Ohio University - Mathematics Department

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1 Introduction

We were tasked to read a paper entitled *Capturing the Interelectron Cusp in the Multiparticle Schrödinger Equation* by Dr. M.J. Mohlenkamp (a draft). We were to understand what was written and present the material to the group we are working with.Our main task was to first understand on how we can represent equations graphical. We were then required to figure out how we could write equations from the graphical representations. The aim is to be able to figure out on how we can compute the costs and to decide which assumptions are more efficient and to consolidate the cost expressions. The computational costs depends on the number of electrons N, the cost to represent a function of γ, denoted M and the cost to perform a convolution (we will explain later) denoted M_*. We will assume that $MN > M_* > M > N$ and we will use this assumptions to decide which orders are more efficient. We were then given individual tasks dertemine the equations, most efficient way of carrying out the operations and how we can contract the given picture and come out with a proposition.

2 Case

My main task was to find out how to contract  . We need to first explain on how we can come out with an equation given a picture. We should note that a dot  represents a variable, which we will denote as $\phi_a(\gamma_a)$. If we have a picture of the form  , we can express it as $\omega_1(|\gamma_a - \gamma_b|)\phi_a(\gamma_a)\phi_b(\gamma_b)$ where the geminal $\omega_1(|\gamma_a - \gamma_b|)$ means γ_a is connected to γ_b. If we have a curve connecting two dots, for example, the picture  , we can represent it as $\phi_m(\gamma_m)\phi_n(\gamma_n)\theta_m(\gamma_n)$ where θ_m denotes our function. Lastly, if the summation index m appears in $\phi_m(\gamma_m)$ and in $\theta_m(\gamma_m)$, both of which are functions of γ_m, so it connects γ_m back to itself and we have a convolution. The picture  can be represented as

$$\int_a \int_b \int_c \int_d \sum_a \sum_b \sum_c \sum_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)\phi_a(\gamma_a)\phi_b(\gamma_b)\phi_c(\gamma_c)\phi_d(\gamma_d)\theta_a(\gamma_c)\theta_c(\gamma_a)\theta_b(\gamma_d)\theta_d(\gamma_b)d\gamma_a d\gamma_b d\gamma_c \tag{1}$$

We then sum over the index a and we get the following

$$\int_a \int_b \int_c \int_d \sum_b \sum_c \sum_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)F(\gamma_a, \gamma_c)\phi_b(\gamma_b)\phi_c(\gamma_c)\phi_d(\gamma_d)\theta_c(\gamma_a)\theta_b(\gamma_d)\theta_d(\gamma_b)d\gamma_a d\gamma_b d\gamma_c d\gamma_d \tag{2}$$

and this costs NM^2.

We then sum over the index b and we get

$$\int_a \int_b \int_c \int_d \sum_c \sum_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)F(\gamma_a, \gamma_c)K(\gamma_b, \gamma_d)\phi_c(\gamma_c)\phi_d(\gamma_d)\theta_c(\gamma_a)\theta_d(\gamma_b)d\gamma_a d\gamma_b d\gamma_c d\gamma_d \tag{3}$$

and this costs NM^2. Summing over the index c, we get

$$\int_a \int_b \int_c \int_d \sum_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)F(\gamma_a, \gamma_c)K(\gamma_b, \gamma_d)G(\gamma_c, \gamma_a)\phi_d(\gamma_d)\theta_d(\gamma_b)d\gamma_a d\gamma_b d\gamma_c d\gamma_d \tag{4}$$

and this costs NM^2. We then sum over d, we get

$$\int_a \int_b \int_c \int_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)F(\gamma_a, \gamma_c)K(\gamma_b, \gamma_d)G(\gamma_c, \gamma_a)R(\gamma_b, \gamma_d)d\gamma_a d\gamma_b d\gamma_c d\gamma_d \quad (5)$$

and this costs NM^2.

Combining $F(\gamma_a, \gamma_c)$ and $G(\gamma_c, \gamma_a)$, we get $H(\gamma_a, \gamma_c)$ and this costs M^2. When we combine $K(\gamma_b, \gamma_d)$ and $R(\gamma_b, \gamma_d)$, we get $P(\gamma_b, \gamma_d)$ and the cost is M^2. Thus equation (5) can be written as

$$\int_a \int_b \int_c \int_d \omega_1(|\gamma_a - \gamma_b|)\omega_2(|\gamma_c - \gamma_d|)H(\gamma_a, \gamma_c)P(\gamma_b, \gamma_d)d\gamma_a d\gamma_b d\gamma_c d\gamma_d \quad (6)$$

We now intergrate the above equation with respect to γ_a and we get a function of γ_b and γ_c and hence we have

$$\int_b \int_c \int_d J(\gamma_b, \gamma_c)\omega_2(|\gamma_c - \gamma_d|)P(\gamma_b, \gamma_d)d\gamma_b d\gamma_c d\gamma_d \quad (7)$$

and this will cost M_*M.

We then intergrate with respect to γ_d and we get a function of γ_b and γ_c and the equation above can be written as

$$\int_b \int_c J(\gamma_b, \gamma_c)W(\gamma_b, \gamma_c)d\gamma_b d\gamma_c \quad (8)$$

and this will cost M_*M.

Since, $J(\gamma_b, \gamma_c)$ and $W(\gamma_b, \gamma_c)$ are both functions of γ_b and γ_c, we combine them and equation (8) can be written as

$$\int_b \int_c R(\gamma_b, \gamma_c)d\gamma_b d\gamma_c \quad (9)$$

and this will cost M^2. We then intergrate with respect to γ_b and equation (9) simplifies to

$$\int_c Z(\gamma_c)d\gamma_c \quad (10)$$

and this will cost M^2. Lastly, we intergrate respect to γ_c and equation (10) simplifies to X where X is a constant and this will cost M^2.

3 Conclusion

We conclude that this order of operations costs NM^2. We are still in the process of finding a propositon for this case. We will continue to look at other cases and try to contract them and find thier costs.