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Direct solution of H_2^+ Schrödinger equation using the hyperspherical coordinate

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Summary. By introducing a Gaussian factor to describe the fact that the nuclei in H_2^+ vibrate around a fixed point, we have modified the method of hyperspherical harmonics recently proposed by us. The modified method has been applied to solve the three-body Schrödinger equation for H_2^+ directly without recourse to the Born–Oppenheimer approximation and the calculations yield well-converged ground-state energies. These are the first-reported results obtained for H_2^+ by the method of hyperspherical harmonics. With 25 hyperspherical harmonics and 40 generalized-Laguerre functions, we obtain a ground-state energy of -0.5945 au, which is close to the exact value of -0.5971 au. A detailed presentation of the method of modified hyperspherical harmonics is presented.

Key words: Three-body problem – Hyperspherical coordinate – Schrödinger equation – H_2^+ – Generalized-Laguerre function

1. Introduction

Recently, Deng et al. [1, 2] have proposed a direct method to solve the many-body Schrödinger equation in the hyperspherical formalism. We tested this method for the atomic system He [1, 2] and the mesomolecular system of $e^+e^-e^+$, ppμ, etc. [3], and we concluded [3] that the method is one of the best available hyperspherical harmonic (HH) methods. However, when we tried to extend the method to the H_2^+ system, we encountered a slow convergence and could not get meaningful results for the size of basis sets we used.

In the past, efforts to perform direct calculations on H_2^+ using the HH method have been made by several authors [4–6], but they all failed. The first effort was made in 1974 by Whitten and Sims [4] who encountered serious convergence difficulties and did not obtain any result. In 1981, Mignaco and Roditi [5] tried to extend their HH method to H_2^+, but reported no results. Using his HH method, Burden [6] in 1983 performed some calculations on the hypothetical systems XY_2 with mass ratios ranging from 1 to 256, and explored the limitations of the method of hyperspherical harmonics. He found that, when the mass ratio was greater than 256, the necessary basis set increased so rapidly that computer storage and time requirements became prohibitive. He, too, failed to complete the direct calculation on H_2^+. Thus, the slow convergence has been a common problem in all calculations of H_2^+ by various methods based on hyperspherical harmonics.

We believe that this slow convergence problem may result from the fact that the two protons in H_2^+ vibrate around their equilibrium position and that this kind of behaviour is difficult to describe by HH and GLF expansions. On the other hand, we know that Gaussian functions can be used to describe such ground-state vibration of heavy particles. Hence, we decided to express the wavefunction as a product of two factors, $\Psi = \Omega\Phi$, where Ω is a Gaussian function. Then, the remaining part Φ may be of such a form that can be easily simulated by an expansion in terms of HH and GLF functions. The idea of correlation function [7, 8] was first introduced into the HH theory by Gorbatov et al. [7] and Haftel and Mandelzweig [8], and the Gaussian function Ω can be regarded as a kind of correlation function.

Programs based on our modified method have been carried out successfully on H_2^+. In the next section we give a detailed description of this method and quantitative results are reported in the third section.

2. Theory

The nonrelativistic Schödinger equation for the H_2^+ system can be written as

$$\left\{ -\tfrac{1}{2} \sum_{i=1}^{3} \nabla_i^2/m_i + V - E \right\} \Psi = 0, \tag{2.1}$$

where atomic units are used, V is the interaction potential and m_i is the mass of the ith particle.

In the process of developing hyperspherical harmonic theory, several coordinate representations [9–14] have been established. Of these the symmetric representations are very convenient for the treatment of the three-body problem. We follow the symmetric representation formalism introduced by Niri [9] and Mandelzweig [10].

In the centre-of-mass system, Eq. (2.1) becomes

$$\{ -\tfrac{1}{2}(\nabla_\xi^2 + \nabla_{\xi'}^2) + V - E\} \Psi = 0, \tag{2.2}$$

$$\xi = 2^{-1/2}(r_1' - r_2'),$$

$$\xi' = [(M/2)/(M+2)]^{1/2}(r_1' + r_2' - 2r_3'), \tag{2.3}$$

where we used the units $m = h = c = 1$; m and M are the masses of protons and electrons respectively; r_i' is the position vector of the ith particle. Let (for $L = 0$),

$$\begin{aligned}
\xi_1 &= -\rho\cos[(\pi/4) - (a/2)]\cos(\lambda/2),\\
\xi_2 &= \rho\sin[(\pi/4) - (a/2)]\sin(\lambda/2),\\
\xi_3 &= 0,\\
\xi_1' &= -\rho\cos([\pi/4) - (a/2)]\sin(\lambda/2),\\
\xi_2' &= -\rho\sin[(\pi/4) - (a/2)]\cos(\lambda/2),\\
\xi_3' &= 0,
\end{aligned} \tag{2.4}$$

with ρ $(0 \leqslant \rho < \infty)$ being the hyperradial variable and a $(0 \leqslant a < \pi/2)$ and λ $(0 \leqslant \lambda < 2\pi)$ being two hyperangles.

Then, Eq. (2.2) can be written in terms of hyperspherical coordinates as follows:

$$\{\tfrac{1}{2}[\partial^2/\partial\rho^2 + (5/\rho)\,\partial/\partial\rho - \Lambda^2/\rho^2] - V + E\}\,\Psi = 0 \tag{2.5}$$

for $L = 0$,

$$\Lambda^2 = -4\,(\partial^2/\partial a^2 + 2\cot 2a\partial/\partial a + (1/\sin^2 a)\,\partial^2/\partial\lambda^2), \tag{2.6}$$

where Λ^2 is the generalized scalar angular-momentum operator.

The interparticle distances of particles j and k can also be expressed by ρ, a and λ,

$$r_i = \rho[\kappa_i(1 + \sin a\cos(\lambda + \omega_i))]^{1/2}, \tag{2.7}$$

where $\kappa_i = 1$, $(M+1)/2M$, $(M+1)/2M$, $\omega_i = 0, \omega, -\omega$ with $\omega = \arccos(-1/(M+1))$, for $i = 3$, 1 and 2, respectively. Particles 1 and 2 correspond to two protons, and r_3 corresponds to the distance between them.

We introduce the Gaussian factor Ω and χ, the exponential of a linear function of r_1 and r_2, to express Ψ as follows:

$$\Psi = \Omega\chi\Phi, \tag{2.8}$$

with

$$\Omega = e^{\alpha_{(3)}r_3 - \beta r_3^2}$$

$$\chi = e^f \tag{2.9}$$

$$f = -\sum_{i=1}^{2} \alpha_{(i)} r_i, \tag{2.10}$$

where the $\alpha_{(i)}$ $(i = 1, 3)$, β are determined by the following physical considerations.

When elliptic coordinates are used, we can get the exact wavefunction of H_2^+ in the Born–Oppenheimer approximation, part of which has the form of $e^{-0.7416(r_1+r_2)}$, at the equilibrium distance between the two nuclei. Hence, we find $\alpha_{(1)} = \alpha_{(2)} = 0.7416 a_0^{-1}$ (let $\alpha_{(1)} = \alpha_{(2)} = \alpha$).

β and $\alpha_{(3)}$ are estimated from the approximate wavefunction of the ground-state vibration of the two nuclei, which can be obtained from the Schrödinger equation describing the motion of the nuclei of H_2^+. We deduce $\beta = (2\pi^2\mu v_0)/h = 4.8 a_0^{-2}$; $\alpha_{(3)} = 19.2 a_0^{-1}$.

Substituting Eq. (2.8) into Eq. (2.5), and carrying out the derivations, we finally arrive at an equation of the following form:

$$[\partial^2/\partial\rho^2 + (5/\rho)\,\partial/\partial\rho - \Lambda^2/\rho^2 + 2(E - V) + W1 + W2\,\partial/\partial\rho + W3/\rho + W4\rho\partial/\partial\rho + W5\rho^2 + W6\rho + W1p]\Phi = 0 \tag{2.11}$$

where $V = -Z/\rho$; Z, $W1$, $W2$, $W3$, $W4$, $W5$, $W6$, $W1p$ are operators which are only related to two hyperangles λ and a.

Φ can now be expanded in terms of hyperspherical harmonic (HH) basis sets $(Y_{\mu,\nu}(\lambda, a))$

$$\Phi = \sum_{\mu,\nu} \Phi_{\mu,\nu}(\rho)\, Y_{\mu,\nu}(\lambda, a). \tag{2.12}$$

Here, $Y_{\mu,\nu}(\lambda, a)$ are solutions (for the S states) of the equation

$$\Lambda^2\psi = K(K+4)\psi \tag{2.13}$$

with the global quantum number $K = 0, 2, 4, \ldots$, and thus can be expressed in terms of the usual Wigner D functions $(D^1_{mm'}(\alpha, \beta, \gamma))$.

The Pauli exclusion principle requires that the wavefunction be antisymmetric under interchange of two idential particles (protons), so $Y_{\mu,\nu}(\lambda, a)$ should be of the form

$$D^{\mu/2}_{\nu/2-\nu/2}(2\lambda, 2a, 0) + (-1)^{s+\nu} D^{\mu/2}_{-\nu/2,\nu/2}(2\lambda. 2a, 0). \tag{2.14}$$

In the space spanned by HH basis sets, Eq. (2.11) yields the matrix equation

$$[\mathrm{d}^2/\mathrm{d}\rho^2 + (5/\rho)\mathrm{d}/\mathrm{d}\rho - \boldsymbol{K}(\boldsymbol{K}+4)/\rho^2 + 2E + 2\boldsymbol{Z}/\rho + \boldsymbol{W1h} + \boldsymbol{W2}(d/d\rho) + \boldsymbol{W3}/\rho + \boldsymbol{W4}\rho d/d\rho + \boldsymbol{W5}\rho^2 + \boldsymbol{W6}\rho]\boldsymbol{\Phi} = 0, \tag{2.15}$$

$$\boldsymbol{W1h} = \boldsymbol{W1} + \boldsymbol{W1p}, \tag{2.16}$$

where $\boldsymbol{\Phi}$ is the $N \times 1$ column matrix; K is the $N \times N$ generalized angular-momentum eigenvalue diagonal matrix, $\boldsymbol{Z}$, $\boldsymbol{W1}$, $\boldsymbol{W2}$, $\boldsymbol{W3}$, $\boldsymbol{W4}$, $\boldsymbol{W5}$, $\boldsymbol{W6}$, $\boldsymbol{W1p}$ are $N \times N$ matrices; N is the dimension of the HH basis. By somewhat complicated derivations, we have obtained analytic expressions (see the Appendix) for all matrix elements (including $\boldsymbol{Z}$, $\boldsymbol{W1}$, $\boldsymbol{W2}$, $\boldsymbol{W3}$, $\boldsymbol{W4}$, $\boldsymbol{W5}$, $\boldsymbol{W6}$, $\boldsymbol{W1p}$), which are used in practical calculations.

Equation (2.15) is a set of coupled hyperradial differential equations, which can be solved by the GLF (generalized-Laguerre function) expansion method as follows.

We expand $\boldsymbol{\Phi}$ in terms of a complete set of GLF functions,

$$\boldsymbol{\Phi}(\rho) = \sum_{n=0}^{\infty} \boldsymbol{C}_n L^{\alpha}_n(\rho), \tag{2.17}$$

where $\boldsymbol{C}_n$ is the column matrix of expansion coefficients, $L^{\alpha}_n(\rho)$ are the generalized-Laguerre functions and we choose $\alpha = 4$. Then Eq. (2.15) becomes

$$\sum_{n=0}^{\infty} \boldsymbol{C}_n[\mathrm{d}^2/\mathrm{d}\rho^2 + (5/\rho)\mathrm{d}/\mathrm{d}\rho - \boldsymbol{K}(\boldsymbol{K}+4)/\rho^2 + 2E + \boldsymbol{W1h} + \boldsymbol{W2}(\mathrm{d}/\mathrm{d}\rho) + (2\boldsymbol{Z} + \boldsymbol{W3})/\rho + \boldsymbol{W4}\rho\mathrm{d}/\mathrm{d}\rho + \boldsymbol{W5}\rho^2 + \boldsymbol{W6}\rho]L^4_n(\rho) = 0. \tag{2.18}$$

Taking into account that

$$[\mathrm{d}^2/\mathrm{d}\rho^2 + (5/\rho - 1)\mathrm{d}/\mathrm{d}\rho + n/\rho]L^4_n(\rho) = 0, \tag{2.19}$$

we can simplify Eq. (2.18) to

$$\sum_{n=0}^{\infty} \boldsymbol{C}_n[-\boldsymbol{K}(\boldsymbol{K}+4)/\rho^2 + 2E + \boldsymbol{W1h} + (\boldsymbol{W2}+1)(\mathrm{d}/\mathrm{d}\rho) + (2\boldsymbol{Z} + \boldsymbol{W3} - n)/\rho]L^4_n(\rho) + \sum_{n=0}^{\infty} \boldsymbol{C}_n[\boldsymbol{W4}\rho\mathrm{d}/\mathrm{d}\rho + \boldsymbol{W5}\rho^2 + \boldsymbol{W6}\rho]L^4_n(\rho) = 0. \tag{2.20}$$

Applying furthermore the following formulae several times,

$$\rho L^4_n = -(n+4)L^4_{n-1} + (2n+5)L^4_n - (n+1)L^4_{n+1}, \tag{2.21}$$

$$\rho(\mathrm{d}/\mathrm{d}\rho)L^4_n = nL^4_n - (n+4)L^4_{n-1}, \tag{2.22}$$

we finally get, from Eq. (2.20), the following recurrence relations for the coefficient matrix:

$$a(C_n)C_n + a(C_{n+1})C_{n+1} + a(C_{n-1})C_{n-1} + a(C_{n+2})C_{n+2} + a(C_{n-2})C_{n-2}$$
$$+ a(C_{n+3})C_{n+3} + a(C_{n-3})C_{n-3} + a(C_{n+4})C_{n+4} + a(C_{n-4})C_{n-4} = 0, \quad (2.23)$$

where

$$\begin{aligned}
a(C_n) = & -K(K+4) + 2(2n+5)Z + 6(n^2+5n+5)W1h \\
& + 3n(n+3)W2 + (2n+5)W3 \\
& + n(n+4) + 6(n^2+5n+5)2E \\
& + ll5(n)W5 + l4(n)W6 + lk4(n)W4, \\
a(C_{n+1}) = & -(n+5)2Z - 4(n+3)(n+5)W1h - 3(n+2)(n+5)W2 - (n+5)W3 \\
& - (n+5)(2n+5) - 4(n+3)(n+5)2E \\
& + ll4(n+1)W5 + l3(n+1)W6 + lk3(n+1)W4, \\
a(C_{n-1}) = & -2nZ - 4(n+2)nW1h - n(n-1)W2 - nW3 - 4n(n+2)2E \\
& + ll6(n-1)W5 + l5(n-1)W6 + lk5(n-1)W4, \\
a(C_{n+2}) = & (n+5)(n+6)(W1h + W2 + 1 + 2E) \\
& + ll3(n+2)W5 + l2(n+2)W6 + lk2(n+2)W4, \\
a(C_{n-2}) = & (n-1)n(W1h + 2E) + ll7(n-2)W5 \\
& + l6(n-2)W6 + lk6(n-2)W4, \\
a(C_{n+3}) = & ll2(n+3)W5 + l1(n+3)W6 + lk1(n+3)W4, \\
a(C_{n-3}) = & ll8(n-3)W5 + l7(n-3)W6, \\
a(C_{n+4}) = & ll1(n+4)W5, \\
a(C_{n-4}) = & ll9(n-4)W5. \qquad (2.24)
\end{aligned}$$

Additionally, $li(j)$ $(i = 1, 7)$, $lki(j)$ $(i = 1, 6)$ and $lli(j)$ $(i = 1, 9)$ are functions in terms of an integral variable j which are defined by us and have the following definitions:

$$\begin{aligned}
l1(j) &= -(j+2)(j+3)(j+4), \\
l2(j) &= 3(2j+3)(j+3)(j+4), \\
l3(j) &= -(15j^2+60j+51)(j+4), \\
l4(j) &= 2(5j^2+27j+25) + 20(j+2)(j+1)(j+4), \\
l5(j) &= -3(5j^2+30j+42)(j+1), \\
l6(j) &= 3(2j+7)(j+1)(j+2), \\
l7(j) &= -(j+2)(j+3)(j+1), \qquad (2.25)
\end{aligned}$$

$$lk1\,(j) = -(j+2)\,(j+3)\,(j+4)$$
$$lk2\,(j) = (5j+4)\,(j+3)\,(j+4),$$
$$lk3\,(j) = -(10j^2+26j+6)\,(j+4),$$
$$lk4\,(j) = 2j\,(5j^2+27j+31),$$
$$lk5\,(j) = -j\,(j+1)\,(5j+16),$$
$$lk6\,(j) = j\,((j+2)\,(j+1), \tag{2.26}$$
$$ll1\,(j) = -(j+1)\,l1\,(j)$$
$$ll2\,(j) = (2j-1)\,l1\,(j) - (j+2)\,l2\,(j),$$
$$ll3\,(j) = -(j-2)\,l1\,(j) + (2j+1)\,l2\,(j) - (j+3)\,l3\,(j),$$
$$ll4\,(j) = -(j-1)\,l2\,(j) + (2j+3)\,l3\,(j) - (j+4)\,l4\,(j),$$
$$ll5\,(j) = -jl3\,(j) + (2j+5)\,l4\,(j) - (j+5)\,l5(\,j),$$
$$ll6\,(j) = -(j+1)\,l4\,(j) + (2j+7)\,l5\,(j) - (j+6)\,l6\,(j),$$
$$ll7\,(j) = -(j+2)\,l5\,(j) + (2j+9)\,l6\,(j) - (j+7)\,l7(j),$$
$$ll8\,(j) = -(j+3)\,l6\,(j) + (2j+11)\,l7\,(j),$$
$$ll9\,(j) = -(j+4)\,l7\,(j). \tag{2.27}$$

From Eq. (2.23), one obtains the generalized eigenvalue equation

$$AC = 2EBC, \tag{2.28}$$

where C is the $M \times 1$ column matrix; A, B are $M \times M$ square matrices; M = NHH (the number of HH) × NGLF (the number of GLF). Equation (2.28) is solved numerically and thereby the wavefunction and the energy eigenvalue are obtained.

3. Calculations and results

We have performed explicit calculations for H_2^+ with the method described above. All calculations were executed on a 4D/25 Personal Iris SiliconGraphics workstation in our laboratory. The programs were written by us. Analytic expressions were used for the calculation of all matrix elements involved. Some of them proved to be very time-consuming (up to a few thousand minutes of CPU).

In view of the storage limitations of our workstation and the CPU time required, the maximum basis set we used was 25 HHs and 40 GLFs.

Some of our quantitative results for the ground-state energies of H_2^+ are displayed in Table 1. The convergence pattern of the ground-state energies is seen to be rather good. Compared with our previous direct calculations on He, $e^+e^-e^+$, ppμ [1–3], more GLFs are required to obtain good convergence. With 25 HHs and 40 GLFs, we obtain a ground-state energy of -0.5945 au, quite close to the exact value of -0.5971 au [15]. By contrast, using the HH–GLF method with 100 HHs and 9 GLFs but without a Gaussian function, we only obtained -0.0317 au for the ground-state energy. Thus, application of our modified method to H_2^+ yields significant improvements of the rate of convergence. Further precise calculations with larger basis sets on H_2^+ are in progress.

Table 1. Energy eigenvalues of the ground state for H_2^+ (au)

		NGLF				
K_m	NHH	10	20	30	35	40
4	4	−0.33297	−0.48397	−0.49528	−0.49528	−0.49528
8	9	−0.45274	−0.55011	−0.55608	−0.55641	−0.55635
12	16	−0.50621	−0.57327	−0.58100	−0.58237	−0.58268
14	20	−0.52347	−0.57685	−0.58704	−0.58924	−0.59012
16	25	−0.53720	−0.58116	−0.58974	−0.59273	−0.59449
Exact value[a]						−0.59714

NHH: the number of hyperspherical harmonics; NGLF: the number of generalized-Laguerre functions. K_m: the maximum global angular momentum
[a] From [15]

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Appendix

The obtained analytic expressions for matrix elements of ***Z***, ***W1***, ***W2***, ***W3***, ***W1p***, ***W4***, ***W5***, ***W6*** are given as follows:

$$\begin{aligned} \boldsymbol{Z}_{\mu\nu\mu'\nu'} = {} & -4/\pi\,[2(\mu'+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2} \\ & (-1)^{(\mu'+\nu'+\mu+\nu)/2} \sum_{\mu''=|\mu-\mu'|}^{(\mu+\mu')} (\mu''+1)/[(2\mu''+1)(2\mu''+3)] \\ & [t_{\nu-\nu'}(\mu'/2, \nu'/2, \mu''/2, (\nu-\nu')/2 \,|\, \mu/2, \nu/2)^2 \\ & + (-1)^s t_{\nu+\nu'}(\mu'/2, -\nu'/2, \mu''/2, (\nu+\nu')/2 \,|\, \mu/2, \nu/2)^2], \end{aligned} \tag{A.1}$$

where the $(l', m', l'', m'' \,|\, l, m)$ are the Clebsch–Gordan coefficients of the su(2) group, and

$$t_\nu = 1 - (2z/k_2^{1/2}) \cos\omega\nu \ (z \text{ is atomic number}). \tag{A.2}$$

$$\begin{aligned} \boldsymbol{W2}_{\mu\nu\mu'\nu'} = {} & 32/\pi\,[2(\mu'+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2}(-1)^{(\mu'+\nu'+\mu+\nu)/2} \\ & \sum_{\mu''=|\mu-\mu'|}^{(\mu+\mu')} (\mu''+1)/[(2\mu''+5)(2\mu''+3)(2\mu''+1)(2\mu''-1)] \\ & [\alpha_{\nu-\nu'}(\mu'/2, \nu'/2, \mu''/2, (\nu-\nu')/2 \,|\, \mu/2, \nu/2)^2 \\ & + (-1)^s \alpha_{\nu+\nu'}(\mu'/2, -\nu'/2, \mu''/2, (\nu+\nu')/2 \,|\, \mu/2, \nu/2)^2], \end{aligned} \tag{A.3}$$

where

$$\alpha_\nu = \alpha_{(3)} + 2\alpha k_2^{1/2} \cos\omega\nu. \tag{A.4}$$

$$W3_{\mu\nu\mu'\nu'} = -16/\pi\,[2(\mu'+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2}(-1)^{(\mu'+\nu'+\mu+\nu)/2}$$
$$\sum_{\mu''=|\mu-\mu'|}^{(\mu+\mu')}(\mu''+1)/[(2\mu''+3)(2\mu''+1)]$$
$$\{\alpha_{\nu-\nu'}(\mu'/2,\nu'/2,\mu''/2,(\nu-\nu')/2|\mu/2,\nu/2)$$
$$\times\{(\mu'/2,\nu'/2,\mu''/2,(\nu-\nu')/2|\mu/2,\nu/2)+4/[(2\mu''+5)(2\mu''-1)]$$
$$\times\sum_{\alpha=-1}^{1}[a^{-\alpha}_{\mu'\nu'}\,a^{\alpha}_{\mu''\nu-\nu'}(\mu'/2,\nu'/2-\alpha,\mu''/2,(\nu-\nu')/2+\alpha|\mu/2,\nu/2)$$
$$+a^{-\alpha}_{\mu'-\nu'}\,a^{\alpha}_{\mu''\nu'-\nu}(\mu'/2,\nu'/2+\alpha,\mu''/2,(\nu-\nu')/2-\alpha|\mu/2,\nu/2)]\}$$
$$+(-1)^{s}\alpha_{\nu+\nu'}(\mu'/2,\ -\nu'/2,\mu''/2,(\nu+\nu')/2|\mu/2,\nu/2)$$
$$\times\{(\mu'/2,-\nu'/2,\mu''/2,(\nu+\nu')/2|\mu/2,\nu/2)+4/[(2\mu''+5)(2\mu''-1)]$$
$$\times\sum_{\alpha=-1}^{1}[a^{-\alpha}_{\mu'-\nu'}\,a^{\alpha}_{\mu''-(\nu+\nu')}(\mu'/2,\ -\nu'/2+\alpha,\mu''/2,(\nu+\nu')/2-\alpha|\mu/2,\nu/2)$$
$$+[a^{-\alpha}_{\mu'-\nu'}\,a^{\alpha}_{\mu''-(\nu+\nu')}(\mu'/2,\ -\nu'/2-\alpha,\mu''/2,(\nu+\nu')/2+\alpha|\mu/2,\nu/2)]\}\},\tag{A.5}$$

where

$$a^{\alpha}_{\mu\nu}=\begin{cases}\nu, & \alpha=0,\\ (2^{-1/2})[(\mu+\alpha\nu+2)(\mu-\alpha\nu)]^{1/2}, & \alpha=\pm 1.\end{cases}\tag{A.6}$$

$$W1_{\mu\nu\mu'\nu'} = 512/\pi^2\,[(\mu'+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2}(-1)^{(\mu'+\nu'+\mu+\nu)/2}$$
$$\sum_{\mu_1=0}^{\infty}\ \sum_{\nu_1=-\mu_1}^{\mu_1}\ \sum_{\mu_3=|\mu_1-\mu|}^{(\mu_1+\mu)}\ \sum_{\mu_2=|\mu'-\mu_3|}^{(\mu'+\mu_3)}$$
$$\times(\mu_1+1)/[2\mu_1+5)(2\mu_1+3)(2\mu_1+1)(2\mu_1-1)]$$
$$\times(\mu_2+1)/[(2\mu_2+5)(2\mu_2+3)(2\mu_1+1)(2\mu_2-1)]$$
$$\times\{\alpha_{\nu_1}\alpha_{\nu-\nu_1-\nu'}(\mu_2/2,(\nu-\nu_1-\nu')/2,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$[(\mu_2/2,(\nu-\nu_1-\nu')/2,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$-4\sum_{\alpha=-1}^{1}a^{\alpha}_{\mu_1\nu_1}\,a^{-\alpha}_{\mu_2\nu-\nu_1-\nu'}(\mu_2/2,(\nu-\nu_1-\nu')/2$$
$$-\alpha,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2-\alpha)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2-\alpha,\mu_1/2,\nu_1/2+\alpha|\mu/2,\nu/2)]$$
$$+\alpha_{\nu_1}\alpha_{\nu'-\nu-\nu_1}(\mu_2/2,(\nu'-\nu-\nu_1)/2,\mu'/2,\ -\nu'/2|\mu_3/2,\ -(\nu+\nu_1)/2)$$
$$\times(\mu_3/2,-(\nu+\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\ -\nu/2)$$

$$[(\mu_2/2, (\nu' - \nu - \nu_1)/2, \mu'/2, -\nu'/2|\mu_3/2, -(\nu + \nu_1)/2)$$
$$\times(\mu_3/2, -(\nu + \nu_1)/2, \mu_1/2, \nu_1/2|\mu/2, -\nu/2)$$
$$-4 \sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1 \nu_1} a^{-\alpha}_{\mu_2 \nu' - \nu - \nu_1} (\mu_2/2, (\nu' - \nu - \nu_1)/2 - \alpha, \mu'/2,$$
$$-\nu'/2|\mu_3/2, -(\nu + \nu_1)/2 - \alpha)$$
$$\times(\mu_3/2, -(\nu_1 + \nu)/2 - \alpha, \mu_1/2, \nu_1/2 + \alpha|\mu/2, -\nu/2)]$$
$$+(-1)^s \alpha_{\nu_1} \alpha_{-\nu-\nu_1-\nu'} (\mu_2/2, -(\nu + \nu_1 + \nu')/2, \mu'/2,$$
$$\nu'/2|\mu_3/2 - (\nu + \nu_1)/2)$$
$$\times(\mu_3/2, -(\nu + \nu_1)/2, \mu_1/2, \nu_1/2|\mu/2, -\nu/2)$$
$$[(\mu_2/2, -(\nu + \nu_1 + \nu')/2, \mu'/2, \nu'/2|\mu_3/2, -(\nu + \nu_1)/2)$$
$$\times(\mu_3/2, -(\nu + \nu_1)/2, \mu_1/2, \nu_1/2|\mu/2, -\nu/2)$$
$$-4 \sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1 \nu_1} a^{-\alpha}_{\mu_2 - \nu - \nu' - \nu_1} (\mu_2/2, (-\nu - \nu_1 - \nu')/2$$
$$-\alpha, \mu'/2, -\nu'/2|\mu_3/2, -(\nu + \nu_1)/2 - \alpha)$$
$$\times(\mu_3/2, -(\nu + \nu_1)/2 - \alpha, \mu_1/2, \nu_1/2 + \alpha|\mu/2, -\nu/2)]$$
$$+(-1)^s \alpha_{\nu_1} \alpha_{+\nu-\nu_1+\nu'} (\mu_2/2, +(\nu - \nu_1 + \nu')/2, \mu'/2,$$
$$-\nu'/2|\mu_3/2, +(\nu - \nu_1)/2)$$
$$\times(\mu_3/2, (\nu - \nu_1)/2, \mu_1/2, +\nu_1/2|\mu/2, +\nu/2)$$
$$[\mu_2/2, (\nu - \nu_1 + \nu')/2, \mu'/2, -\nu'/2|\mu_3/2, (\nu - \nu_1)/2)$$
$$\times(\mu_3/2, (\nu - \nu_1)/2, \mu_1/2, \nu_1/2|\mu/2, \nu/2)$$
$$-4 \sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1 \nu_1} a^{-\alpha}_{\mu_2 \nu + \nu' - \nu_1} (\mu_2/2, (\nu + \nu' - \nu_1)/$$
$$2 - \alpha, \mu'/2, -\nu'/2|\mu_3/2, (\nu - \nu_1)/2 - \alpha)$$
$$\times(\mu_3/2, (\nu - \nu_1)/2 - \alpha, \mu_1/2, \nu_1/2 + \alpha|\mu/2, \nu/2)]\} \tag{A.7}$$

$$\boldsymbol{W1p} = \boldsymbol{W1p1} + \boldsymbol{W1p2}. \tag{A.8}$$

$$\boldsymbol{W1p1}_{\mu\nu\mu'\nu'} = 2\beta[(\mu' + 1)(2 - \delta_{\nu o})(2 - \delta_{\nu' o})/(\mu + 1)]^{1/2} \sum_{\alpha=-1}^{1}$$
$$\{\delta_{\nu\nu'}[a^{-\alpha}_{\mu'\nu'} a^{\alpha}_{0,\nu-\nu'} (\mu'/2, \nu'/2, 0, (\nu - \nu')/2|\mu/2, \nu/2)$$
$$\times\{\mu'/2, \nu'/2 - \alpha, 0, (\nu - \nu')/2 + \alpha|\mu/2, \nu/2)$$
$$+ a^{-\alpha}_{\mu' - \nu'} a^{\alpha}_{0,\nu'-\nu} (\mu'/2, \nu'/2, 0, (\nu - \nu')/2|\mu/2, \nu/2)$$
$$\times(\mu'/2, \nu'/2 + \alpha, 0, (\nu - \nu')/2 - \alpha|\mu/2, \nu/2)]$$
$$+ \delta_{\nu,-\nu'} [a^{-\alpha}_{\mu'\nu'} a^{\alpha}_{0,-(\nu+\nu')} (\mu'/2, -\nu'/2, 0, (\nu + \nu')/2|\mu/2, \nu/2)$$

$$\times(\mu'/2,\ -\nu'/2+\alpha, 0, (\nu+\nu')/2-\alpha\,|\,\mu/2, \nu/2)$$
$$+\ a^{-\alpha}_{\mu'-\nu'}\, a^{\alpha}_{0,\nu'+\nu}(\mu'/2,\ -\nu'/2, 0, (\nu+\nu')/2\,|\,\mu/2, \nu/2)$$
$$\times(\mu'/2,\ -\nu'/2-\alpha, 0, (\nu+\nu')/2+\alpha\,|\,\mu/2, \nu/2)]\times(-1)^{s+\nu}$$
$$+\ (\delta_{\nu,\nu'+1}-\delta_{\nu,\nu'-1})\,[a^{-\alpha}_{\mu'\nu'} a^{\alpha}_{1,\nu-\nu'})$$
$$\times(\mu'/2, \nu'/2, 1/2, (\nu-\nu')/2\,|\,\mu/2, \nu/2)$$
$$\times(\mu'/2, \nu'/2-\alpha, 1/2, (\nu-\nu')/2+\alpha\,|\,\mu/2, \nu/2)$$
$$+\ a^{-\alpha}_{\mu'-\nu'}\, a^{\alpha}_{1,\nu'-\nu}(\mu'/2, \nu'/2, 1/2, (\nu-\nu')/2\,|\,\mu/2, \nu/2)$$
$$\times(\mu'/2, \nu'/2+\alpha, 1/2, (\nu-\nu')/2-\alpha\,|\,\mu/2, \nu/2)]\times(-1)^{(\mu'-\mu+1)/2}/2$$
$$+\ (\delta_{-\nu,\nu'+1}-\delta_{\nu,\nu'-1})\,[a^{-\alpha}_{\mu'\nu'} a^{\alpha}_{1,-\nu-\nu'}(\mu'/2,\ -\nu'/2,$$
$$1/2, (\nu+\nu')/2\,|\,\mu/2, \nu/2)$$
$$\times(\mu'/2, \nu'/2-\alpha, 1/2, (\nu-\nu')/2-\alpha\,|\,\mu/2, \nu/2)$$
$$+\ a^{-\alpha}_{\mu'-\nu'}\, a^{\alpha}_{1,\nu+\nu'}(\mu'/2,\ -\nu'/2, 1/2, (\nu+\nu')/2\,|\,\mu/2, \nu/2)$$
$$\times(\mu'/2,\ -\nu'/2-\alpha, 1/2, (\nu+\nu')/2+\alpha\,|\,\mu/2, \nu/2)]$$
$$\times(-1)^{s+\nu}(-1)^{(\mu'-\mu+1)/2}/2\}. \tag{A.9}$$

$$\boldsymbol{W1p2}_{\mu\nu\mu'\nu'} = -6\beta\,[(2-\delta_{\nu o})(2-\delta_{\nu' o})]^{1/2}$$
$$[\delta_{\nu\nu'}(\mu'/2, \nu'/2, 0, (\nu-\nu')/2\,|\,\mu/2, \nu/2)^2$$
$$+\ \delta_{\nu,-\nu'}(\mu'/2,\ -\nu'/2, 0, (\nu+\nu')/2\,|\,\mu/2, \nu/2)^2(-1)^{s+\nu}]. \tag{A.10}$$

$$\boldsymbol{W4}_{\mu\nu\mu'\nu'} = -2\beta\,[(\mu'+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2}$$
$$[\delta_{\nu\nu'}(\mu'/2, \nu'/2, 0, (\nu-\nu')/2\,|\,\mu/2, \nu/2)^2$$
$$+\ \delta_{\nu,-\nu'}(\mu'/2,\ -\nu'/2, 0, (\nu+\nu')/2\,|\,\mu/2, \nu/2)^2(-1)^{s+\nu}$$
$$+\ \delta_{\nu,\nu'+1}(\mu'/2, \nu'/2, 1/2, (\nu-\nu')/2\,|\,\mu/2, \nu/2)^2(-1)^{(\mu'-\mu+1)/2}/2$$
$$+\ \delta_{\nu,-\nu'-1}(\mu'/2,\ -\nu'/2, 1/2, (\nu+\nu')/2\,|\,\mu/2,$$
$$\nu/2)^2(-1)^{s+\nu}(-1)^{(\mu'-\mu+1)/2}/2$$
$$-\ \delta_{\nu,\nu'-1}(\mu'/2, \nu'/2, 1/2, (\nu-\nu')/2\,|\,\mu/2, \nu/2)^2(-1)^{(\mu'-\mu+1)/2}/2$$
$$-\ \delta_{\nu,1-\nu'}(\mu'/2,\ -\nu'/2, 1/2, (\nu+\nu')/2\,|\,\mu/2, \nu/2)^2$$
$$(-1)^{s+\nu}(-1)^{(\mu'-\mu+1)/2}/2]. \tag{A.11}$$

$$\boldsymbol{W5}_{\mu\nu\mu'\nu'} = f4cg(0,0,0,0) + (2^{1/2}/4)f4cg(0,0,1,1) - (2^{1/2}/4)f4cg(0,0,1,-1)$$
$$+\ (2^{1/2}/4)f4cg(1,1,0,0) + (1/8)f4cg(1,1,1,1) - (1/8)f4cg(1,1,1,-1)$$
$$-(2^{1/2}/4)f4cg(1,-1,0,0) - (1/8)f4cg(1,-1,1,1) + (1/8)f4cg(1,-1,1,-1), \tag{A.12}$$

where

$$f4cg(\mu_1,\nu_1,\mu_2,\nu_2)=\beta^2[(\mu'+1)(\mu_1+1)(\mu_2+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2} \times(-1)^{(\mu_1+\mu_2+\mu'-\mu)/2}$$

$$\sum_{\mu_3=|\mu-\mu_1|}^{(\mu+\mu_1)}\{\delta_{\nu,\nu_1+\nu_2+\nu'}(\mu_2/2,\nu_2/2,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$[(\mu_2/2,\nu_2/2,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$-\sum_{\alpha=-1}^{1}a^{\alpha}_{\mu_1\nu_1}a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2,\nu_2/2-\alpha,\mu'/2,\nu'/2|\mu_3/2,(\nu-\nu_1)/2-\alpha)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2-\alpha,\mu_1/2,\nu_1/2+\alpha|\mu/2,\nu/2)]$$
$$+(-1)^{\nu+\nu'}\delta_{\nu,\nu'-\nu_1-\nu_2}(\mu_2/2,\nu_2/2,\mu'/2-\nu'/2|\mu_3/2,-(\nu+\nu_1)/2)$$
$$\times(\mu_3/2,-(\nu+\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,-\nu/2)$$
$$[(\mu_2/2,\nu_2/2,\mu'/2,-\nu'/2|\mu_3/2,-(\nu+\nu_1)/2)$$
$$\times(\mu_3/2,-(\nu+\nu_1)/2,\mu_1/2,\nu_1/2,|\mu/2,-\nu/2)$$
$$-\sum_{\alpha=-1}^{1}a^{\alpha}_{\mu_1\nu_1}a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2,\nu_2/2-\alpha,\mu'/2,-\nu'/2|\mu_3/2,-(\nu_1+\nu)/2-\alpha)$$
$$\times(\mu_3/2-(\nu_1+\nu)/2-\alpha,\mu_1/2,\nu_1/2+\alpha|\mu/2,-\nu/2)]$$
$$+(-1)^{s+\nu}\delta_{\nu,-\nu'-\nu_1-\nu_2}(\mu_2/2,\nu_2/2,\mu'/2,\nu'/2|\mu_3/2,-(\nu+\nu_1)/2)$$
$$\times(\mu_3/2,-(\nu+\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,-\nu/2)$$
$$[(\mu_2/2,\nu_2/2,\mu'/2,\nu'/2|\mu_3/2,-(\nu+\nu_1)/2)$$
$$\times(\mu_3/2,-(\nu+\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,-\nu/2)$$
$$-\sum_{\alpha=-1}^{1}a^{\alpha}_{\mu_1\nu_1}a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2,\nu_2/2-\alpha,\mu'/2,\nu'/2|\mu_3/2,-(\nu+\nu_1)/2-\alpha)$$
$$\times(\mu_3/2-(\nu+\nu_1)/2-\alpha,\mu_1/2,\nu_1/2+\alpha|\mu/2,-\nu/2)]$$
$$+(-1)^{s+\nu'}\delta_{\nu,\nu_2+\nu_1-\nu'}(\mu_2/2,\nu_2/2,\mu'/2,-\nu'/2,|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$[(\mu_2/2,\nu_2/2,\mu'/2,-\nu'/2|\mu_3/2,(\nu-\nu_1)/2)$$
$$\times(\mu_3/2,(\nu-\nu_1)/2,\mu_1/2,\nu_1/2|\mu/2,\nu/2)$$
$$-\sum_{\alpha=-1}^{1}a^{\alpha}_{\mu_1\nu_1}a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2,\nu_2/2-\alpha,\mu'/2,-\nu'/2|\mu_3/2,(\nu-\nu_1)/2-\alpha)$$
$$\times(\mu_3/2,[(\nu-\nu_1)/2-\alpha,\mu_1/2,\nu_1/2+\alpha|\mu/2,\nu/2)]\} \quad (A.13)$$

$$W6_{\mu\nu\mu'\nu'}=f4cgp(0,0)+(2^{1/2}/4)\,f4cgp(1,1)-(2^{1/2}/4)\,f4cgp(1,-1), \quad (A.14)$$

where

$$f4cgp(\mu_2, \nu_2) = -32\beta/\pi\,[2(\mu'+1)(\mu_2+1)(2-\delta_{\nu o})(2-\delta_{\nu' o})/(\mu+1)]^{1/2}$$
$$\times(-1)^{(\mu_2+\mu'-\mu)/2}$$
$$\sum_{\mu_3=|\mu_2-\mu'|}^{(\mu_2+\mu')} \sum_{\mu_1=|\mu_3-\mu|}^{(\mu_3+\mu)} \sum_{\nu_1=-\mu_1}^{\mu_1} (\mu_1+1)/[(2\mu_1+5)(2\mu_1+3)(2\mu_1+1)(2\mu_1-1)]$$
$$\times(-1)^{-\nu_1/2}\alpha_{\nu_1}$$
$$\{\delta_{\nu,\nu_1+\nu_2+\nu'}(\mu_2/2, \nu_2/2, \mu'/2, \nu'/2 \,|\, \mu_3/2, (\nu-\nu_1)/2)$$
$$\times(\mu_3/2, (\nu-\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, \nu/2)$$
$$[(\mu_2/2, \nu_2/2, \mu'/2, \nu'/2 \,|\, \mu_3/2, (\nu-\nu_1)/2)$$
$$\times(\mu_3/2, (\nu-\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, \nu/2)$$
$$-2\sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1\nu_1} a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2, \nu_2/2-\alpha, \mu'/2, \nu'/2 \,|\, \mu_3/2, (\nu-\nu_1)/2-\alpha)$$
$$\times(\mu_3/2, +(\nu-\nu_1)/2-\alpha, \mu_1/2, \nu_1/2+\alpha \,|\, \mu/2, \nu/2)]$$
$$+(-1)^{\nu+\nu'}\delta_{\nu,\nu'-\nu_1-\nu_2}(\mu_2/2, \nu_2/2, \mu'/2, -\nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, -\nu/2)$$
$$[(\mu_2/2, \nu_2/2, \mu'/2, -\nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2, \mu_1/2 \nu_1/2 \,|\, \mu/2, -\nu/2)$$
$$-2\sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1\nu_1} a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2, \nu_2/2-\alpha, \mu'/2, -\nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2-\alpha)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2-\alpha, \mu_1/2, \nu_1/2+\alpha \,|\, \mu/2, -\nu/2)]$$
$$+(-1)^{s+\nu'}\delta_{\nu,\nu'-\nu_1-\nu_2}(\mu_2/2, \nu_2/2, \mu'/2, \nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, -\nu/2)$$
$$[(\mu_2/2, \nu_2/2, \mu'/2, \nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2, \mu_1/2, \nu_1|2 \,|\, \mu/2, -\nu/2)$$
$$-2\sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1\nu_1} a^{-\alpha}_{\mu_2\nu_2}(\mu_2/2, \nu_2/2-\alpha, \mu'/2, \nu'/2 \,|\, \mu_3/2, -(\nu+\nu_1)/2-\alpha)$$
$$\times(\mu_3/2, -(\nu+\nu_1)/2-\alpha, \mu_1/2, \nu_1/2+\alpha \,|\, \mu/2, -\nu/2)]$$
$$+(-1)^{s+\nu'}\delta_{\nu,\nu_2+\nu_1-\nu'}(\mu_2/2, \nu_2/2, \mu'/2, -\nu'/2 \,|\, \mu_3/2, (\nu-\nu_1)/2)$$
$$\times(\mu_3/2, (\nu-\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, \nu/2)$$
$$[(\mu_2/2, \nu_2/2, \mu'/2, -\nu'/2 \,|\, \mu_3/2, (\nu-\nu_1)/2)$$
$$\times(\mu_3/2, (\nu-\nu_1)/2, \mu_1/2, \nu_1/2 \,|\, \mu/2, \nu/2)$$

$$-2 \sum_{\alpha=-1}^{1} a^{\alpha}_{\mu_1 \nu_1} a^{-\alpha}_{\mu_2 \nu_2} (\mu_2/2, \nu_2/2 - \alpha, \mu'/2, \ -\nu'/2 \,|\, \mu_3/2, (\nu - \nu_1)/2 - \alpha)$$

$$\times (\mu_3/2, (\nu - \nu_1)/2 - \alpha, \mu_1/2, \nu_1/2 + \alpha \,|\, \mu/2, \nu/2)]\}. \qquad (A.15)$$

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