Final Report for Fall 2009

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1 Introduction

The first task for this quarter was to read the paper "Capturing the Interelectron Cusp in the Multiparticle Schrödinger Equation*" by Dr. Mohlenkamp. The paper gives possible graphical representations of electron interactions. The next task was to figure out how the equations corresponded to the graphical representations.

The first thing to note is that  represents a variable, which in our equations is denoted as $\phi_a(\gamma_a)$. Next, we denote two variables, or coordinates, being connected by a geminal as a straight line. So, if our equation has $\phi_a(\gamma_a)\phi_b(\gamma_b)w_1(|\gamma_a - \gamma_b|)$, then we graphically represent it as  . The final possibiltity is that two of our coordinates may be connected by a function that is not a geminal, then we represent this connection as a curve. If we let our function be denoted by θ_a, then $\phi_a(\gamma_a)\phi_b(\gamma_b)\theta_a(\gamma_b)$ is graphically represented as  .

2 First Proposition

The next task was to figure out how to contract  . We already had one proposition that said we could contract it to  . That representation can be contracted by the following method:

We have to compute

$$\int_a \int_b \int_m \sum_a \sum_b \sum_m \phi_a(\gamma_a)\phi_b(\gamma_b)\phi_m(\gamma_m)\theta_a(\gamma_b)\theta_b(\gamma_m)\theta_m(\gamma_a)w_1(|\gamma_b - \gamma_m|)d\gamma_m d\gamma_b d\gamma_a.$$

If we first integrate in γ_a at a cost of $\mathcal{O}(N^2M)$, we are left with

$$\int_b \int_m \sum_a \sum_b \sum_m C_{a,m}\phi_b(\gamma_b)\phi_m(\gamma_m)\theta_a(\gamma_b)\theta_b(\gamma_m)w_1(|\gamma_b - \gamma_m|)d\gamma_m d\gamma_b.$$

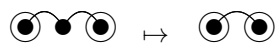
Next, we sum over a at a cost of $\mathcal{O}(N^2M)$, and are left with

$$\int_b \int_m \sum_b \sum_m F_m(\gamma_b)\phi_b(\gamma_b)\phi_m(\gamma_m)\theta_b(\gamma_m)w_1(|\gamma_b - \gamma_m|)d\gamma_m d\gamma_b.$$

which can be graphically represented as  .

We can generalize this as a new proposition.

Proposition 2.1 *We can contract*



with cost $\mathcal{O}(NM^2)$.

We have to compute

$$\int_a \int_b \int_m \sum_a \sum_b F(\gamma_a)G(\gamma_m)\phi_b(\gamma_b)\theta_b(\gamma_m)\theta_a(\gamma_b)d\gamma_m d\gamma_b d\gamma_a.$$

If we first sum over b at a cost of $\mathcal{O}(NM^2)$, we are left with

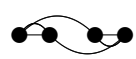
$$\int_a \int_b \int_m \sum_a F(\gamma_a)G(\gamma_m)H(\gamma_b, \gamma_m)\theta_a(\gamma_b)d\gamma_m d\gamma_b d\gamma_a.$$

Next, we integrate in γ_b at a cost of $\mathcal{O}(NM^2)$, and are left with

$$\int_a \int_m \sum_a F(\gamma_a)G(\gamma_m)J_a(\gamma_m)d\gamma_m d\gamma_a,$$

which can be graphically represented as  .

3 Second Proposition

My next task was to find out how to contract  . We have to compute

$$\int_a \int_b \int_m \int_n \sum_a \sum_b \sum_m \sum_n \phi_a(\gamma_a)\phi_b(\gamma_b)\phi_m(\gamma_m)\phi_n(\gamma_n)\theta_a(\gamma_b)\theta_b(\gamma_n)\theta_m(\gamma_a)\theta_n(\gamma_m)w_1(|\gamma_a-\gamma_b|)w_2(|\gamma_m-\gamma_n|)d\gamma_n d$$

If we first integrate in γ_a at a cost of $\mathcal{O}(N^2M_*)$, we are left with

$$\int_b \int_m \int_n \sum_a \sum_b \sum_m \sum_n F_{a,m}(\gamma_b)\phi_b(\gamma_b)\phi_m(\gamma_m)\phi_n(\gamma_n)\theta_a(\gamma_b)\theta_b(\gamma_n)\theta_n(\gamma_m)w_2(|\gamma_m-\gamma_n|)d\gamma_n d\gamma_m d\gamma_b.$$

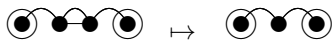
Next, we sum over a at a cost of $\mathcal{O}(N^2M)$, and are left with

$$\int_b \int_m \int_n \sum_b \sum_m \sum_n G_m(\gamma_b)\phi_b(\gamma_b)\phi_m(\gamma_m)\phi_n(\gamma_n)\theta_b(\gamma_n)\theta_n(\gamma_m)w_2(|\gamma_m-\gamma_n|)d\gamma_n d\gamma_m d\gamma_b.$$

which can be graphically represented as  which we already know how to contract.

This method can also be generalized as a new proposition.

Proposition 3.1 *We can contract*



with cost $\mathcal{O}(N^2 M_*)$.

We have to compute

$$\int_a \int_b \int_m \int_n \sum_a \sum_b \sum_m \sum_n F(\gamma_a) G(\gamma_n) \phi_b(\gamma_b) \phi_m(\gamma_m) \theta_a(\gamma_b) \theta_b(\gamma_m) \theta_m(\gamma_n) w_1(|\gamma_b - \gamma_m|) d\gamma_m d\gamma_b d\gamma_a.$$

If we first integrate in γ_b at a cost of $\mathcal{O}(N^2 M_*)$, we are left with

$$\int_a \int_m \int_n \sum_a \sum_b \sum_m \sum_n F(\gamma_a) G(\gamma_n) J_{a,b}(\gamma_m) \phi_m(\gamma_m) \theta_b(\gamma_m) \theta_m(\gamma_n) d\gamma_m d\gamma_a.$$

Next, we sum over b at a cost of $\mathcal{O}(N^2 M)$, and are left with

$$\int_a \int_m \int_n \sum_a \sum_m \sum_n F(\gamma_a) G(\gamma_n) J_a(\gamma_m) \phi_m(\gamma_m) \theta_m(\gamma_n) d\gamma_m d\gamma_a.$$

which can be graphically represented as  .

4 Conclusion

After working on determinants for the past two and a half years, switching topics was both welcoming and scary. I had finally gotten comfortable with our work on determinants and felt confident that I could help in the computations. So, in that respect, I was sad to switch topics because it would be like starting from scratch all over again. On the other hand, it was nice to branch out and start something fresh and new. The theory behind the math was difficult to grasp at first. I'm sure there are parts of it I still do not understand. The first read through the paper was difficult, and the pictures were confusing at first. However, once I was able to place parts of each picture with part of an equation, understanding the pictures and how to contract them became easy. I still cannot tell how a picture will contract just by sight. I have to write the corresponding expression down before I can tell what can be done to the graphical representation. Hopefully, working with this topic more will let me see how to contract the pictures without needing the expressions.