Notes for Master Thesis

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Contents

Abstract

The purpose of this note is to gather what I've found in one single note, such that information is easy to come by and read. This should help greatly when writing the actual thesis.

1 Introduction

2 General method

To eventually calculate the energy of our system, we use a variational method. We approximate the system using Taylor expansions and minimize the system until it converges to the expected energy. To accomplish this, we use the method of Shifted Correlated Gaussians.

2.1 Shifted Correlated Gaussians

The method of Shifted Correlated Gaussians relies on writing our wave function in the non-orthonormal basis of shifted Gaussians.

$$|\psi\rangle = \sum_{i=1}^{n_g} c_i e^{-\mathbf{r}^T A \mathbf{r} + \mathbf{s}^T \mathbf{r}} = \sum_{i=1}^{n_g} c_i |g_i\rangle \tag{1}$$

Here, c_i are coefficients, $\mathbf{r}$ is a *size-N* vector of coordinates, A is an *NxN* matrix of parameters, and $\mathbf{s}$ is a *size-N* column of "shift" vectors. The goal is then, as stated in section 2.1 to minimize the energy with respect to this wavefunction. That is, we use the variational method.

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{2}$$

The benefit of using the Shifted Correlated Gaussians is the the matrix elements in equation 2 become analytical. As such, the matrix elements can be solved by hand, and afterwards the minimization routine can be performed using numerical programming.[2]

2.2 Solving the variational system

In order to find the minimal energy, we turn the problem into an optimization problem. Let us differentiate equation 2 with respect to the coefficients, c_k in equation 2.

$$\frac{\partial E_0}{\partial c_k} = \frac{\partial}{\partial c_k} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{3}$$

We can simplify this by writing out the wavefunctions in equation 3 as was done in equation 1

$$\frac{\partial}{\partial c_k} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\partial}{\partial c_k} \frac{\sum_{k,k'} c_k c_{k'} \langle g_k|H|g_{k'}\rangle}{\sum_{k,k'} c_k c_{k'} \langle g_k|g_{k'}\rangle} = \frac{\partial}{\partial c_k} \frac{c^T H c}{c^T N C} \tag{4}$$

The last line in equation 4 is the sums being rewritten into a matrix form, where c is a vector of all the possible c_k's in the sum. Now, we can perform the differentiation, using our rules for differentiating a fraction.

$$\frac{\partial E}{\partial c_k} = \frac{\left(\frac{\partial}{\partial c_k} c^T H c\right) c^T N c - c^T H c \left(\frac{\partial}{\partial c_k} c^T N c\right)}{\left(c^T N c\right)^2} \tag{5}$$

We then use the following result from matrix calculus.[3]

$$\frac{d\mathbf{x}^T A \mathbf{x}}{d\mathbf{x}^T} = 2A\mathbf{x} \tag{6}$$

Plugging equation 6 into equation 5 and setting to zero, we get.

$$\begin{aligned} &\frac{\partial E}{\partial c_k} = 2\frac{(Hc)_k \, c^T N c - c^T H c \, (Nc)_k}{\left(C^T N c\right)^2} = 2\frac{(Hc)_k - E\,(Nc)_k}{C^T N c} = 0 \\ &\implies Hc - ENc = 0 \implies Hc = ENc \end{aligned} \tag{7}$$

The second equality on the first line of equation 7 comes from the fact that $c^T H c = E c^T N c$.

We see that minimizing the energy comes down to solving a generalized eigenvalue problem. One must however note, that the energy in equation 2 not only depends on the value of the coefficients, c_k but also the parameterization matrices, A being used. These parameterization matrices are constructed according to equation 8

$$A = \sum_{i<j}^{n} \alpha_{ij} w_{ij} w_{ij}^T \tag{8}$$

where $\alpha_{ij} = \frac{1}{b_{ij}^2}$ with b_{ij} typically being chosen stochastically, as is done in [1], where the b_{ij}'s are samples from an exponential distribution.

$$b_{ij} = -ln(u)b_{max} \tag{9}$$

with the quasi-random number $u \in]0,1[$ being chosen from a Van-der-Corput sequence, and b_max having roughly the same dimension as the system being evaluated.

So, when optimizing the energy, one must vary both the linear coefficients, c_k and the non-linear parameters α_{ij}. We can find the optimal paramters, c_k, by solving the generalized eigenvalue problem while keeping the α's constant. Then, we can find the optimal *alpha*'s using a minimization routine, such as a Quasi-Newton method.

3 Matrix elements

The matrix elements can be calculated explicitly given the expression in equation 1. We are interested in the matrix elements for $\langle g'|g\rangle$ and $\langle g'|H|g\rangle$, where H is a sum of some kinetic energy operator and a central field potential.[1] These matrix elements are fairly straight forward to calculate. The detailed calculations are described in [2], and will be outlined below.

3.1 Overlap

The calculation of the matrix elements goes as follows: We begin by integrating the product of two Gaussians.

$$\langle g'|g\rangle = \int d^3\vec{r_1}...d^3\vec{r_N} exp(-\mathbf{r}^T B\mathbf{r} + s'^T\mathbf{r}) exp(-\mathbf{r}^T A\mathbf{r} + s^T\mathbf{r}) \tag{10}$$

We integrate over each of the spacial coordinates. To simplify this, we recall that multiplying two exponential functions together is the same as summing the exponents.

$$\langle g'|g\rangle = \int d^3\vec{r_1}...d^3\vec{r_N} exp(-\mathbf{r}^T D\mathbf{r} + (s' + s)^T\mathbf{r}) \tag{11}$$

With $D = A + B$. Now, we can rewrite the exponent. We note that since A and A' are real and symmetric. As such, the matrix D is real and symmetric, and it has N (the dimension of D) real eigenvalues. We can rewrite D in a basis where it is diagonal.

$$D = QCQ^T \tag{12}$$

where Q is a vector of eigenvalues for D, such that $Q^TQ = 1$. In this basis, we also have $\mathbf{r} = Q\mathbf{x}$. Plugging this into equation 11, we can use the fact that C is diagonal to write.

$$\langle g'|g\rangle = \int d^3\vec{x_1}...d^3\vec{x_N} exp\left(-\sum_{i=1}^{N} \vec{x_i}C_{ii}\vec{x_i} + \sum_{i=1}^{N}(\vec{s_i'} + \vec{s_i})\vec{x_i}\right) \tag{13}$$

Now, the sum in the exponential can be seen as a product of several exponential functions. As such, we can rewrite into the much simpler form.

$$\langle g'|g\rangle = \prod_{i=1}^{N} \int d^3\vec{x_i} exp\left(-\vec{x_i}C_{ii}\vec{x_i} + (\vec{s_i'} + \vec{s_i})\vec{x_i}\right) \tag{14}$$

It is now straightforward to calculate the integral using a standard CAS tool. The result is.

$$\langle g'|g\rangle = \prod_{i=1}^{N} exp\left(\frac{1}{4B_{ii}}(\vec{s_i'} + \vec{s_i})^2\right)\left(\frac{\pi^N}{C_{ii}}\right)^{3/2} \tag{15}$$

Finally, transforming back and writing everything on matrix form, we get the result.

[1] Note that since the Gaussian basis that we use is linearly dependent, we have $\langle g'|g\rangle \neq 0$.

$$\langle g'|g\rangle = e^{\frac{1}{4}(\mathbf{s}'+\mathbf{s})^T R(\mathbf{s}'+\mathbf{s})} \left(\frac{\pi^N}{det(D)}\right)^{3/2} \tag{16}$$

with $R = D^{-1}$.

3.2 Kinetic energy

Getting the kinetic energy follows the same concept, but the calculations are a bit trickier nonetheless. The kinetic energy operator is as follows.

$$\hat{K} = -\frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^T} \tag{17}$$

Where K is a symmetric positive definite matrix. Before we consider the expectation value of this operator, we introduce some intermediate results.

$$\langle g'|\mathbf{r}|g\rangle = \langle e^{-\mathbf{r}^T B\mathbf{r}+\mathbf{s}'^T\mathbf{r}}|\mathbf{r}|e^{-\mathbf{r}^T A\mathbf{r}+\mathbf{s}^T\mathbf{r}}\rangle = \frac{\partial}{\partial \mathbf{s}^T}\langle g'|g\rangle \tag{18}$$

Since we have calculated the overlap in equation 16, we can easily calculate this derivative using rules from matrix calculus.

$$\frac{\partial}{\partial \mathbf{s}^T}\langle g'|g\rangle = \frac{\partial}{\partial \mathbf{s}^T} e^{\frac{1}{4}(\mathbf{s}'+\mathbf{s})^T R(\mathbf{s}'+\mathbf{s})} \left(\frac{\pi^N}{det(D)}\right)^{3/2} = \frac{1}{2}R(\mathbf{s}+\mathbf{s}')\langle g'|g\rangle \tag{19}$$

The second derivative we wish to calculate is.

$$\langle g'|\mathbf{r}^T F\mathbf{r}|g\rangle = \left(\frac{\partial}{\partial \mathbf{s}} F \frac{\partial}{\partial \mathbf{s}^T}\right)\langle g'|g\rangle \tag{20}$$

Here, F is a real, symmetric and positive definite matrix. The first derivative is taken care of in a similar fashion to equation 19.

$$\left(\frac{\partial}{\partial \mathbf{s}} F \frac{\partial}{\partial \mathbf{s}^T}\right)\langle g'|g\rangle = \frac{\partial}{\partial \mathbf{s}}\left(\frac{1}{2}FR(\mathbf{s}+\mathbf{s}')e^{\frac{1}{4}(\mathbf{s}'+\mathbf{s})^T R(\mathbf{s}'+\mathbf{s})}\left(\frac{\pi^N}{det(D)}\right)^{3/2}\right) \tag{21}$$

The second part is a bit trickier and requires some explanation. We can see that the differential will yield two terms. Let us consider the term $\frac{\partial}{\partial \mathbf{s}} FR\mathbf{s}$. We recall that each entry in $\mathbf{s}$ is a shift vector, $\vec{s_i}$. As such, we can write.

$$FR\mathbf{s} = \begin{bmatrix}(FR)_{11}\vec{s_1} + ... + (FR)_{1n}\vec{s_n} & (FR)_{21}\vec{s_1} + ... + (FR)_{2n}\vec{s_n} & ... & (FR)_{n1}\vec{s_1} + ... + (FR)_{nn}\vec{s_n}\end{bmatrix}^T \tag{22}$$

Now, the derivative can be written as.

$$\frac{\partial}{\partial \mathbf{s}} = \begin{bmatrix}\frac{\partial}{\partial \vec{x_1}} & \frac{\partial}{\partial \vec{x_2}} & ... & \frac{\partial}{\partial \vec{x_n}}\end{bmatrix} \tag{23}$$

As such, when multiplying the vectors together, we get.

$$\frac{\partial}{\partial \mathbf{s}} = \left((FR)_{11} + (FR)_{22} + ... + (FR)_{nn}\right)\mathbb{1}_3 = 3Trace(FR) \tag{24}$$

[2]

The second term, where we differentiate the exponential function is the same as before. Hence, we end up with.

$$\left(\frac{\partial}{\partial \mathbf{s}} F \frac{\partial}{\partial \mathbf{s}^T}\right)\langle g'|g\rangle = \left(\frac{3}{2}Trace(FR) + \frac{1}{4}(\mathbf{s}+\mathbf{s}')^T RFR(\mathbf{s}+\mathbf{s}'\right)\langle g'|g\rangle \tag{25}$$

[2] How do we get the last equality? Ask Dmitri.

Now, we are ready to look at the original expression, with $\hat{K} = -\frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^T}$. Taking the derivative out on either side, we get the following expression.

$$\langle g' | - \frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^T} | g \rangle = \langle g' | (\mathbf{s'}^T - 2\mathbf{r}^\mathbf{T} B) K (\mathbf{s}^T - 2\mathbf{r}^\mathbf{T} A) | g \rangle \tag{26}$$

We can now write out the terms.

$$\langle g' | (\mathbf{s'}^T - 2\mathbf{r}^\mathbf{T} B) K (\mathbf{s}^T - 2\mathbf{r}^\mathbf{T} A) | g \rangle = \left(\mathbf{s'}^T K \mathbf{s} - \mathbf{s'}^T K A R (\mathbf{s} + \mathbf{s'}) - (\mathbf{s} + \mathbf{s'})^T R B K \mathbf{s} + 4 \mathbf{r}^T B K A \mathbf{r} \right) \langle g' | g \rangle \tag{27}$$

We notice that the last term, since BKA is symmetric, is exactly equal to the expression in equation 20, the result of which we derived in equation 26. As such, we can write the final form as.

$$\langle g' | - \frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^T} | g \rangle = \left(6 Trace(BKAR) + (\mathbf{s'} - BR(\mathbf{s} + \mathbf{s'}))^T K (\mathbf{s} - AR(\mathbf{s} + \mathbf{s'})) \right) \langle g' | g \rangle \tag{28}$$

3.3 Coulomb potential

We can write a one-body central potential, $V(\vec{r_i})$ and a two-body central potential $V(\vec{r_i} - \vec{r_j})$ in a convenient form $V(w^T \mathbf{r})$. Here, w^T is a size-N column vector where the $i'th$ component is -1 while the $j'th$ component is 1. The overlap of two Gaussian functions with respect to some central potential is of the form.

$$\langle g' | f(|w^T \mathbf{r}|) | g \rangle = \langle g' | g \rangle \left(\frac{\beta}{\pi} \right)^{\frac{3}{2}} 2\pi \frac{e^{-\beta q^2}}{\beta q} \int_0^\infty r dr f(r) e^{-\beta r^2} sinh(2\beta q r) \tag{29}$$

Where $\beta = (w^T R w)^{-1}$ and $q = \frac{1}{2} w^T R (\mathbf{s'} + \mathbf{s})$. For the coulomb potential, this turns out to have a very simple form.

$$\langle g' | \frac{1}{r} | g \rangle = \frac{erf(\sqrt{\beta} q)}{q} e^{\frac{1}{4}(\mathbf{s}+\mathbf{s'})^T R (\mathbf{s}+\mathbf{s'})} \left(\frac{\pi^N}{det(D)} \right)^{\frac{3}{2}} \tag{30}$$

4 Taylor expanding the matrix elements

In order to incorporate the these matrix elements into our project, we want to expand to the elements to different orders of magnitude. This gives us an approximate model that is, hopefully, good enough to describe our phenomena while being a bit simpler. We wish to expand our matrix elements to third order at the very least. The calculations for the different orders is done below.

4.1 S-wave expansion

This is by far the simplest of the expansions. Lets us cosider the overlap as in equation 16.

4.1.1 Overlap

By Taylor expanding both sides, we get the following results. The left side reads.

$$\langle g' | g \rangle = \langle e^{-\mathbf{r}^T B \mathbf{r} + \mathbf{s'}^T \mathbf{r}} | e^{-\mathbf{r}^T A \mathbf{r} + \mathbf{s}^T \mathbf{r}} \rangle \approx \langle e^{-\mathbf{r}^T B \mathbf{r}} \left(1 + \mathbf{s'}^T \mathbf{r} + ... \right) | e^{-\mathbf{r}^T A \mathbf{r}} \left(1 + \mathbf{s}^T \mathbf{r} + ... \right) \rangle \tag{31}$$

For S-waves, we are only interested in the 1st order of magnitude. As such, we simply write.

$$\langle B | A \rangle = \langle e^{-\mathbf{r}^T B \mathbf{r}} | e^{-\mathbf{r}^T A \mathbf{r}} \rangle \tag{32}$$

Now, for the right side, we have the expansion.

$$e^{\frac{1}{4}(\mathbf{s}+\mathbf{s'})^T R (\mathbf{s}+\mathbf{s'})} \approx \left(1 + \frac{1}{4} (\mathbf{s}+\mathbf{s'})^T R (\mathbf{s}+\mathbf{s'}) + \frac{1}{32} (\mathbf{s}+\mathbf{s'})^T R (\mathbf{s}+\mathbf{s'}) (\mathbf{s}+\mathbf{s'})^T R (\mathbf{s}+\mathbf{s'}) \right) \left(\frac{\pi^N}{det(D)} \right)^{\frac{3}{2}} \tag{33}$$

The expression in equation 33 is the full taylor expansion of the overlap on the right hand side. We only need the first order term, which then reads.

$$\langle B|A\rangle = \left(\frac{\pi^N}{det(D)}\right)^{\frac{3}{2}} = M_0 \tag{34}$$

4.1.2 Kinetic energy

Just as before, we simply Taylor expand both sides. From equation 28, it is clear that while Taylor expanding and keeping terms of order 0 in s, only the first term surives.

$$\langle B| - \frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^T}|A\rangle = 6Trace(BKAR)M_0 \tag{35}$$

4.1.3 Coulomb

For the Coulomb potential, we have the full expression as in equation 30. We look at the terms that depend on **s**.

$$\frac{erf(\sqrt{\beta}q)}{\sqrt{\beta}q}\sqrt{\beta} \approx \frac{2\sqrt{\beta}}{\sqrt{\pi}}\left(1 - \frac{\beta q^2}{3} + ...\right) \tag{36}$$

I have written out the value of q in its entirety, where $\mathbf{v} = \mathbf{s} + \mathbf{s}'$. The second term we consider is the Taylor expansion of the overlap, which we discussed in equation 33. We consider a product of these where we only keep the zeroth order terms, so.

$$\langle B|\frac{1}{|\mathbf{w}^T\mathbf{r}|}|A\rangle = \frac{2\sqrt{\beta}}{\sqrt{\pi}}M_0 \tag{37}$$

4.2 P-wave expansion

We can use much of what we have already written in the section on S-waves. We now need to take the shift vectors, **s** into account. To distinguish all possible shift vectors, we label these b and a.

4.2.1 Overlap

We write the full overlap as.

$$\langle g'|g\rangle = e^{\frac{1}{4}(a+b)^T R(a+b)}M_0 \tag{38}$$

Taylor expanding this to order of ab, we get.

$$\langle bB|aA\rangle = \frac{1}{2}\left(b^T Ra\right)M_0 = M_1 \tag{39}$$

4.2.2 Kinetic

The Taylor expansion for the kinetic energy reads term wise (with $M = e^{\frac{1}{4}(a+b)^T R(a+b)}M_0$).

$$6Trace(BKAR)M \to 6Trace(BKAR)M_0 \tag{40}$$
$$b^T KaM \to b^T KaM_0 \tag{41}$$
$$(a+b)^T RBKAR(a+b)M \to a^T RBKARbM_0 + b^T RBKARaM_0 \tag{42}$$
$$-(a+b)^T RBKaM \to -b^T RBKaM_0 \tag{43}$$
$$-(a+b)^T RAKbM \to -a^T RAKbM_0 \tag{44}$$

These are all the terms for the p-wave expansion.

4.2.3 Coulomb

As before, we multiply the Taylor expansion of the potential function, equation 36, with the expansion of the overlap, equation 33, and keep only terms of order ab. The result is.

$$\langle bB|\frac{1}{|\mathbf{w}^T\mathbf{r}}|aA\rangle = 2sqrt\frac{b}{\pi}M_1 - \frac{\beta^{\frac{3}{2}}}{3\sqrt{\pi}}\left(a^T R\mathbf{w}\right)\left(b^T R\mathbf{w}\right) \tag{45}$$

4.3 D-wave expansion

Finally, for the D-waves, we follow much of the same pattern as in the P-wave expansion, only a bit more complicated.

4.3.1 Overlap

In this basis, we write the full overlap as.

$$\langle g'|g\rangle = e^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \tag{46}$$

Taylor expanding to order $abcd$ we get.

,

$$\langle (cd)B|(ab)A\rangle = \frac{1}{4}\left((a^T Rb)(c^T Rd) + (a^T Rc)(b^T Rd) + (a^T Rd)(b^T Rc)\right)M_0 = M_2 \tag{47}$$

4.3.2 Kinetic

Doing the similar expansion keeping terms of order $abcd$ only, we get the following terms.

The 6Trace(BKAR)M term

$$6Trace(BKAR)M \rightarrow 6Trace(BKAR)M_2 \tag{48}$$

The $(\mathbf{c}+\mathbf{d})^\mathbf{T}\mathbf{K}(\mathbf{a}+\mathbf{b})\mathbf{M}$ term

$$\begin{aligned}&(c+d)^T K(a+b)Me^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \rightarrow \\ &\frac{1}{2}\left[(a^T Kc)(b^T Rd) + (a^T Kd)(b^T Rc) + (b^T Kc)(a^T Rd) + (b^T Kd)(a^T Rc)\right]M_0\end{aligned} \tag{49}$$

The $-(\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d})^\mathbf{T}\mathbf{RBK}(\mathbf{a}+\mathbf{b})\mathbf{M}$ term

$$\begin{aligned}&-(a+b+c+d)RBK(a+b)e^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \rightarrow \\ &-\left[(a^T RBKb)(c^T Rd) + (b^T RBKa)(c^T Rd)\right]\frac{1}{2}M_0 \\ &-\left[(c^T RBKa)(b^T Rd) + (c^T RBKb)(a^T Rd)\right]\frac{1}{2}M_0 \\ &-\left[(d^T RBKa)(b^T Rc) + (d^T RBKb)(c^T Ra)\right]\frac{1}{2}M_0\end{aligned} \tag{50}$$

The $-(\mathbf{c}+\mathbf{d})^\mathbf{T}\mathbf{RBK}(\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d})\mathbf{M}$ term

$$\begin{aligned}&-(c+d)RBK(a+b+c+d)e^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \rightarrow \\ &-\left[(c^T KARa)(b^T Rd) + (c^T KARb)(a^T Rd) + (c^K ARd)(a^T Rb)\right]\frac{1}{2}M_0 \\ &-\left[(d^T KARa)(b^T Rc) + (d^T KARb)(a^T Rc) + (d^T KARc)(a^T Rb)\right]\frac{1}{2}M_0\end{aligned} \tag{51}$$

The $(\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d})^\mathbf{T}\mathbf{RBKAR}(\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d})\mathbf{M}$ term

$$
\begin{aligned}
&(a+b+c+d)RBKAR(a+b+c+d)e^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \rightarrow \\
&\left[(a^T RBKARb)(c^T Rd)+(a^T RBKARc)(b^T Rd)+(a^T RBKARd)(b^t Rc)\right]\frac{1}{2}M_0 \\
&+\left[(b^T RBKARa)(c^T Rd)+(b^T RBKARc)(a^T Rd)+(b^T RBKARd)(a^t Rc)\right]\frac{1}{2}M_0 \\
&+\left[(c^T RBKARa)(b^T Rd)+(c^T RBKARb)(a^T Rd)+(c^T RBKARd)(a^t Rc)\right]\frac{1}{2}M_0 \\
&+\left[(d^T RBKARa)(b^T Rc)+(d^T RBKARb)(a^T Rc)+(d^T RBKARc)(a^t Rb)\right]\frac{1}{2}M_0
\end{aligned}
\tag{52}
$$

4.3.3 Coulomb

Finally, the Coulomb potential reads

$$
\langle (cd)B|\frac{1}{|\mathbf{w}^T\mathbf{r}}|(ab)A\rangle = 2\sqrt{\frac{\beta}{\pi}}\left(1-\frac{\beta q^2}{3}+\frac{\beta^2 q^4}{10}+\dots\right)e^{\frac{1}{4}(a+b+c+d)^T R(a+b+c+d)}M_0 \tag{53}
$$

Writing out q^2 and q^4 and expanding to order $abcd$ yields the result.

$$
\begin{aligned}
&\langle (cd)B|\frac{1}{|\mathbf{w}^T\mathbf{r}}|(ab)A\rangle = 2\sqrt{\frac{\beta}{\pi}}M_2+ \\
&-\frac{2\sqrt{\beta}}{\sqrt{\pi}}\frac{\beta}{3}\frac{1}{2}\begin{bmatrix} a^T Rww^T Rbc^T Rd+ \\ a^T Rww^T Rcb^T Rd+ \\ a^T Rww^T Rdb^T Rc+ \\ b^T Rww^T Rca^T Rd+ \\ b^T Rww^T Rda^T Rc+ \\ c^T Rww^T Rda^T Rb \end{bmatrix}M_0+\frac{2\sqrt{\beta}}{\sqrt{\pi}}\beta^2\frac{1}{10}\frac{1}{2}\begin{bmatrix} a^T Rww^T Rbc^T Rww^T Rd+ \\ a^T Rww^T Rcb^T Rww^T Rd+ \\ a^T Rww^T Rdb^T Rww^T Rc \end{bmatrix}M_1
\end{aligned}
\tag{54}
$$

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