SUPPLEMENTARY INFO FOR:

A Critical Review of the two-temperature theory and the derivation of matrix elements. High field Ion mobility and energy calculation for all-atom structures in light gases using a 4-6-12 potential.

1. Introduction

This supplementary information includes.

a) The derivation of the collisional term for the calculation of moments of the Boltzmann equation.

b) The derivation of the recursive relation for the different moments of the Boltzmann equation.

c) Calculation of several matrix elements up to the third approximation.

d) Aisbett's Formula for the calculation of the matrix elements.

S.1 The derivation of the collisional term for the calculation of moments of the Boltzmann equation.

Given eqs. (1b) and (2) of the manuscript (repeated here):

$$F = F^{(0)} \sum\nolimits_p a_p \phi_p$$

$$\frac{eE}{Mn}\frac{\partial F}{\partial w} = \iiint (f'F' - fF) g db d\epsilon dc_i,$$

one would like to arrive to eqs. (3-4). Since the gas velocity distribution is unchanged, $f' = f$ and replacing $\sum_p a_p \phi_p$ with Φ, one arrives at:

$$\frac{eE}{Mn}\frac{\partial F}{\partial w} = \iiint fF^{(0)}(\Phi' - \Phi) g db d\epsilon dc_i$$

Labeling the operator: $\mathcal{J}\Phi = \int\int\int f(\Phi - \Phi') gbdbd\epsilon dc_i$ and substituting

$$\frac{eE}{Mn}\frac{\partial F}{\partial w} = -F^{(0)}\ \mathcal{J}\Phi$$

To find the moments of the equation, we multiply both sides by a function of the ion's velocity $\psi_{lm}^{(r)}$ and integrate over all possible velocities z_i:

$$\frac{eE}{Mn}\int_{-\infty}^{\infty} \frac{\partial F}{\partial w}\ \psi_{lm}^{(r)}\ \partial z_i = -F^{(0)} \int_{-\infty}^{\infty} \psi_{lm}^{(r)}\ \mathcal{J}\Phi\, \partial z_i$$

For simplicity, one can drop the indices in $\psi_{lm}^{(r)}$. Thus,

$$\frac{eE}{Mn}\int_{-\infty}^{\infty} \frac{\partial F}{\partial w}\ \psi\ \partial z_i = -F^{(0)} \int_{-\infty}^{\infty} \psi\ \mathcal{J}\Phi\, \partial z_i$$

Integrating by parts on LHS, and assuming that the linear operator $\mathcal{J}$ is symmetric, i.e., $(\psi, \mathcal{J}\Phi) = (\mathcal{J}\Phi, \psi)$ on RHS (where (a, b) represents the inner product):

$$\frac{eE}{Mn}\iint \left[\psi F|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} F\left(\frac{\partial \psi}{\partial w}\right)\partial w\right] \partial z_2 \partial z_3 = -F^{(0)} \int_{-\infty}^{\infty} \Phi\ \mathcal{J}\psi\, \partial z_i$$

with $z_i = z_1 = w$,

$$\frac{eE}{Mn}\iint\left[\psi\big(F(\infty)-F(-\infty)\big)-\int_{-\infty}^{\infty}F\left(\frac{\partial\psi}{\partial w}\right)\partial w\right]\partial z_2\partial z_3 = -\int_{-\infty}^{\infty}F^{(0)}\Phi\ \mathcal{J}\psi\,\partial z_i$$

Given that $F(\infty)=0\quad ; F^{(0)}\Phi = F$,

$$-\frac{eE}{Mn}\iiint F\left(\frac{\partial\psi}{\partial w}\right)\partial z_i = -\int_{-\infty}^{\infty}F\ \mathcal{J}\psi\,\partial z_i$$

Thus,

$$\frac{eE}{Mn}\left\langle\frac{\partial\psi}{\partial w}\right\rangle_{Av} = \langle\mathcal{J}\psi\rangle_{Av}$$

The symmetry condition has been proven to be unnecessary to arrive at the final equation used.

S.2 The derivation of the recursive relation for the different moments of the Boltzmann equation.

Given the recursive eq. (11)

$$\left(l+\frac{1}{2}\right)\sum_s a_{rs}(l)\,\langle\psi_l^{(s)}\rangle = \mathcal{E}\left[l\left(l+\frac{1}{2}+r\right)\langle\psi_{l-1}^{(r)}\rangle-(l+1)\,\langle\psi_{l+1}^{(r-1)}\rangle\right]$$

From eq. (3) using eq. (8) and recursive relations of the polynomials (10a-d):

$$\frac{eE}{Mn}\left\langle\frac{\partial\psi_{lm}^{(r)}}{\partial w}\right\rangle_{Av} = \langle\mathcal{J}\psi_{lm}^{(r)}\rangle_{Av} \tag{3}$$

$$\mathcal{J}\psi_{lm}^{(r)} = \sum_s a_{rs}(l)\,\psi_{lm}^{(s)} \tag{8}$$

$$\psi_l^{(r)} = \left(\frac{Mz^2}{2kT_b}\right)^{\frac{l}{2}} P_l\left(\frac{w}{z}\right) S_{l+\frac{1}{2}}^{(r)}\left(\frac{Mz^2}{2kT_b}\right)$$

From the left-hand side of eq. (3) we need to calculate the derivative of $\psi_{lm}^{(r)}$ with respect to $w = z_1$. Using the chain rule, one arrives at:

$$\frac{\partial\psi_l^{(r)}}{\partial z_1} = \frac{\partial(Az^2)^{\frac{l}{2}}}{\partial z_1}P_l\left(\frac{z_1}{z}\right)S_{l+\frac{1}{2}}^{(r)}(Az^2) + (Az^2)^{\frac{l}{2}}\frac{\partial}{\partial z_1}P_l\left(\frac{z_1}{z}\right)S_{l+\frac{1}{2}}^{(r)}(Az^2) + (Az^2)^{\frac{l}{2}}P_l\left(\frac{z_1}{z}\right)\frac{\partial}{\partial z_1}S_{l+\frac{1}{2}}^{(r)}(Az^2)$$

With $A = \frac{M}{2kT_b}$ and $z^2 = z_1^2 + z_2^2 + z_3^2$. Let's calculate each of the three derivatives separately first. The derivatives for the Legendre and Sonine Polynomials follow the recursive equations (10a-b) but in order to do so, one has to modify the derivatives.

$$\rightarrow \frac{\partial(Az^2)^{\frac{l}{2}}}{\partial z_1} = A^{l/2}\frac{l}{2}2z_1(z_1^2+z_2^2+z_3^2)^{\frac{l}{2}-1} = \frac{lz_1}{z^2}(Az^2)^{l/2}$$

$$\rightarrow \frac{\partial}{\partial z_1} P_l\left(\frac{z_1}{z}\right) = \frac{\partial\left(\frac{z_1}{z}\right)}{\partial z_1} \frac{\partial}{\partial\left(\frac{z_1}{z}\right)} P_l\left(\frac{z_1}{z}\right) = \frac{\partial\left(\frac{z_1}{z}\right)}{\partial z_1} \frac{l}{\left(\frac{z_1}{z}\right)^2 - 1}\left(\frac{z_1}{z} P_l\left(\frac{z_1}{z}\right) - P_{l-1}\left(\frac{z_1}{z}\right)\right) =$$

$$\frac{z_2^2 + z_3^2}{(z^2)^{\frac{3}{2}}} \frac{lz^2}{z_1^2 - z^2}\left(\frac{z_1}{z} P_l\left(\frac{z_1}{z}\right) - P_{l-1}\left(\frac{z_1}{z}\right)\right) = -\frac{l}{z}\left(\frac{z_1}{z} P_l\left(\frac{z_1}{z}\right) - P_{l-1}\left(\frac{z_1}{z}\right)\right)$$

$$\rightarrow \frac{\partial}{\partial z_1} S_{l+\frac{1}{2}}^{(r)}(Az^2) = \frac{\partial Az^2}{\partial z_1} \frac{\partial}{\partial Az^2} S_{l+\frac{1}{2}}^{(r)}(Az^2) = -2Az_1 S_{l+\frac{3}{2}}^{(r-1)}(Az^2)$$

Substituting the derivatives in the equation above:

$$\frac{\partial \psi_l^{(r)}}{\partial z_1} = \frac{lz_1}{z^2}\psi_l^{(r)} - \frac{lz_1}{z^2}\psi_l^{(r)} + \frac{l}{z}(Az^2)^{\frac{l}{2}} P_{l-1}\left(\frac{z_1}{z}\right) S_{l+\frac{1}{2}}^{(r)}(Az^2) - 2Az_1 (Az^2)^{\frac{l}{2}} P_l\left(\frac{z_1}{z}\right) S_{l+\frac{3}{2}}^{(r-1)}(Az^2)$$

Using the recursive relations eqs. (10c-d):

$$\frac{\partial \psi_l^{(r)}}{\partial z_1} = -\frac{(l+1)zA}{\left(l+\frac{1}{2}\right)}(Az^2)^{\frac{l}{2}} P_{l+1}\left(\frac{z_1}{z}\right) S_{l+\frac{3}{2}}^{(r-1)}(Az^2) - \frac{lzA}{\left(l+\frac{1}{2}\right)}(Az^2)^{\frac{l}{2}} P_{l-1}\left(\frac{z_1}{z}\right) S_{l+\frac{3}{2}}^{(r-1)}(Az^2)$$
$$+ \frac{lzA}{\left(l+\frac{1}{2}\right)}(Az^2)^{\frac{l}{2}} P_{l-1}\left(\frac{z_1}{z}\right) S_{l+\frac{3}{2}}^{(r-1)}(Az^2) + \frac{l\left(l+\frac{1}{2}+r\right)}{z\left(l+\frac{1}{2}\right)}(Az^2)^{\frac{l}{2}} P_{l-1}\left(\frac{z_1}{z}\right) S_{l-\frac{1}{2}}^{(r-1)}(Az^2)$$

And canceling terms and simplifying:

$$\frac{\partial \psi_l^{(r)}}{\partial z_1} = -\frac{(l+1)}{\left(l+\frac{1}{2}\right)} A^{\frac{1}{2}} \psi_{l+1}^{(r-1)} + \frac{l\left(l+\frac{1}{2}+r\right)}{\left(l+\frac{1}{2}\right)} A^{\frac{1}{2}} \psi_{l-1}^{(r)}$$

Substituting into eq. (3) yields:

$$\frac{eE}{Mn} A^{\frac{1}{2}}\left(\frac{l\left(l+\frac{1}{2}+r\right)}{\left(l+\frac{1}{2}\right)}\langle\psi_{l-1}^{(r)}\rangle - \frac{(l+1)}{\left(l+\frac{1}{2}\right)}\langle\psi_{l+1}^{(r-1)}\rangle\right) = \sum_s a_{rs}(l)\langle\psi_l^{(s)}\rangle$$

And rearranging:

$$\left(l+\frac{1}{2}\right)\sum_s a_{rs}(l)\langle\psi_l^{(s)}\rangle = \mathcal{E}\left[l\left(l+\frac{1}{2}+r\right)\langle\psi_{l-1}^{(r)}\rangle - (l+1)\langle\psi_{l+1}^{(r-1)}\rangle\right] \; q.e.d.$$

S.3 Calculation of Matrix elements.

Calculation of $a_{10}(0)$

Given that $\psi_0^{(1)} = \frac{3}{2} - z^2\left(\frac{M}{2kT_b}\right)$; $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}|_{l=0,s=0}=1$$

$$\psi_0^{(0)}\left(\vec{W}+d\vec{g}\right)\left[\psi_0^{(1)}\left(\vec{W}+e_\mu\vec{g}+f\vec{g}\right)-\psi_0^{(1)}\left(\vec{W}+e_\mu\vec{g}'+f\vec{g}\right)\right]=-\frac{e_\mu M\left[f(g^2-\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}-\vec{g}')\right]}{kT_b}$$

and:

$$a_{10}(0)=-\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int\int e^{\left(-\left(\frac{m}{2dkT}\right)W^2-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{e_\mu M\left[f(g^2-\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}-\vec{g}')\right]}{kT_b}gbdbd\epsilon d\vec{W}d\vec{g} \qquad (52)$$

Integrating over the center of mass velocities yields:

$$a_{10}(0)=-\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2d\pi kT}{m}\right)^{\frac{3}{2}}\frac{e_\mu Mf(g^2-\vec{g}\cdot\vec{g}')}{kT_b}gbdbd\epsilon d\vec{g} \qquad (53)$$

Integrating ϵ from 0 to 2π:

$$a_{10}(0)=-e_\mu f\left(\frac{M}{kT_b}\right)\left(\frac{dM}{2\pi kT_b}\right)^{\frac{3}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g^3(1-cos\chi)2\pi bdbd\vec{g} \qquad (54)$$

Where following eq. (42):

$$\int_0^{2\pi}\vec{g}\cdot\vec{g}'\,d\epsilon=2\pi g^2cos\chi$$

Using the aforementioned relations and rearranging:

$$a_{10}(0)=-\frac{2}{\pi^{\frac{3}{2}}}e_\mu\frac{f}{d}\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g^3(1-cos\chi)2\pi bdbd\vec{g}$$

Integrating in the angles of velocity:

$$a_{10}(0)=-8\frac{f}{d}\sqrt{\frac{1}{\pi}}\;e_\mu\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g^5Q^{(1)}(g)dg$$

Multiply and divide by $\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{1}{2}}$ and rearranging

$$a_{10}(0)=-8\frac{f}{d}\;e_\mu\left(\frac{2kT_{eff}}{\pi\mu}\right)^{\frac{1}{2}}\left[\left(\frac{\mu}{2kT_{eff}}\right)^3\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g^5Q^{(1)}(g)dg\right]=-8\frac{f}{d}\;e_\mu\left(\frac{2kT_{eff}}{\pi\mu}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})$$

$$a_{10}^*(0)=-8\frac{f}{d} \qquad (55)$$

Calculation of $a_{20}(0)$

Given that $\psi_0^{(2)}=\frac{1}{2}\left(\frac{15}{4}+\frac{M^2z^4}{4k^2T_b^2}-\frac{5Mz^2}{2kT_b}\right)$; $\vec{z}=(z_1=w,z_2,z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}|_{l=0,s=0}=1$$

$$\psi_0^{(0)}(\vec{W}+d\vec{g})\left[\psi_0^{(2)}(\vec{W}+e_\mu\vec{g}+f\vec{g})-\psi_0^{(2)}(\vec{W}+e_\mu\vec{g}'+f\vec{g})\right]=$$
$$-\frac{e_\mu M[f(g^2-\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}-\vec{g}')]}{4k^2T_b^2}\left[-10kT_b+M\left(2e_\mu^2g^2+2e_\mu\left(f(g^2-\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}+\vec{p})\right)+2\big(f^2g^2+W^2+2f\vec{g}\cdot\vec{W}\big)\right)\right]$$

Integrating over the center of mass velocities yields:

$$a_{20}(0)=\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2d\pi kT}{m}\right)^{\frac{3}{2}}\frac{e_\mu M[fg^2mM(e_\mu^2+f^2)(g^2-\vec{g}\cdot\vec{g}\prime)+e_\mu f^2Mm(g^2-\vec{g}\cdot\vec{g}\prime)(g^2+\vec{g}\cdot\vec{g}\prime)+5fk(g^2-\vec{g}\cdot\vec{g}\prime)(dMT-mT_b)]}{2k^2mT_b^2}gbdbd\epsilon d\vec{g}$$
(56)

Integrating ϵ from 0 to 2π:

$$a_{20}(0)=\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2d\pi kT}{m}\right)^{\frac{3}{2}}\frac{e_\mu M[fg^4mM(e_\mu^2+f^2)(1-cos\chi)+e_\mu f^2Mmg^4(1-cos^2\chi)+5fkg^2(1-cos\chi)(dMT-mT_b)]}{2k^2mT_b^2}g2\pi bdbd\vec{g} \quad (57)$$

Rearranging:

$$a_{20}(0)=\frac{e_\mu}{d\pi^{\frac{3}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{\left[fg^5mM(e_\mu^2+f^2)Q^{(1)}(g)+\frac{2}{3}e_\mu f^2Mmg^5Q^{(2)}(g)+5fkg^3Q^{(1)}(dMT-mT_b)\right]}{kmT_b}d\vec{g}$$

Where the $\frac{2}{3}$ that multiplies the second term in brackets comes from eq. (42). Integrating in the angles of velocity,

$$a_{20}(0)=\frac{4e_\mu}{d^2\pi^{\frac{1}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left[f\frac{Md}{kT_b}g^7\ (e_\mu^2+f^2)Q^{(1)}(g)+\frac{2}{3}e_\mu f^2\frac{Md}{kT_b}\ \ g^7Q^{(2)}(g)+5fdg^5Q^{(1)}\left(d\frac{MT}{mT_b}-1\right)\right]dg$$

With the identities $\frac{Md}{kT_b}=\frac{\mu}{kT_{eff}}$ and $\frac{dMT}{mT_b}=(1-d)$, one gets:

$$a_{20}(0)=\frac{4}{d^2}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left[f2\left(\frac{\mu}{2kT_{eff}}\right)^4g^7\ \left(e_\mu^2+f^2\right)Q^{(1)}(g)+\frac{2}{3}e_\mu f^22\left(\frac{\mu}{2kT_{eff}}\right)^4\ \ g^7Q^{(2)}(g)-5fd^2g^5Q^{(1)}\right]dg$$

Using eq. (41), one arrives at:

$$a_{20}(0)=\frac{4}{d^2}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)\left[6f\ \left(e_\mu^2+f^2\right)\Omega^{(1,2)}(T_{eff})+4e_\mu f^2\Omega^{(2,2)}(T_{eff})-5fd^2\Omega^{(1,1)}(T_{eff})\right]$$

Factoring $\Omega^{(1,1)}(T_{eff})$ and labeling $A^*=\frac{\Omega^{(2,2)}(T_{eff})}{\Omega^{(1,1)}(T_{eff})}$ and $C^*=\frac{\Omega^{(1,2)}(T_{eff})}{\Omega^{(1,1)}(T_{eff})}$

It yields:

$$a_{20}(0)=\frac{4}{d^2}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)\Omega^{(1,1)}(T_{eff})\left[6f\ \left(e_\mu^2+f^2\right)C^*+4e_\mu f^2A^*-5fd^2\right]$$

Due to the fact that for a Maxwell potential $C^*=5/6$, one can reorder the equations to give:

$$a_{20}(0)=\frac{4}{d^2}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)\Omega^{(1,1)}(T_{eff})\left[f\ \left(e_\mu^2+f^2\right)(6C^*-5)+4e_\mu f^2A^*+5f\ \left(e_\mu^2+f^2-d^2\right)\right]$$

And $\left(e_\mu^2+f^2-d^2\right)=-2*e_\mu f$ so that:

$$a_{20}^{*}(0)=\frac{4}{d^2}\left[f\ \left(e_\mu^2+f^2\right)(6C^*-5)+4e_\mu f^2A^*-10f^2e_\mu\right] \tag{56}$$

Calculation of $a_{01}(1)$

Given that $\psi_1^{(1)}=z_1\left(\frac{M}{2kT_b}\right)^{1/2}\left[\frac{5}{2}-\frac{Mz^2}{2kT_b}\right]$; $\psi_1^{(0)}=z_1\left(\frac{M}{2kT_b}\right)^{1/2}$ $\vec{z}=(z_1=w,z_2,z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}|_{l=1,s=1}=\frac{4}{5}$$

$$\psi_1^{(1)}(\vec{W}+d\vec{g})\left[\psi_1^{(0)}(\vec{W}+e_\mu\vec{g}+f\vec{g})-\psi_1^{(0)}(\vec{W}+e_\mu\vec{g}'+f\vec{g})\right]=-\frac{e_\mu M(g_1-g_1')(dg_1+W_1)\left(M\left(d^2g^2+W^2+2d\vec{g}\cdot\vec{W}\right)-5kT_b\right)}{4k^2T_b^2}$$

Integrating over the center of mass velocities yields:

$$a_{01}(1)=-\frac{4}{5}\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2\pi kT}{m}\right)^{3/2}\frac{e_\mu Md^{\frac{5}{2}}g_1(g_1-g_1')\left[d^2Mg^2+\frac{5dkMT}{m}-5kT_b\right]}{4k^2T_b^2}gbdbd\epsilon d\vec{g}$$

Integrating ϵ from 0 to 2π:

$$a_{01}(1)=-\frac{4}{5}\frac{e_\mu}{2\pi^{\frac{3}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{g_1^2\left[d^2Mg^2+\frac{5dkMT}{m}-5kT_b\right]}{kT_b}g2\pi(1-cos\chi)bdbd\vec{g}$$

Using eq. (42):

$$a_{01}(1)=-\frac{4}{5}\frac{e_\mu}{2\pi^{\frac{3}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g_1^2\left[d\left(\frac{Md}{kT_b}\right)g^2+\frac{5dMT}{mT_b}-5\right]gQ^{(1)}(g)d\vec{g}$$

Changing to spherical coordinates:

$$a_{01}(1)=-\frac{4}{5}\frac{e_\mu}{2\pi^{\frac{3}{2}}}\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}g^5\left[d\left(\frac{\mu}{kT_{eff}}\right)g^2+\frac{5dMT}{mT_b}-5\right]\cos^2\theta_g\,sin\theta_g Q^{(1)}(g)dgd\theta_g d\phi_g$$

And integrating over the angles:

$$a_{01}(1)=-\frac{4}{5}\frac{e_\mu}{2\pi^{\frac{3}{2}}}\frac{4\pi}{3}\left(\frac{2kT_{eff}}{\mu}\right)^{\frac{1}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{\mu}{2kT_{eff}}\right)^3g^5\left[2d\left(\frac{\mu}{2kT_{eff}}\right)g^2+\frac{5dMT}{mT_b}-5\right]Q^{(1)}(g)dgd\theta_g d\phi_g$$

Rearranging:

$$a_{01}(1)=-\frac{8}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\left[6d\Omega^{(1,2)}(T_{eff})+5d\left(\frac{1}{d}-1\right)\Omega^{(1,1)}(T_{eff})-5\Omega^{(1,1)}(T_{eff})\right]$$

And:

$$a_{01}(1)=-\frac{8d}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[6C^*-5]$$

Finally:

$$a_{01}^{*}(1)=-\frac{8d}{15}[6C^*-5]$$

Calculation of $a_{11}(0)$

Given that $\psi_0^{(1)} = \left[\frac{3}{2} - \frac{Mz^2}{2kT_b}\right]$ $\quad \vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=0,s=1} = \frac{2}{3}$$

$$\psi_0^{(1)}(\vec{W} + d\vec{g})\left[\psi_0^{(1)}(\vec{W} + e_\mu\vec{g} + f\vec{g}) - \psi_0^{(1)}(\vec{W} + e_\mu\vec{g}' + f\vec{g})\right] = \frac{e_\mu M(\vec{g}-\vec{g}')(3f\vec{g}-\vec{W})\left(3kT_b - M\left(3d^2g^2 + W^2 - 2d\vec{g}\cdot\vec{W}\right)\right)}{2k^2T_b^2}$$

Integrating over the center of mass velocities yields:

$$a_{11}(0) = \frac{2}{3}\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}} \int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)} \frac{e_\mu M d^{\frac{3}{2}}(g^2 - \vec{g}\cdot\vec{g}')[3dfkMT + d^2M(fmg^2 + 2kT) - 3fkmT_b]}{2k^2T_b^2 m} gbdbd\epsilon d\vec{g}$$

Integrating ϵ from 0 to 2π:

$$a_{11}(0) = \frac{2}{3\pi^{\frac{3}{2}}} e_\mu \left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}} \int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)} \frac{\left[3fkMT + dM(fmg^2 + 2kT) - \frac{3f}{d}kmT_b\right]}{kT_b m} g^3(1 - \cos(\chi))2\pi bdbd\vec{g}$$

Using eq. (42):

$$a_{11}(0) = \frac{2}{3\pi} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \left(\frac{\mu}{2kT_{eff}}\right)^3 \int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)} \left[\frac{3f}{d}\frac{dMT}{mT_b} + f\frac{dM}{kT_b}g^2 + 2\frac{dMT}{mT_b} - \frac{3f}{d}\right] g^3 Q^{(1)}(g) d\vec{g}$$

Using previously known relations and integrating over the angles of velocity:

$$a_{11}(0) = \frac{8}{3} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \left(\frac{\mu}{2kT_{eff}}\right)^3 \int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)} \left[\frac{3f}{d}(1-d) + 2f\left(\frac{\mu}{2kT_{eff}}\right)g^2 + 2(1-d) - \frac{3f}{d}\right] g^5 Q^{(1)}(g) dg$$

Using CCS and simplifying:

$$a_{11}(0) = \frac{8}{3} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}(T_{eff})[6fC^* + 2(1-d) - 3f]$$

Adding and subtracting $2f$ and using the identity $2(f-d) = -2e_\mu$:

$$a_{11}(0) = \frac{8}{3} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}(T_{eff})\left[f(6C^* - 5) + 2\left(1 - e_\mu\right)\right]$$

And hence:

$$a_{11}^*(0) = \frac{8}{3}\left[f(6C^* - 5) + 2\left(1 - e_\mu\right)\right]$$

Calculation of $a_{10}(1)$

Given that $\psi_1^{(1)} = z_1\left(\frac{M}{2kT_b}\right)^{1/2}\left[\frac{5}{2} - \frac{Mz^2}{2kT_b}\right]$, $\psi_1^{(0)} = z_1\left(\frac{M}{2kT_b}\right)^{1/2}$ $\quad \vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=1,s=0} = 2$$

$$\psi_1^{(0)}(\vec{W} + d\vec{g})\left[\psi_1^{(1)}(\vec{W} + e_\mu\vec{g} + f\vec{g}) - \psi_1^{(1)}(\vec{W} + e_\mu\vec{g}' + f\vec{g})\right] = \ldots too\ long$$

Integrating over the center of mass velocities yields:

$$a_{10}(1) = 2\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2\pi kT}{m}\right)^{\frac{3}{2}}$$

$$\times\frac{e_\mu M d^{\frac{5}{2}}}{4k^2T_b^2 m}\Big[-e_\mu^2 mMg^2(g_1^2-g_1g_1') - f^2mM\Big(g^2(g_1^2-g_1g_1') + 2g_1^2(g^2-\vec{g}\cdot\vec{g}')\Big) - 2fkMT\Big(g^2-\vec{g}\cdot\vec{g}' + 2(g_1^2-g_1g_1')\Big) + e_\mu M\left(-2fm(g^2g_1^2-g_1g_1'(\vec{g}\cdot\vec{g}')) - 2kT\big(g_1^2-{g_1'}^2\big)\right) - 5k(dMT-mT_b)(g_1^2-g_1g_1')\Big]\,gbdbd\epsilon d\vec{g}$$

Integrating ϵ from 0 to 2π:

$$a_{10}(1) = \frac{e_\mu}{\pi^{\frac{3}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$\times\frac{1}{kT_b m}\Big[-e_\mu^2 mMg^3g_1^2(1-\cos(\chi)) - 3f^2mMg^3g_1^2(1-\cos(\chi)) - 2fkMT\Big(g^3(1-\cos(\chi)) + 2g_1^2g(1-\cos(\chi))\Big) + e_\mu M\Big(-2fmg^3g_1^2(1-\cos^2(\chi)) - kT(3g_1^2-g^2)g(1-\cos^2(\chi))\Big) - 5k(dMT-mT_b)g_1^2g(1-\cos(\chi))\Big]\,2\pi bdbd\vec{g}$$

Note that the term $\left(g_1^2-{g_1'}^2\right)$ has to be carefully integrated using eqs. (45-48). Using eq. (42):

$$a_{10}(1) = \frac{e_\mu}{d\pi^{\frac{3}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$\times\Big[-2e_\mu^2\frac{Md}{2kT_b}\,g^3g_1^2Q^{(1)}(g) - 6f^2\frac{Md}{2kT_b}g^3g_1^2Q^{(1)}(g) - 2f\frac{MTd}{mT_b}\Big(g^3Q^{(1)}(g) + 2g_1^2gQ^{(1)}(g)\Big) - \frac{8}{3}fe_\mu\frac{Md}{2kT_b}\,g^3g_1^2Q^{(2)}(g) - \frac{2}{3}e_\mu\frac{MTd}{mT_b}\,(3g_1^2-g^2)gQ^{(2)}(g) - 5d\left(\frac{dMT}{mT_b}-1\right)g_1^2gQ^{(1)}(g)\Big]\,d\vec{g}$$

Using previously known relations and integrating over the angles of velocity:

$$a_{10}(1) = \frac{4e_\mu}{d\pi^{\frac{1}{2}}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$\times\Big[-\frac{2}{3}e_\mu^2\frac{Md}{2kT_b}\,g^7Q^{(1)}(g) - \frac{6}{3}f^2\frac{Md}{2kT_b}g^7Q^{(1)}(g) - \frac{6}{3}f\frac{MTd}{mT_b}\Big(g^5Q^{(1)}(g) + \frac{2}{3}g^5Q^{(1)}(g)\Big) - \frac{8}{9}fe_\mu\frac{Md}{2kT_b}\,g^7Q^{(2)}(g) - \frac{5}{3}d\left(\frac{dMT}{mT_b}-1\right)g^5Q^{(1)}(g)\Big]\,d\vec{g}$$

Where the integration of the $(3g_1^2-g^2)$ over θ_g becomes 0. Using CCS and simplifying:

$$a_{10}(1) = \frac{4}{3d}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[-6e_\mu^2C^* - 18f^2C^* - 10f(1-d) - 8fe_\mu A^* + 5d^2]$$

Reorganizing the terms:

$$a_{10}(1) = -\frac{4}{3d}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[(e_\mu^2+3f^2)6C^* + 5(2f-2fd-d^2) + 8fe_\mu A^*]$$

Adding and subtracting $5(e_\mu^2+3f^2)$ and using $2(f-d) = -2e_\mu$ and $e_\mu^2 - d^2 + f^2 = -2e_\mu f$:

$$a_{10}(1) = -\frac{4}{3d}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[(e_\mu^2+3f^2)(6C^*-5) + 5(2f-4ef) + 8fe_\mu A^*]$$

And hence:

$$a_{10}^*(1) = -\frac{4}{3d}[(e_\mu^2+3f^2)(6C^*-5) + 10f(1-2e) + 8fe_\mu A^*]$$

Calculation of $a_{12}(0)$

Given that $\psi_0^{(1)} = \left[\frac{3}{2} - \frac{Mz^2}{2kT_b}\right]$, $\psi_0^{(2)} = \frac{1}{2}\left(\frac{15}{4} + \frac{M^2z^4}{4k^2T_b^2} - \frac{5Mz^2}{2kT_b}\right)$, $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}|_{l=0,s=2} = \frac{8}{15}$$

$\psi_0^{(2)}(\vec{W} + d\vec{g})\left[\psi_0^{(1)}(\vec{W} + e_\mu\vec{g} + f\vec{g}) - \psi_0^{(1)}(\vec{W} + e_\mu\vec{g}' + f\vec{g})\right] = -\frac{e_\mu M}{16k^3T_b^3}(\vec{g} - \vec{g}')\left(3e_\mu(\vec{g} + \vec{g}') + 2(3f\vec{g} + \vec{W})\right)\left[9d^4g^4M^2 + 15k^2T_b^2 + 12d^3M^2g^2\vec{g}\cdot\vec{W} - 10kMT_bW^2 + M^2W^4 + 4dM(\vec{g}\cdot\vec{W})(MW^2 - 5kT_b) + 2d^2g^2M\left(M\left(5W^2 + 4(W_1W_2 + W_1W_3 + W_2W_3)\right) - 15kT_b\right)\right]$

Integrating over the center of mass velocities yields:

$$a_{12}(0) = -\frac{8}{15}\left(\frac{M}{2\pi kT_b}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\left(\frac{2\pi kT}{m}\right)^{\frac{3}{2}}$$

$\times\frac{e_\mu Md^{\frac{5}{2}}}{8k^3T_b^3m^2}(g^2 - \vec{g}\cdot\vec{g}')\left[10d^2kM^2T(fg^2m + 2kT) + d^3g^2mM^2(fg^2m + 4kT) - 30fk^2mMTT_b + 15\frac{f}{d}k^2m^2T_b^2 + 5dkM\left(3fkMT^2 - 2mT_b(fg^2m + 2kT)\right)\right]gbdbd\epsilon d\vec{g}$

Integrating ϵ from 0 to 2π:

$$a_{12}(0) = -\frac{2}{15}\frac{e_\mu}{\pi^{3/2}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$\times\left[10d^2\left(fg^2\frac{M}{kT_b}\frac{MT}{mT_b} + 2\frac{M^2T^2}{m^2T_b^2}\right) + d^3fg^4\frac{M^2}{k^2T_b^2} + 4d^3g^2\frac{M}{kT_b}\frac{MT}{mT_b} - 30f\frac{MT}{mT_b} + 15\frac{f}{d} + 5d\left(3f\frac{M^2T^2}{m^2T_b^2} - 2\left(fg^2\frac{M}{kT_b} + 2\frac{MT}{mT_b}\right)\right)\right]g^3(1 - \cos(\chi))2\pi bdbd\vec{g}$

Using eq. (42) and simplifying the terms:

$$a_{12}(0) = -\frac{2}{15}\frac{e_\mu}{\pi^{3/2}}\left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}}\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$\times\left[10\left(2fg^2\frac{Md}{2kT_b}(1-d) + 2(1-d)^2\right) + 4dfg^4\frac{M^2d^2}{4k^2T_b^2} + 8dg^2\frac{Md}{2kT_b}(1-d) - 30\frac{f}{d}(1-d) + 15\frac{f}{d} + 5\left(3\frac{f}{d}(1-d)^2 - 2\left(2fg^2\frac{Md}{2kT_b} + 2(1-d)\right)\right)\right]g^3Q^{(1)}(g)d\vec{g}$

Integrating over the angles of velocity:

$$a_{12}(0) = -\frac{8}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\left(\frac{\mu}{2kT_{eff}}\right)^3\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$\times\left[10\left(2fg^2\left(\frac{\mu}{2kT_{eff}}\right)(1-d) + 2(1-d)^2\right) + 4dfg^4\left(\frac{\mu}{4kT_{eff}}\right)^2 + 8dg^2\left(\frac{\mu}{2kT_{eff}}\right)(1-d) - 30\frac{f}{d}(1-d) + 15\frac{f}{d} + 15\frac{f}{d}(1-d)^2 - 10\left(2fg^2\left(\frac{\mu}{2kT_{eff}}\right) + 2(1-d)\right)\right]g^5Q^{(1)}(g)dg$

Using collision integrals:

$$a_{12}(0) = -\frac{8}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})$$

$$\times\left[10(6f(1-d)C^{*}+2(1-d)^{2})+48df\frac{\Omega^{(1,3)}(T_{eff})}{\Omega^{(1,1)}(T_{eff})}+24d(1-d)C^{*}-30\frac{f}{d}(1-d)+15\frac{f}{d}+15\frac{f}{d}(1-d)^{2}-10(6fC^{*}+2(1-d))\right]$$

Simplifying:

$$a_{12}(0)=-\frac{8}{15}e_{\mu}\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})\left[-60fdC^{*}-20d+20d^{2}+48df\frac{\Omega^{(1,3)}(T_{eff})}{\Omega^{(1,1)}(T_{eff})}+24d(1-d)C^{*}+15fd\right]$$

Given that $B^{*}=5C^{*}-4\frac{\Omega^{(1,3)}(T_{eff})}{\Omega^{(1,1)}(T_{eff})}$:

$$a_{12}(0)=-\frac{8}{15}e_{\mu}\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[-3fd(4B^{*}-5)-4d(1-d)5+4d(1-d)6C^{*}]$$

Rearranging:

$$a_{12}(0)=-\frac{8d}{15}e_{\mu}\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}(T_{eff})[4(1-d)(6C^{*}-5)-3f(4B^{*}-5)]$$

Hence:

$$a_{12}^{*}(0)=-\frac{8d}{15}[4(1-d)(6C^{*}-5)-3f(4B^{*}-5)]$$

Calculation of $a_{00}(2)$

Given that $\psi_{2}^{(0)}=\frac{1}{2}\left[\frac{3}{2}\frac{Mz_{1}^{2}}{kT_{b}}-\frac{Mz^{2}}{2kT_{b}}\right]$, , $\vec{z}=(z_{1}=w,z_{2},z_{3})$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=2,s=0}=\frac{4}{3}$$

$$\psi_{2}^{(0)}(\vec{W}+d\vec{g})\left[\psi_{2}^{(0)}(\vec{W}+e_{\mu}\vec{g}+f\vec{g})-\psi_{2}^{(0)}(\vec{W}+e_{\mu}\vec{g}'+f\vec{g})\right]=\frac{e_{\mu}M^{2}\left(d^{2}(3g_{1}^{2}-g^{2})+3W_{1}^{2}+W^{2}+2d(3g_{1}W_{1}-\vec{g}\cdot\vec{W})\right)\left(3e_{\mu}\left(g_{1}^{2}-g_{1}^{2\prime}\right)+2\left(f\left(3g_{1}(g_{1}-g_{1}')-\vec{g}\cdot(\vec{g}-\vec{g}')\right)+3W_{1}(g_{1}-g_{1}')-\vec{W}\cdot(\vec{g}-\vec{g}')\right)\right)}{16k^{2}T_{b}^{2}}$$

Integrating over the center of mass velocities yields:

$$a_{00}(2)=\frac{4}{3}\left(\frac{M}{2\pi kT_{b}}\right)^{\frac{3}{2}}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\int\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^{2}\right)}\left(\frac{2\pi kT}{m}\right)^{\frac{3}{2}}$$

$$\times\frac{e_{\mu}M^{2}d^{\frac{7}{2}}}{16k^{2}T_{b}^{2}m}\left[(3g_{1}^{2}-g^{2})m\left(e_{\mu}(3g_{1}^{2}-3g_{1}'^{2})+2f(3g_{1}(g_{1}-g_{1}')-\vec{g}\cdot(\vec{g}-\vec{g}'))\right)+4kT\left(3(g_{1}^{2}-g_{1}g_{1}')+(g^{2}-\vec{g}\cdot\vec{g}')\right)\right]gbdbd\epsilon d\vec{g}$$

Integrating ϵ from 0 to 2π:

$$a_{00}(2)=\frac{1}{6\pi^{3/2}}e_{\mu}\left(\frac{Md}{2kT_{b}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^{2}\right)}$$

$$\times\frac{Md}{kT_{b}m}\left[(3g_{1}^{2}-g^{2})m\left(\frac{3e_{\mu}}{2}(3g_{1}^{2}-g^{2})(1-\cos^{2}(\chi))+2f\left(3g_{1}^{2}(1-\cos(\chi))-g^{2}(1-\cos(\chi))\right)\right)+4kT\left(3g_{1}^{2}(1-\cos(\chi))+g^{2}(1-\cos(\chi))\right)\right]g2\pi bdbd\vec{g}$$

Integrating over the angles of velocity:

$$a_{00}(2) = \frac{8}{15\pi^{1/2}} e_\mu \left(\frac{Md}{2kT_b}\right)^{\frac{5}{2}} \int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)} \left[3eg^4\left(\frac{Md}{2kT_b}\right)(1-\cos^2(\chi)) + 4fg^4\left(\frac{Md}{2kT_b}\right)(1-\cos(\chi)) + 10g^2 d\frac{MT}{mT_b}(1-\cos(\chi))\right] g^3 2\pi b db dg$$

Using CCS integrals and the appropriate ratios:

$$a_{00}(2) = \frac{16}{15} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}(T_{eff})[3eA^* + 6fC^* + 5(1-d)]$$

Simplifying and rearranging with $f - d = -e$:

$$a_{00}(2) = \frac{16}{15} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}(T_{eff})[3eA^* + f(6C^* - 5) + 5(1-e)]$$

And hence:

$$a_{00}^*(2) = \frac{16}{15}[3eA^* + f(6C^* - 5) + 5(1-e)]$$

Calculation of $a_{01}(2)$

Given that $\psi_2^{(0)} = \frac{1}{2}\left[\frac{3}{2}\frac{Mz_1^2}{kT_b} - \frac{Mz^2}{2kT_b}\right]$, $\psi_2^{(1)} = \frac{1}{2}\left[\frac{7}{2} - \frac{M}{2kT_b}z^2\right]\left[\frac{3}{2}\frac{Mz_1^2}{kT_b} - \frac{Mz^2}{2kT_b}\right]$, $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=2,s=1} = \frac{8}{21}$$

$$\psi_2^{(1)}(\vec{W} + d\vec{g})\left[\psi_2^{(0)}(\vec{W} + e_\mu\vec{g} + f\vec{g}) - \psi_2^{(0)}(\vec{W} + e_\mu\vec{g}' + f\vec{g})\right] = \frac{e_\mu M^2\left(d^2(3g_1^2 - g^2) + 3W_1^2 + W^2 + 2d(3g_1W_1 - \vec{g}\cdot\vec{W})\right)\left(3e_\mu\left(g_1^2 - g_1^{2\prime}\right) + 2\left(f\left(3g_1(g_1 - g_1') - \vec{g}\cdot(\vec{g} - \vec{g}')\right) + 3W_1(g_1 - g_1') - \vec{W}\cdot(\vec{g} - \vec{g}')\right)\right)}{32k^3T_b^3}$$

$$\times\left(-7kT_b + M\left(d^2g^2 + W^2 + 2d\vec{g}\cdot\vec{W}\right)\right)$$

Integrating over the center of mass velocities, epsilon, and the angles of velocity yields:

$$a_{01}(2) = -\frac{4}{105\pi^{\frac{1}{2}}} e_\mu \left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}} \int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$\times g^2\left[\left(3e_\mu dg^4\left(\frac{dM}{kT_b}\right)^2 + 21e_\mu g^2\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) - 21e_\mu g^2\left(\frac{dM}{kT_b}\right)\right)(1+\cos(\chi)) + 4fdg^4\left(\frac{dM}{kT_b}\right)^2 + 28(d+f)g^2\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) + 140\left(\left(\frac{MTd}{mT_b}\right)^2 - \left(\frac{MTd}{mT_b}\right)\right)\right](1-\cos(\chi))g^3 2\pi b db dg$$

Using the definitions of CCS:

$$a_{01}(2) = -\frac{16}{105} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}\left[24e_\mu d\frac{\Omega^{(2,3)}}{\Omega^{(1,1)}} + 48fd\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}} - 21e_\mu d\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}} + 42[(d+f)(1-d) - f]\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}} + 35d(d-1)\right]$$

Using the definitions of A^*, B^*, C^* and $E^* = \frac{\Omega^{(2,3)}}{\Omega^{(2,2)}}$ and rearranging:

$$a_{01}(2) = \frac{16d}{105} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)}\left[(6C^* - 5)(7(d-1) - 3f) + 3f(4B^* - 5) - 3e_\mu(8E^* - 7)A^*\right]$$

Hence:

$$a_{01}^{*}(2) = \frac{16d}{105}\left[(6C^{*} - 5)(7(d-1) - 3f) + 3f(4B^{*} - 5) - 3e_{\mu}(8E^{*} - 7)A^{*}\right]$$

Calculation of $\boldsymbol{a_{02}(1)}$

Given $\psi_1^{(0)} = w\left(\frac{M}{2kT_b}\right)^{1/2}$ $, \psi_1^{(2)} = \frac{1}{2}w\left(\frac{M}{2kT_b}\right)^{1/2}\left[\frac{35}{4} - 7\frac{M}{2kT_b}z^2 + \left(\frac{M}{2kT_b}\right)^2 z^4\right]$, $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=1,s=2} = \frac{16}{35}$$

$$\psi_1^{(2)}(\vec{W} + d\vec{g})\left[\psi_1^{(0)}(\vec{W} + e_{\mu}\vec{g} + f\vec{g}) - \psi_1^{(0)}(\vec{W} + e_{\mu}\vec{g}' + f\vec{g})\right] =$$
$$\frac{e_{\mu}M(g_1 - g_1')(dg_1 + W_1)\left(d^4M^2g^2 + 35k^2T_b^2 + 4d^3M^2g^2\vec{g}\cdot\vec{W} - 14kMT_bW^2 + M^2W^4 + 4dM\vec{g}\cdot\vec{W}(MW^2 - 7kT_b) + 2d^2M(Mg^2W^2 - 7g^2kT_b + 2M(\vec{g}\cdot\vec{W})(\vec{g}\cdot\vec{W})\right)}{16k^3T_b^3}$$

Integrating over the center of mass velocities and over epsilon yields:

$$a_{02}(1) = \frac{4}{35\pi^{\frac{1}{2}}}e_{\mu}\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{1}{m^2k^2T_b^2}$$
$$\times\left[d^2M^2(d^2g^2m^2 + 14dg^2kmT + 35k^2T^2) - 14dkmMT_b(dg^2m + 5kT) + 35m^2k^2T_b^2\right]g_1^2(1 - \cos(\chi))g2\pi bdbd\vec{g}$$

Integrating over the velocity angles and arranging:

$$a_{02}(1) = \frac{8}{105\pi^{\frac{1}{2}}}e_{\mu}\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$
$$\times\left[d^2g^4\left(\frac{dM}{kT_b}\right)^2 + 14dg^2\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) + 35\left(\frac{MTd}{mT_b}\right)^2 - 14\left(dg^2\left(\frac{dM}{kT_b}\right) + 5\left(\frac{MTd}{mT_b}\right)\right) + 35\right]g^5(1 - \cos(\chi))2\pi bdbdg$$

Using the CCS relations

$$a_{02}(1) = \frac{8}{105}e_{\mu}\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}\left[48d^2\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}} + 84d(1-d)\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}} + 35(1-d)^2 - 84d\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}} - 70(1-d) + 35\right]$$

Simplifying, rearranging and using the common relations:

$$a_{02}(1) = -\frac{8d^2}{105}e_{\mu}\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}\left[3(4B^{*} - 5) + 4(6C^{*} - 5)\right]$$

Hence:

$$a_{02}^{*}(1) = -\frac{8d^2}{105}\left[3(4B^{*} - 5) + 4(6C^{*} - 5)\right]$$

Calculation of $\boldsymbol{a_{11}(1)}$

Given $\psi_1^{(1)} = z_1\left(\frac{M}{2kT_b}\right)^{1/2}\left[\frac{5}{2} - \frac{Mz^2}{2kT_b}\right]$, $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=1,s=1} = \frac{4}{5}$$

$$\psi_1^{(1)}(\vec{W}+d\vec{g})\left[\psi_1^{(1)}(\vec{W}+e_\mu\vec{g}+f\vec{g})-\psi_1^{(1)}(\vec{W}+e_\mu\vec{g}'+f\vec{g})\right]=\frac{e_\mu M(dg_1+W_1)(Md^2g^2+MW^2+2Md\vec{g}\cdot\vec{W})}{8k^3T_b^3}[f^2M\left(g^2(g_1-g_1')+2g_1(g^2-\vec{g}\cdot\vec{g}')\right)+e_\mu{}^2M\left(g^2(g_1-g_1')-5kT_b(g_1-g_1')+MW^2(g_1-g_1')+2MW_1\vec{W}\cdot(\vec{g}-\vec{g}')+e_\mu M\big(2f(g^2g_1-\vec{g}\cdot\vec{g}'g_1')+2g_1\vec{g}\cdot\vec{W}-2g_1'\vec{g}'\cdot\vec{W}'\big)+2fM\left(2g_1(\vec{g}\cdot\vec{W}-\vec{g}'\cdot\vec{W})+g^2W_1-g_1'(\vec{g}\cdot\vec{W})\right)\right)\Big]$$

Integrating over the center of mass velocities, over epsilon and over the angles in velocity yields:

$$a_{11}(1)=\frac{4}{15\pi^{\frac{1}{2}}}e_\mu\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{1}{m^2k^2T_b^2}$$

$$\times\left[g^4\left(\frac{dM}{kT_b}\right)^2(e_\mu{}^2+3f^2)+g^2\left(\frac{dM}{kT_b}\right)\left(5\frac{(d^2+e_\mu{}^2+3f^2)}{d}\left(\left(\frac{MTd}{mT_b}\right)-1\right)+22f\left(\frac{MTd}{mT_b}\right)\right)+5\left(\frac{MTd}{mT_b}\right)^2\left(11+\frac{10f}{d}\right)-50\left(\frac{MTd}{mT_b}\right)\left(1+\frac{f}{d}\right)+25+\left[2g^4\left(\frac{dM}{kT_b}\right)^2e_\mu f+4g^2\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)e_\mu+10g^2\left(\frac{dM}{kT_b}\right)\frac{e_\mu f}{d}\left(\left(\frac{MTd}{mT_b}\right)-1\right)\right](1+cos(\chi))\right]g^5(1-\cos(\chi))2\pi bdbdg$$

Using the CCS relations:

$$a_{11}(1)=\frac{4}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}[48(e_\mu{}^2+3f^2)\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}}+6(1-d)\left(5d+22f+\frac{5(e_\mu{}^2+3f^2)}{d}\right)\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}}+5(1-d)^2\left(11+\frac{10f}{d}\right)-6\left(5d+\frac{5(e_\mu{}^2+3f^2)}{d}\right)\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}}-50(1-d)\left(1+\frac{f}{d}\right)+25+\left(64e_\mu f\frac{\Omega^{(2,3)}}{\Omega^{(1,1)}}+16e_\mu(1-d)\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}+\frac{40e_\mu f}{d}(1-d)\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}-\frac{40e_\mu f}{d}\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}\right)$$

Simplifying and rearranging:

$$a_{11}(1)=\frac{4}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}\left[8e_\mu A^*\left(f(8E^*-7)+2(1-e_\mu)\right)-3(e_\mu{}^2+3f^2)(4B^*-5)+[5(e_\mu{}^2+3f^2)-5d^2+22f(1-d)](6C^*-5)+30+60f(1-d)-60d(1-d)-30d^2+10(e_\mu{}^2+3f^2)\right]$$

And hence:

$$a_{11}^*(1)=\frac{4}{15}\left[8e_\mu A^*\left(f(8E^*-7)+2(1-e_\mu)\right)-3(e_\mu{}^2+3f^2)(4B^*-5)+[5(e_\mu{}^2+3f^2)-5d^2+22f(1-d)](6C^*-5)+10(3-6e_\mu+4e_\mu^2)\right]$$

Calculation of $a_{21}(0)$

Given that $\psi_0^{(1)}=\frac{3}{2}-z^2\left(\frac{M}{2kT_b}\right)$, $\psi_0^{(2)}=\frac{1}{2}\left(\frac{15}{4}+\frac{M^2z^4}{4k^2T_b^2}-\frac{5Mz^2}{2kT_b}\right)$, $\vec{z}=(z_1=w,z_2,z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l+s+\frac{3}{2}\right)}\Big|_{l=0,s=1}=\frac{2}{3}$$

$$\psi_0^{(1)}(\vec{W}+d\vec{g})[\psi_0^{(2)}(\vec{W}+e_\mu\vec{g}+f\vec{g})-\psi_0^{(2)}(\vec{W}+e_\mu\vec{g}'+f\vec{g})]=-\frac{e_\mu M\left(f(g^2-\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}-\vec{g}')\right)\left(M(d^2g^2+W^2+2d(\vec{g}\cdot\vec{W})\right)}{8k^3T_b^3}\left(M\left(2e_\mu g^2+2e_\mu\left(f(g^2+\vec{g}\cdot\vec{g}')+\vec{W}\cdot(\vec{g}+\vec{g}')\right)+2(f^2g^2+W^2+2f\vec{g}\cdot\vec{W})\right)-10kT_b\right)$$

Integrating over the center of mass velocities, over epsilon and over the angles in velocity yields:

$$a_{21}(0)=-\frac{4}{3d\pi^{\frac{1}{2}}}e_\mu\left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}}\int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}\frac{1}{m^2k^2T_b^2}$$

$$\times\left[5d^3kM^2T(fg^2m+2kT)+3dfkmMT\left((e_\mu^2+f^2)g^2M-10kT_b\right)-3fkm^2T_b\left((e_\mu^2+f^2)g^2M-5kT_b\right)+d^2M\big(M(f(e^2+f^2)g^4m^2+2(e^2+3f^2)g^2kmT+25fk^2T^2)-5kmT_b(fg^2m+2kT)\big)+e_\mu fg^2mM(dM(dfg^2m+4dkT+3fkT)-3fkmT_b)(1+\cos(\chi))\right]g^5(1-\cos(\chi))2\pi bdbdg$$

Rearranging:

$$a_{21}(0) = -\frac{4}{3d\pi^{\frac{1}{2}}} e_\mu \left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}} \int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$\times \Bigg[5\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) fdg^2 + 10\left(\frac{MTd}{mT_b}\right)^2 d + 3\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)\frac{f}{d}\left(e_\mu^2 + f^2\right)g^2 - 30\left(\frac{MTd}{mT_b}\right) f - 3\left(\frac{dM}{kT_b}\right)\frac{f}{d}\left(e_\mu^2 + f^2\right)g^2 - 15f + \left(\frac{dM}{kT_b}\right)^2 f\left(e_\mu^2 + f^2\right)g^4 + 2\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)\left(e_\mu^2 + 3f^2\right)g^2 + 25\left(\frac{MTd}{mT_b}\right)^2 f - 5\left(\frac{dM}{kT_b}\right) dfg^2 - 10\left(\frac{MTd}{mT_b}\right) d + e_\mu f\left(\left(\frac{dM}{kT_b}\right)^2 fg^4 + 4\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) g^2 + 3\left(\frac{dM}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)\frac{f}{d} g^2 - 3\left(\frac{dM}{kT_b}\right)\frac{f}{d} g^2\right)(1 + \cos(\chi))\Bigg] g^5(1 - \cos(\chi))2\pi bdbdg$$

Using CCS expressions:

$$\begin{aligned} a_{21}(0) = -\frac{4}{3d} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)} \Bigg[& e_\mu f\left(32f\frac{\Omega^{(2,3)}}{\Omega^{(1,1)}} + 16(1-d)\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}} + 12(1-d)\frac{f}{d}\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}} - 12\frac{f}{d}\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}\right) \\ & + 48f\left({e_\mu}^2 + f^2\right)\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}} + \left(12(1-d)\left({e_\mu}^2 + 3f^2\right) - 18f\left({e_\mu}^2 + f^2\right) - 30d^2 f\right)\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}} + 10d(1-d)^2 \\ & - 30(1-d)f + 15f + 25(1-d)^2 f - 10(1-d)d\Bigg] \end{aligned}$$

Using the known ratio expressions:

$$\begin{aligned} a_{21}(0) = -\frac{4}{3d} e_\mu \left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}} \Omega^{(1,1)} \Big[& 4e_\mu f A^*\left(f(8E^* - 7) + 4\left(1 - e_\mu\right)\right) - 3f\left({e_\mu}^2 + f^2\right)(4B^* - 5) \\ & + 2\left(d^2(1-d) - fd(2 - 3d + 11f) + f^2(4 + 7f)\right)(6C^* - 5) + 10f\left(1 - 2e_\mu\right)^2\Big] \end{aligned}$$

Hence:

$$\begin{aligned} a_{21}^*(0) = -\frac{4}{3d}\Big[& 4e_\mu f A^*\left(f(8E^* - 7) + 4\left(1 - e_\mu\right)\right) - 3f\left({e_\mu}^2 + f^2\right)(4B^* - 5) \\ & + 2\left(d^2(1-d) - fd(2 - 3d + 11f) + f^2(4 + 7f)\right)(6C^* - 5) + 10f\left(1 - 2e_\mu\right)^2\Big] \end{aligned}$$

Calculation of $a_{22}(0)$

Given that $\psi_0^{(2)} = \frac{1}{2}\left(\frac{15}{4} + \frac{M^2 z^4}{4k^2 T_b^2} - \frac{5Mz^2}{2kT_b}\right)$, $\vec{z} = (z_1 = w, z_2, z_3)$

$$\frac{(2l+1)s!\,\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(l + s + \frac{3}{2}\right)}\Big|_{l=0,s=2} = \frac{8}{15}$$

$$\psi_0^{(2)}(\vec{W} + d\vec{g})[\psi_0^{(2)}(\vec{W} + e_\mu\vec{g} + f\vec{g}) - \psi_0^{(2)}(\vec{W} + e_\mu\vec{g}' + f\vec{g})] = \frac{e_\mu M\left(f(g^2 - \vec{g}\cdot\vec{g}') + \vec{W}\cdot(\vec{g} - \vec{g}')\right)}{32k^4 T_b^4}\left(M\left(2e_\mu g^2 + 2e_\mu\left(f(g^2 + \vec{g}\cdot\vec{g}') + \vec{W}\cdot(\vec{g} + \vec{g}')\right) + 2\left(f^2 g^2 + W^2 + 2f\vec{g}\cdot\vec{W}\right)\right) - 10kT_b\right)\left(d^4 g^4 M^2 + 15k^2 T^2 + 4d^3 g^2 M^2(\vec{g}\cdot\vec{W}) - 10kMT_b W^2 + M^2 W^4 + 4dM(\vec{g}\cdot\vec{W})(MW^2 - 5kT_b) + 2d^2 M\left(g^2(MW^2 - 5kT_b) + 2M(\vec{W}\cdot\vec{g})\right)\right)$$

Integrating over the center of mass velocities, over epsilon and over the angles in velocity yields:

$$a_{22}(0) = \frac{4}{15d\pi^{\frac{1}{2}}} e_\mu \left(\frac{\mu}{2kT_{eff}}\right)^{\frac{5}{2}} \int\int e^{\left(-\left(\frac{\mu}{2kT_{eff}}\right)g^2\right)}$$

$$
\begin{aligned}
\Bigg[&\left(\frac{Md}{kT_b}\right)^3 g^6 df\left(e_\mu^2+f^2\right)+\left(\frac{Md}{kT_b}\right)^2\left(\frac{MTd}{mT_b}\right) g^4\left(4de_\mu^2+5d^2f+10e_\mu^2 f+12df^2+10f^3\right)-\left(\frac{Md}{kT_b}\right)^2 g^4\left(5d^2f+10e_\mu^2 f+10f^3\right)\\
&+\left(\frac{Md}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)^2 g^2\left(20d^2+20e_\mu^2+94df+15e_\mu^2\frac{f}{d}+60f^2+15f^2\frac{f}{d}\right)\\
&-\left(\frac{Md}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) g^2\left(20d^2+20e_\mu^2+100df+30e_\mu^2\frac{f}{d}+60f^2+30f^2\frac{f}{d}\right)+\left(\frac{Md}{kT_b}\right) g^2 f\left(50d+15\frac{e_\mu^2}{d}+15\frac{f^2}{d}\right)\\
&+\left(\frac{MTd}{mT_b}\right)^3(140d+175f)-\left(\frac{MTd}{mT_b}\right)^2(200d+325f)+\left(\frac{MTd}{mT_b}\right)(100d+225f)-75f\\
&+\Bigg(\left(\frac{Md}{kT_b}\right)^3 g^6 de_\mu f^3+\left(\frac{Md}{kT_b}\right)^2\left(\frac{MTd}{mT_b}\right) g^4\left(8de_\mu f+10e_\mu f^2\right)-\left(\frac{Md}{kT_b}\right)^2 g^4\left(10e_\mu f^2\right)\\
&+\left(\frac{Md}{kT_b}\right)\left(\frac{MTd}{mT_b}\right)^2 g^2\left(8de_\mu+40e_\mu f+15e_\mu\frac{f^2}{d}\right)-\left(\frac{Md}{kT_b}\right)\left(\frac{MTd}{mT_b}\right) g^2\left(40e_\mu f+30e_\mu\frac{f^2}{d}\right)+\left(\frac{Md}{kT_b}\right) g^2\left(15e_\mu\frac{f^2}{d}\right)\Bigg)(1\\
&+\cos(\chi))\Bigg] g^5(1-\cos(\chi))2\pi b\,db\,dg
\end{aligned}
$$

Using the known relations for CCS:

$$
\begin{aligned}
a_{22}(0)=\frac{4}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}\Bigg[&320e_\mu f^2\frac{\Omega^{(2,4)}}{\Omega^{(1,1)}}+32\left(8(1-d)e_\mu f+10e_\mu\frac{f^2}{d}(1-d)-10e_\mu\frac{f^2}{d}\right)\frac{\Omega^{(2,3)}}{\Omega^{(1,1)}}\\
&+4\Bigg(8e_\mu(1-d)^2+40e_\mu\frac{f}{d}(1-d)^2+15e_\mu\frac{f^2}{d^2}(1-d)^2-40e_\mu\frac{f}{d}(1-d)-30e_\mu\frac{f^2}{d^2}(1-d)\\
&+15e_\mu\frac{f^2}{d^2}\Bigg)\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}+480f\left(e_\mu^2+f^2\right)\frac{\Omega^{(1,4)}}{\Omega^{(1,1)}}\\
&+48\left(\left(4e_\mu^2+5df+10e_\mu^2\frac{f}{d}+12f^2+10\frac{f^3}{d}\right)(1-d)-5df-10e_\mu^2\frac{f}{d}-10\frac{f^3}{d}\right)\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}}\\
&+6\Bigg(\left(20d+20\frac{e_\mu^2}{d}+94f+15e_\mu^2\frac{f}{d^2}+60\frac{f^2}{d}+15f^2\frac{f}{d^2}\right)(1-d)^2\\
&-\left(20d+20\frac{e_\mu^2}{d}+100f+30e_\mu^2\frac{f}{d^2}+60\frac{f^2}{d}+30f^2\frac{f}{d^2}\right)(1-d)+\left(50f+15e_\mu^2\frac{f}{d^2}+15\frac{f^3}{d^2}\right)\Bigg)\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}}\\
&+\left(140+175\frac{f}{d}\right)(1-d)^3-\left(200+325\frac{f}{d}\right)(1-d)^2+\left(100+225\frac{f}{d}\right)(1-d)-75\frac{f}{d}\Bigg]
\end{aligned}
$$

Using the well-known relations and $D^*=\frac{\Omega^{(1,4)}}{\Omega^{(1,1)}}\ and\ G^*=\frac{\Omega^{(2,4)}}{\Omega^{(2,2)}}$:

$$
\begin{aligned}
a_{22}(0)=\frac{4}{15}e_\mu\left(\frac{2kT_{eff}}{\mu\pi}\right)^{\frac{1}{2}}\Omega^{(1,1)}\Big[&4e_\mu A^*\left[8\left(1-e_\mu\right)^2+2f(4(1-d)-5f)(8E^*-7)+f^2(80G^*-63)\right]\\
&+15f\left(e_\mu^2+f^2\right)(32D^*-21)+3\left[5f\left(d^2+2e_\mu^2+2f^2\right)-4(1-d)\left(e_\mu^2+3f^2\right)\right](4B^*-5)\\
&+f\left[44-128d-d^2+(80+90d)f-170f^2\right](6C^*-5)+40\left(1-e_\mu\right)\left(1-2e_\mu\left(1-e_\mu\right)\right)\Big]
\end{aligned}
$$

Hence:

$$
\begin{aligned}
a_{22}^*(0)=\frac{4}{15}\Big[&4e_\mu A^*\left[8\left(1-e_\mu\right)^2+2f(4(1-d)-5f)(8E^*-7)+f^2(80G^*-63)\right]+15f\left(e_\mu^2+f^2\right)(32D^*-21)\\
&+3\left[5f\left(d^2+2e_\mu^2+2f^2\right)-4(1-d)\left(e_\mu^2+3f^2\right)\right](4B^*-5)\\
&+f\left[44-128d-d^2+(80+90d)f-170f^2\right](6C^*-5)+40\left(1-e_\mu\right)\left(1-2e_\mu\left(1-e_\mu\right)\right)\Big]
\end{aligned}
$$

$$
a_{13}^*(0)=\frac{8d^2}{35}\left(5f(32D^*-21)+\left(6\left(e_\mu-1\right)+27f\right)(4B^*-5)+\left(8\left(e_\mu-1\right)-27f\right)(6C^*-5)\right)
$$

Other elements:

$$\begin{aligned} a_{23}^{*}(0) = \frac{4}{35}d\Big(&-4\mathrm{A}^{*}e_\mu\left((8\mathrm{E}^{*}-7)\big(8e_\mu(e_\mu+9f-2)+9f(11f-8)+8\big)+f(80\mathrm{G}^{*}-63)(-4e_\mu-11f+4)+f^2(320\mathrm{I}^{*}-231)\right) \\ &+6(4\mathrm{B}^{*}-5)\left(e_\mu\left(e_\mu(19e_\mu+81f-19)+2f(63f-22)\right)+f(9f(11f-9)+17)\right) \\ &-2(6\mathrm{C}^{*}-5)\big(e_\mu\big(e_\mu(57e_\mu+222f-1)+2f(189f+88)-84\big)+f(3f(176f-81)-68)+28\big) \\ &+10(32\mathrm{D}^{*}-21)\big(e_\mu\big(e_\mu(3e_\mu+16f-3)+14f^2\big)+(22f-9)f^2\big)-15f(128\mathrm{H}^{*}-77)(e_\mu^2+f^2)\Big) \end{aligned}$$

$$\begin{aligned} a_{30}^{*}(0) = \frac{f}{d^3}\Big(&-8\mathrm{A}^{*}e_\mu\left((8\mathrm{E}^{*}-7)f(e_\mu^2+f^2)-14f^2e_\mu\right)+3(4\mathrm{B}^{*}-5)(e_\mu^2+f^2)^2+4(6\mathrm{C}^{*}-5)(e_\mu^2+f^2)(7fe_\mu+e_\mu^2+f^2)-64f^2\mathrm{F}^{*}e_\mu^2 \\ &-140f^2e_\mu^2\Big) \end{aligned}$$

$$\begin{aligned} & a_{32}^{*}(0) = \tfrac{1}{15d}\Big(-8\mathrm{A}^{*}e_\mu\left((8\mathrm{E}^{*}-7)\big(e_\mu\big(e_\mu\big(8e_\mu(e_\mu+14f-2)+f(377f-112)+8\big)+12(45f-22)f^2\big)+(9f(33f-32)+76)f^2\big)-\right. \\ & f(80\mathrm{G}^{*}-63)\big(e_\mu\big(e_\mu(8e_\mu+25f-8)+30f^2\big)+(33f-16)f^2\big)+3f^2(320\mathrm{I}^{*}-231)(e_\mu^2+f^2)-112f(e_\mu-1)\big(3(e_\mu-1)e_\mu+1\big)\Big)+ \\ & 6(4\mathrm{B}^{*}-5)\left(e_\mu\left(e_\mu\left(e_\mu\left(e_\mu(38e_\mu+241f-38)+2f(271f-80)\right)+4f(3f(60f-23)+13)\right)+8(81f-38)f^3\right)+\right. \\ & \left.(27f(11f-10)+68)f^3\right)-4(6\mathrm{C}^{*}-5)\,\big(e_\mu\big(e_\mu\big(e_\mu\big(e_\mu(57e_\mu+372f-1)+561f^2+96f-84\big)+6f(f(96f+85)-8)+28\big)+ \\ & 4(f(243f+152)-140)f^2\big)+(f(9f(88f-45)-136)+84)f^2\big)+60(32\mathrm{D}^{*}-21)(e_\mu^2+f^2)\big(e_\mu\big(e_\mu(e_\mu+7f-1)+12f^2\big)+ \\ & (11f-5)f^2\big)-64f\mathrm{F}^{*}e_\mu^2\left(-2f(10\mathrm{V}^{*}-9)(6e_\mu+11f-6)+24(e_\mu-1)^2+3f^2(40\mathrm{W}^{*}-33)\right)-45f(128\mathrm{H}^{*}-77)(e_\mu^2+f^2)^2- \\ & 280f\big(2(e_\mu-1)e_\mu+1\big)\big(6(e_\mu-1)e_\mu+1\big)\Big) \end{aligned}$$

$$\begin{aligned} & a_{33}^{*}(0) = \tfrac{1}{35}\Big(-8\mathrm{A}^{*}e_\mu\Big((8\mathrm{E}^{*}-7)\left(2e_\mu\left(2e_\mu\big(e_\mu(28e_\mu+261f-56)+f(762f-377)+28\big)+f(9f(209f-180)+320)\right)+\right. \\ & \left.4f(3f(11f(13f-18)+93)-44)\right)+(320\mathrm{I}^{*}-231)\big(38f^3e_\mu+4fe_\mu^2(3e_\mu+10f-3)+4(13f-6)f^3\big)-2(80\mathrm{G}^{*}- \\ & 63)\big(e_\mu\big(e_\mu\big(2e_\mu(2e_\mu+25f-4)+f(147f-50)+4\big)+(209f-90)f^2\big)+(11f(13f-12)+31)f^2\big)-7f^2(640\mathrm{S}^{*}-429)(e_\mu^2+f^2)- \\ & 112(e_\mu-1)^2\big(2(e_\mu-1)e_\mu+1\big)\Big)+6(4\mathrm{B}^{*}-5)\big(e_\mu\big(e_\mu\big(e_\mu\big(e_\mu(338e_\mu+2001f-482)+4f(1215f-542)+216\big)+ \\ & 2f(24f(143f-90)+409)-72\big)+2(9f(319f-288)+610)f^2\big)+(3f(55f(13f-18)+486)-248)f^2\big)+(6\mathrm{C}^{*}- \\ & 5)\left(e_\mu\left(e_\mu\big(93(32-193f)e_\mu^2+48(f(187-835f)+8)e_\mu-3232e_\mu^3+2f(-30063f^2+6912f+2026)-128\big)-\right.\right. \\ & \left.\left.32f(f(6f(319f-162)-305)+168)\right)+f\big(952-f(3f(55f(169f-192)+2916)+1984)\big)\right)+10(32\mathrm{D}^{*}-21)\left(e_\mu\left(e_\mu\left(e_\mu\big(84e_\mu+\right.\right.\right. \\ & \left.\left.\left.499f-84\big)+8f(137f-39)\right)+6f(2f(121f-54)+19)\right)+4(319f-144)f^3\right)+(55f(13f-12)+162)f^3\Big)- \\ & 15(128\mathrm{H}^{*}-77)(e_\mu^2+f^2)\big(e_\mu\big(e_\mu(6e_\mu+41f-6)+58f^2\big)+5(13f-6)f^2\big)+105f(256\mathrm{R}^{*}-143)(e_\mu^2+f^2)^2- \\ & 64\mathrm{F}^{*}e_\mu^2\left(3f^2(40\mathrm{W}^{*}-33)(6e_\mu+13f-6)-f(10\mathrm{V}^{*}-9)\big(12e_\mu(2e_\mu+11f-4)+11f(13f-12)+24\big)+16(e_\mu-1)^3-\right. \\ & \left.f^3(560\mathrm{P}^{*}-429)\right)-560(e_\mu-1)\big(2(e_\mu-1)e_\mu+1\big)^2\Big) \end{aligned}$$

Collision Cross Section Ratios

$$A^{*}=\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}},\qquad C^{*}=\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}},\qquad B^{*}=5C^{*}-4\frac{\Omega^{(1,3)}}{\Omega^{(1,1)}},\qquad D^{*}=\frac{\Omega^{(1,4)}}{\Omega^{(1,1)}},\qquad E^{*}=\frac{\Omega^{(2,3)}}{\Omega^{(2,2)}}$$

$$F^{*}=\frac{\Omega^{(3,3)}}{\Omega^{(1,1)}},\qquad G^{*}=\frac{\Omega^{(2,4)}}{\Omega^{(2,2)}},\qquad H^{*}=\frac{\Omega^{(1,5)}}{\Omega^{(1,1)}},\qquad I^{*}=\frac{\Omega^{(2,5)}}{\Omega^{(2,2)}},$$

$$R^{*}=\frac{\Omega^{(1,6)}}{\Omega^{(1,1)}},\qquad S^{*}=\frac{\Omega^{(2,6)}}{\Omega^{(2,2)}},\qquad P^{*}=\frac{\Omega^{(3,6)}}{\Omega^{(3,3)}},\qquad V^{*}=\frac{\Omega^{(3,4)}}{\Omega^{(3,3)}},\qquad W^{*}=\frac{\Omega^{(3,5)}}{\Omega^{(3,3)}},$$

S.4 Aisbett's Formula

The Aisbett's formula is given by:

$$a_{rs}(l) = 2\left(\frac{2\,k_b\,T_{eff}}{\pi\mu}\right)^{1/2}\sum c_{Long}(\lambda'',p_2,p_3,p_4,p_5,L,\lambda,\nu,L'',r,s,l)\times\bar{\omega}_{T_{eff}}(\lambda'',p_2)\times d^{p_3}\times(1-d)^{p_4}\times f^{p_5} \times e_\mu^{(\lambda''+p_2-p_3-p_5)}$$

And the normalized $a^*_{rs}(l)$.

$$a^*_{rs}(l) = 2\left(\frac{1}{e_\mu\,\Omega^{(1,1)}_{T_{eff}}}\right)\sum c_{Long}(\lambda'',p_2,p_3,p_4,p_5,L,\lambda,\nu,L'',r,s,l)\times\bar{\omega}_{T_{eff}}(\lambda'',p_2)\times d^{p_3}\times(1-d)^{p_4}\times f^{p_5} \times e_\mu^{(\lambda''+p_2-p_3-p_5)}$$

Where a 2 factor has been added to the formula given by Viehland as a correction. This expression is a complicated sum of different indexes as clarified below. The p_i are given by:

$$p_2 = k + k'' + \nu'' + \frac{(L + L'' - \lambda'')}{2}$$

$$p_3 = k - k'' - \nu'' + \frac{(L - L'' - \lambda'')}{2}$$

$$p_4 = \lambda + \nu + \nu'$$

$$p_5 = L'' + 2k''$$

Where the different p_i contain the different loop indexes. These are the loops, from the innermost to the outermost given by:

$$0 \le \lambda \le Min(l + 2r\,, l + 2s)$$

$$|\lambda - l| \le L \le Min(l + 2r, l + 2s, \lambda + l)$$

$$0 \le \nu' \le r + \frac{(l - L - \lambda)}{2}$$

$$1 \le \lambda'' \le 2(r - \nu') + l - \lambda$$

$$|\lambda'' - L| \le L'' \le Min(2r - 2\nu' + l - \lambda, \lambda'' + L)$$

$$0 \le \nu'' \le r - \nu' + \frac{(l - \lambda - L'' - \lambda'')}{2}$$

$$0 \le \nu \le s + \frac{(l - L - \lambda)}{2}$$

$$0 \le k \le s - \nu + \frac{(l - L - \lambda)}{2}$$

$$0 \le k'' \le r - \nu' - \nu'' + \frac{(l - \lambda - L'' - \lambda'')}{2}$$

The c_{Long} is a complicated expression that contains p_i and summation indices.

$$c_{Long}(\lambda'',p_2,p_3,p_4,p_5,L,\lambda,\nu,L'',r,s,l) = (-1)^{(l+p_3-p_4+p_5-L-L'')}\,s!\,\,(\lambda''+p_2+1)!\,\Gamma\left(l+r+\tfrac{3}{2}\right)\Gamma\left(p_4+\tfrac{3}{2}\right)\left(\Gamma\left(\tfrac{3}{2}\right)\right)^3(2\lambda+1)\,(2L+1)\,(2\lambda''+1)(2L''+1)\begin{pmatrix}\lambda'' & L'' & L\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}L & \lambda & l\\ 0 & 0 & 0\end{pmatrix}^2\left(\Gamma\left(\lambda''+\tfrac{p_2-p_3-p_5+3}{2}\right)\Gamma\left(\tfrac{\lambda''+p_2+p_3+L+3}{2}\right)\Gamma\left(\tfrac{p_5+L''+3}{2}\right)\Gamma\left(p_4-\right.\right.$$

$\nu + \frac{3}{2}\Big)\ \Gamma\left(\lambda + \nu + \frac{3}{2}\right)\left(s - \nu + \frac{l-\lambda-\lambda''-p_2-p_3}{2}\right)!\ \ \left(\frac{\lambda''+p_2+p_3-L}{2}\right)!\ \ \nu!\ \ \Big(r + \nu - p_4 + \frac{l+\lambda-\lambda''-p_2+p_3}{2}\Big)!\ \ \left(\frac{p_5-L''}{2}\right)!\ \ \left(\frac{p_2-p_3-p_5}{2}\right)!\ \ (p_4 - \lambda - \nu)!\Big)^{-1}$

In this expression, the $\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}$ are the 'Three J Symbol' functions.

The $\overline{\omega}_{T_{eff}}$ term is a function of $\overline{\Omega}_{T_{eff}}$ which can be written as (in this case the sums are directly shown)

$$\overline{\omega}_{T_{eff}}(\lambda'', p_2) = \sum_{r_2=1}^{\lambda''} c_{Short}(\lambda'', r_2)\ \overline{\Omega}_{T_{eff}}^{(r_2,\ \lambda''+p_2)}$$

This term also includes the coefficient c_{Short} given by:

$$c_{Short}(\lambda'', r_2) = \left(1 - \frac{1 + (-1)^{\mathrm{r}_2}}{2(\mathrm{r}_2 + 1)}\right) \sum_{k_2=r_2}^{\lambda''} \frac{(-1)^{(k_2+r_2)}\ \ (\lambda'' + k_2)!}{2^{k_2}\ \ k_2!\ \ (\lambda'' - k_2)!\ \ r_2!\ \ (k_2 - r_2)!}$$

S.5 Programs

The authors have programs available to calculate matrix elements regularly and through Aisbett's formula for any matrix element. The calculation of all-atom ions at high fields using a 4-6-12 potential up to the 4th approximation is available free of charge at www.imospedia.com.