only one of the powers is $= -1$, the integral is a sum of elementary functions, but this closed form is numerically useless for large $l + m + n$ because of huge cancellations between positive and negative terms. Therefore both types of integrals were calculated by a combination of one-dimensional numerical integration and numerically stable (strictly positive) recurrence (see the Appendix).

Each set of nonlinear parameters $\alpha_i, \beta_i, \gamma_i$ requires separate numerical integration, which consumes considerable computation time. Therefore we decided for a basis with only one set of nonlinear parameters. Further, for each triplet of powers (l_i, m_i, n_i) we included all $J + 1$ angular factors G_{J,j_i}. Such basis functions were used successfully for large-scale $td\mu$ upper-bound calculations [8].

IV. BINDING ENERGIES OF $td\mu$

The muonic molecular ion $(td\mu)^+$ consists of a tritium nucleus t^+, a deuteron d^+, and a negative muon μ^-. The respective masses in units of electron masses are $m_1 = m_t = 5496.918$, $m_2 = m_d = 3670.481$, and $m_3 = m_\mu = 206.7686$. Upper-bound calculations for $td\mu$ were pushed to extreme accuracy [9]. From these calculations we know that the spectrum contains five bound states: The three lowest states with angular momentum $J = 0$, 1, and 2, respectively, and the first excited states with $J = 0$ and 1. The latter state, denoted $td\mu(11)$, has attracted the most attention, since it is extremely weakly bound with 1.2×10^{-4} n.a.u. (which is only $\sim 0.5\%$ of the binding energy of the ground state) and plays a key role in the process of muon catalyzed fusion [2]. As can be inferred from Eq. (11), one prerequisite for formula (9) to give a good lower bound on E_k is that the variance of H computed with the optimal trial function obtained by diagonalizing (9) is $< E_s - E_k$. This unfortunately disqualifies the $td\mu(11)$ state for the method due to its tiny binding energy.

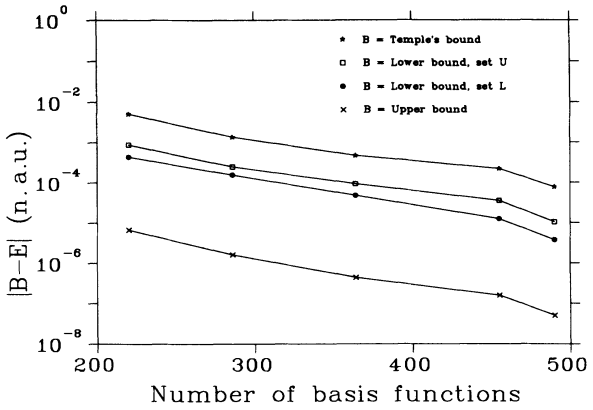

FIG. 2. Convergence of upper and lower bounds to the exact $td\mu(01)$ energy E.

Of the remaining states we mainly discuss the exited J=0 state $td\mu(01)$. We used a single set of exponents α, β, γ and choose the powers by the prescription

$$l_i \leq l_{\max},\ m_i \leq m_{\max},\ n_i \leq n_{\max},\ l_i + m_i + n_i \leq p_{\max}. \quad (15)$$

The shift energy E_s was chosen at the dissociation energy $E_s = -0.5$ n.a.u. The nonlinear parameters α, β, γ were once optimized to give best upper bounds (referred to as "set U") and secondly for the best lower bound ("set L") with powers $l_{\max} = m_{\max} = n_{\max} = p_{\max} = 9$ (220 basis functions).

Figure 2 shows the convergence behavior of the lower in comparison with the upper bounds to the energy of $td\mu(01)$. The very accurate upper bound from Ref. [9] was used as the reference "exact" energy. One observes that the convergence of all bounds goes roughly in parallel. Yet the best lower bounds (set L) are worse by a

TABLE I. Bounds to $td\mu$ energies (n.a.u.). Highly accurate upper bounds [9] are used as reference "exact" energies E. L denotes the variational lower bound with N basis functions, U the Rayleigh-Ritz upper bound with the same number of basis functions. Temple's bound T was calculated with the trial function from the calculation of U. The basis sets used are defined in Table II.

$(J\,v)$	E	N	$U-E$	$E-L$	$E-T$
(00)	−0.55885433	364	3.0×10^{-9}	4.6×10^{-7}	1.4×10^{-6}
(01)	−0.50642402	490	0.5×10^{-7}	3.7×10^{-6}	0.8×10^{-4}
(10)	−0.54287138	572	4.0×10^{-9}	3.5×10^{-7}	5.0×10^{-7}
(20)	−0.51893005[a]	660		2.6×10^{-6}	4.2×10^{-6}

[a] No E available, replaced by U.

TABLE II. Definition of the basis sets used for Table I. Note that the basis contains $J+1$ different angular symmetry factors G_{J,j_i}, hence N can increase with J, although $l_{\max}$, $m_{\max}$, $n_{\max}$, and $p_{\max}$ decrease.

(Jv)	Bound	N	α	β	γ	$l_{\max}$	$m_{\max}$	$n_{\max}$	$p_{\max}$
(00)	U, L	364	0.767	0.690	1.449	11	11	11	11
(01)	U	490	0.682	0.512	0.794	8	8	13	13
(01)	L	490	0.800	0.640	0.824	8	8	13	13
(10)	U, L	572	0.802	0.770	0.988	10	10	10	10
(20)	U, L	660	0.612	0.535	1.078	9	9	9	9

factor of ~ 70 than the best upper bounds comparing at the same number of basis functions. One also sees that optimization of the nonlinear parameters in set L gave only moderate improvement over the lower bounds obtained with set U. The ordinary Temple's bound using the trial function from the upper bound calculation is worse by a factor of ~ 20 than the lower bounds with set L.

Quite similar convergence behavior was found for the remaining three states (Jv)= (00), (10), and (20). As with the (01) state, the various bounds for a given state converge with the number of basis functions approximately exponentially at the same rate, but the lower bounds are constantly poorer than the upper bounds by roughly two orders of magnitude. Optimization of the nonlinear parameters for the lower bound did not give significant improvements. Differently from the (01) state, for these states the ordinary Temple's bound is only farther by factors ~ 2 from the exact eigenvalues than the variatonal lower bound. Table I summarizes the best bounds for all four states. Definition of the basis sets used is in Table II.

V. CONCLUSIONS

For cases where the more powerful projection methods are inapplicable to calculate lower bounds to eigenvalues, we derived an optimal variational form of the standard Temple's bound. We showed that this lower bound to eigenvalues of H can be straightforwardly understood as a Rayleigh-Ritz variational upper bound to eigenvalues of the inverse Hamiltonian H^{-1}.

As is generally true for lower bounds, the numerical quality of the lower bounds is much poorer than that of the corresponding upper bounds. Yet once one decides for the calculation of Temple's bound, one should use the optimal form given in this paper, since it may improve the bound by more than one order of magnitude. The main labor in such a calculation goes into the evaluation of $\langle H^2 \rangle$, while the additional effort to obtain the optimal bound consists only in the solution of a finite-dimensional eigenvalue problem. In the given examples, the use of the basis which was optimized for the upper-bound calculation proved quite adequate also for the lower bound, although minor improvements could be achieved by optimizing the basis for the lower bounds. In practical considerations this small improvement must be weighed against the considerable computational effort which may be connected with repeated calculations of $\langle H^2 \rangle$ in the course of an optimization of the basis.

In the given examples of four bound states of the muonic molecular ion $(td\mu)^+$ the optimal lower bounds are poorer than the upper bounds by about two orders of magnitude. For the (01) state the improvement by the variational bound over Temple's bound amounts to a factor of 20. Although, in view of the superiority of the upper bounds, no attempt was made to push the lower bounds to convergence, in all four cases the differences between upper and lower bounds could be reduced to below 10^{-5} n.a.u.

APPENDIX: CALCULATION OF THE INTEGRALS

We need to compute integrals of the form

$$J_{l,m,n}(\lambda,\mu,\nu) = \int_0^\infty dr_1 \int_0^\infty dr_2 \int_{|r_1-r_2|}^{r_1+r_2} dr_{12} r_1^l r_2^m r_{12}^n \times e^{-\lambda r_1 - \mu r_2 - \nu r_{12}}, \quad \text{(A1)}$$

where the coordinate r_{12} has been distinguished arbitrarily, since the three coordinates are simply related by the triangular inequality. Obviously, the integrals for different powers l, m, n are related by

$$\begin{aligned} J_{l,m,n}(\lambda,\mu,\nu) &= \frac{d}{d(-\lambda)} J_{l-1,m,n}(\lambda,\mu,\nu) \\ &= \frac{d}{d(-\mu)} J_{l,m-1,n}(\lambda,\mu,\nu) \\ &= \frac{d}{d(-\nu)} J_{l,m,n-1}(\lambda,\mu,\nu). \end{aligned} \quad \text{(A2)}$$

These relations prove to be useful for the computation of some of the integrals and for checks.

There arise three different types of $J_{l,m,n}$, either with all three powers l, m, $n \geq 0$, or with exactly one of the powers $=-1$, or with two of the powers $=-1$.

A numerically stable recurrence relation for the J's with non-negative l, m, n is obtained by partial integration with respect to the coordinate $r_1 + r_2$

$$J_{l,m,n} = \frac{1}{\lambda+\mu}(A_{l,m,n} + l\, J_{l-1,m,n} + m\, J_{l,m-1,n}). \quad \text{(A3)}$$

By differentiating Eq. (A3) with respect to $-\lambda$, $-\mu$, and $-\nu$ and using Eqs. (A2) one readily sees that the surface terms $A_{l,m,n}$ also obey differential relations

$$A_{l,m,n} = \frac{d}{d(-\lambda)} A_{l-1,m,n} = \frac{d}{d(-\mu)} A_{l,m-1,n} = \frac{d}{d(-\nu)} A_{l,m,n-1}. \quad \text{(A4)}$$

For the $A_{l,m,n}$ one finds the recurrence relation

$$A_{l,m,n} = \frac{1}{\lambda+\mu+2\nu}[\, l\, A_{l-1,m,n} + m\, A_{l,m-1,n} + 2n\, A_{l,m,n-1} + \delta_{0m} 2(n+l)!(\lambda+\nu)^{-(n+l+1)} + \delta_{0l} 2(n+m)!(\mu+\nu)^{-(n+m+1)}]. \quad \text{(A5)}$$

For $n = -1$, relation (A3) is equally valid, but relation (A5) must be replaced by

$$A_{l,m,-1} = \frac{1}{\lambda-\mu}[\, l\, A_{l-1,m,-1} - m\, A_{l,m-1,-1} - \delta_{0m} 2l!(\lambda+\nu)^{-(l+1)} + \delta_{0l} 2m!(\mu+\nu)^{-(m+1)}]. \quad \text{(A6)}$$

For general λ, μ, ν the alternating sign leads to huge cancellations and makes this recurrence useless for upward use. The downward version of relation (A6) (assuming without loss of generality $\lambda \geq \mu$)

$$A_{l-1,m,-1} = \frac{1}{l}[(\lambda-\mu) A_{l,m,-1} + m\, A_{l,m-1,-1}] \quad \text{(A7)}$$

is strictly positive and therefore numerically stable.

As starting values for the latter recurrence one needs to compute $m_{\max}+1$ integrals $A_{l_{\max},m,-1}$, $m = 0, \ldots, m_{\max}$. For that purpose one observes that

$$A_{0,0,0} = \frac{2}{(\lambda+\nu)(\mu+\nu)} \quad \text{(A8)}$$

and integrates relation (A4)

$$A_{0,0,-1}(\lambda,\mu,\nu) = \int_\nu^\infty dx \frac{2}{(\lambda+x)(\mu+x)}. \quad \text{(A9)}$$

We differentiate (A9) l and m times with respect to $-\lambda$ and $-\mu$, respectively, to obtain

$$A_{l,m,-1}(\lambda,\mu,\nu) = \int_\nu^\infty dx \frac{2\, l!m!}{(\lambda+x)^{l+1}(\mu+x)^{m+1}}, \quad \text{(A10)}$$

which can easily be integrated numerically. [The closed analytical form of the integral (A10) is equivalent to the recurrence (A6) and therefore equally numerically useless.]

The third type of integrals of the form $J_{-1,-1,n}$ cannot be expressed through known functions and therefore requires numerical integrations. Again the recurrence starting from $J_{-1,-1,0}$

$$J_{-1,-1,n} = \frac{1}{\nu}[\, -\lambda J_{0,-1,n-1} - \mu J_{-1,0,n-1} + (n+1) J_{-1,-1,n-1}] \quad \text{(A11)}$$

is too unstable for general use. Therefore we directly calculate $J_{-1,-1,n}$ for each n by using the differential relations (A2) and their inverse integral form to obtain

$$J_{-1,-1,n}(\lambda,\mu,\nu) = \int_\lambda^\infty dx \int_\mu^\infty dy \left(\frac{d}{d(-\nu)}\right)^n \times J_{0,0,0}(x,y,\nu). \quad \text{(A12)}$$

Observing that $J_{0,0,0}(x,y,\nu) = 2/[(\nu+x)(x+y)(y+\nu)]$ the differentiations with respect to $-\nu$ and the integration with respect to y can be performed explicitly. The integration over x was performed numerically for each n using a self-adapting Gauss-Legendre quadrature procedure. We could verify the results using the relations (A2) to a relative accuracy of at least 10^{-25} when calculating with 31 decimal digits (FORTRAN REAL*16).

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