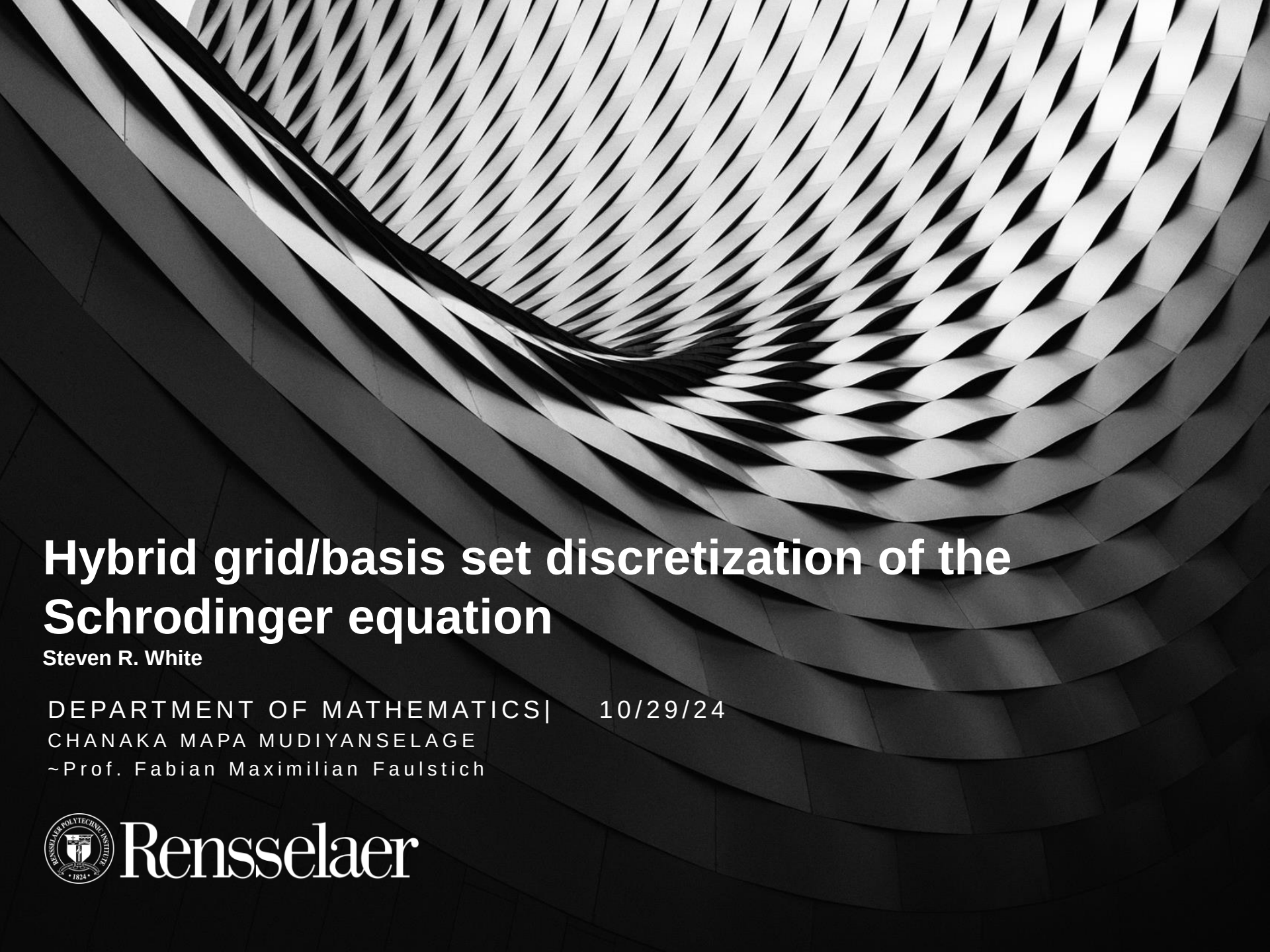

Hybrid grid/basis set discretization of the Schrodinger equation

Steven R. White

DEPARTMENT OF MATHEMATICS| 10/29/24

CHANAKA MAPA MUDIYANSELAGE

~Prof. Fabian Maximilian Faulstich

Rensselaer

Outline

- Overview
- Key details
- Previous methods
- Arrays of Gaussians
- Wavelets and Guasslets
- Diagonal Approximation

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- **Overview**
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I. Overview

- **Problem:** Solving the Schrödinger equation for large systems with complex electron-electron interactions, specifically the N^4 scaling of two-electron Coulomb integrals.
- **Objective:** Reduce computational complexity to make large electronic structure calculations feasible.
- **Significance:** Addressing this problem is crucial for advancing computational quantum chemistry and enabling simulations of larger and more complex molecular systems.

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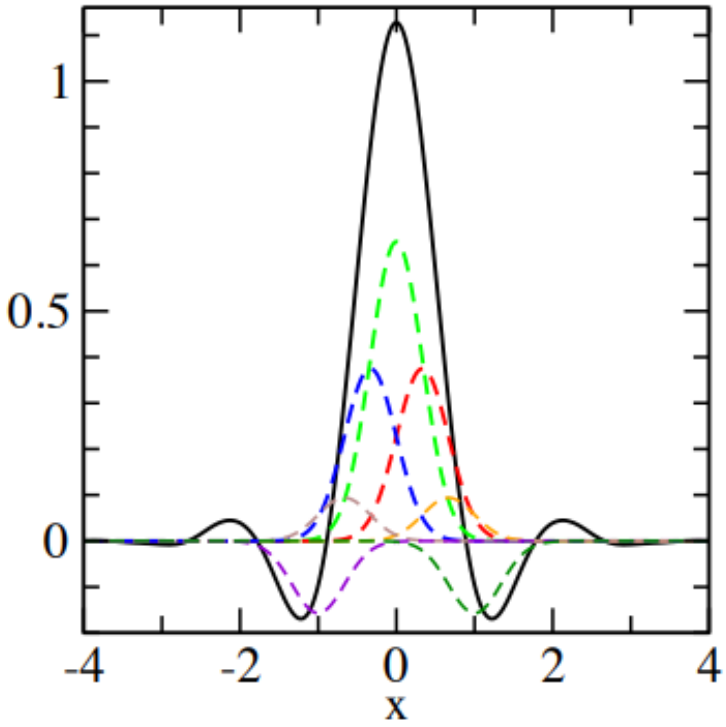
II. Key details

- **Objective**:
  - Use of Guasslets
  - Introduction of diagonal approximations
- **Motivation**:
- **Key Contributions**:
  - Development of gausslets
  - Diagonal approximations for two-electron terms
  - Tests and examples are provided in one-dimensional cases

II. Key details

Guasslets

- **What are them?**
- **How they are**
  - ❖ Orthogonal
    - Partial orthogonalization
    - Wavelet transformation
  - ❖ Smooth
  - ❖ Localized
  - ❖ Composed of Sums of Gaussians ???



Diagonal approximations for two-electron terms

- **Two-electron coulomb interaction integral**

$$V_{ijkl} = \int_{\mathbf{r}_1} \int_{\mathbf{r}_2} \frac{\phi_i(\mathbf{r}_1)\phi_l(\mathbf{r}_1)\phi_j(\mathbf{r}_2)\phi_k(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- **Scaling Complexity: From N^4 to N^2**
- **How it works?**
- **Advantages of the Diagonal Approximation**

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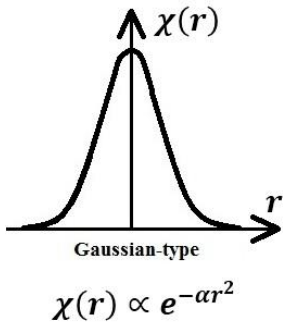
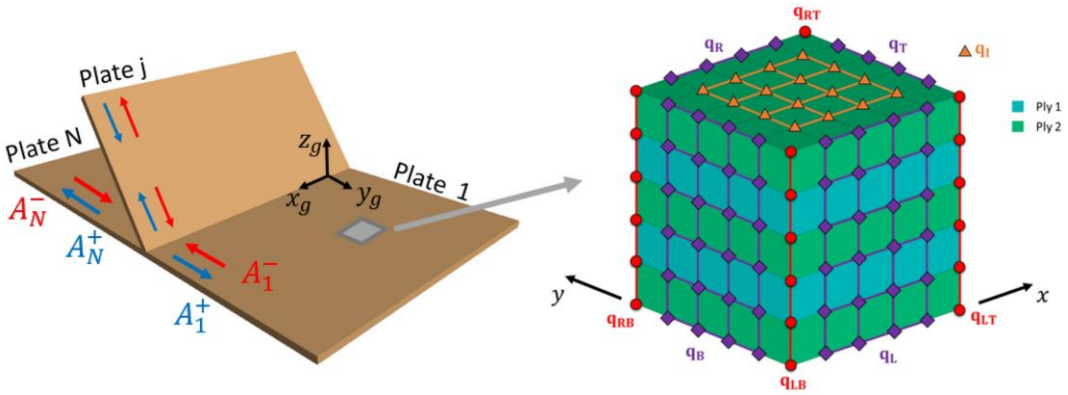
III. Previous methods, DMRG and SMDMRG

- **Gaussian-type Orbitals (GTOs)**
- **Plane Waves**
- **Finite Elements**
- **Grids**
- **Wavelets**





Method(Their approach)

- Problem Identification (Why this is important?)
- Exploring Gaussian Arrays
- Wavelet Transformation (Fixing Gaussian issues)
- Gausslets (Creating the new tool)
- Diagonal Approximation (Reducing complexity)
- Future Applications

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IV. Arrays of Gaussians

Put Gaussians in a uniform grid with identical width “w” and this Advantages with:

- **Analytic integrals**
- **Smoothness**
- **Having a product space which is greatly reduced**
- **Polynomial completeness to a higher order**

IV. Arrays of Gaussians

Having a product space which is greatly reduced

- **How?**
  - **Size of the space**
  - **No. of functions in product space**

Define a Gaussian $g_i(x)$:

$$g_i(x) = a\, exp(-(x-b)^2/2c^2)$$

- **Importance**

IV. Arrays of Gaussians

Consider a unit-spaced 1D grid, and on each integer point j put a Gaussian with width “w”

$$g_j(x) \equiv \exp[-\frac{1}{2}\frac{(x-j)^2}{w^2}]$$

To see the completeness of the set $\{g_i\}$ consider the sum;

$$C(x) = \sum_j g_j(x).$$

- **Proportionality to a constant function**

IV. Arrays of Gaussians

Let us show $C(x)$ is nearly a constant for sufficiently large w

Note: C is periodic and expand it in Fourier series(with coefficients)

$$c(k = 2\pi n)$$

Then;

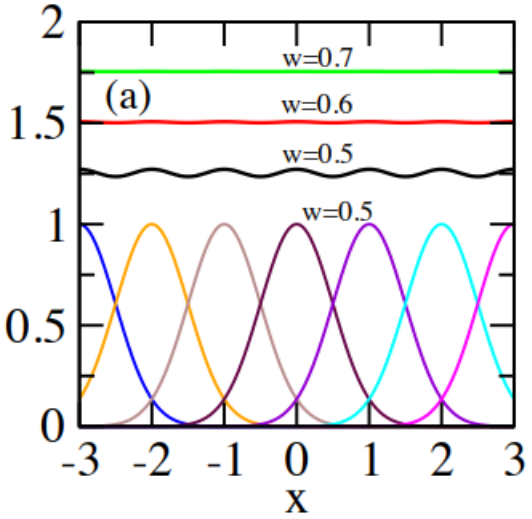
$$c(k) = \int_0^1 dx\ C(x) \exp(-ikx)$$
$$= \sqrt{2\pi} w \exp(-\frac{1}{2} k^2 w^2).$$

IV. Arrays of Gaussians

Polynomial completeness to a higher order

- **Completeness**
  - **Linear combination statement**
  - **Special property of Gaussians**

$$g_j^{(n)}(x) = P(x-j,n)g_j(x)$$
$$= \sum_{l,m} C_{l,m} j^l x^m g_j(x)$$



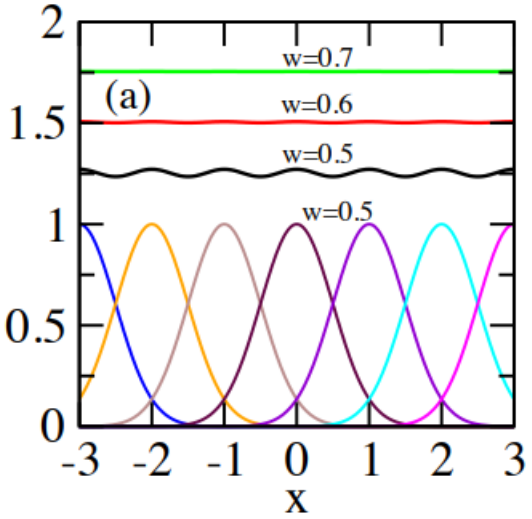
IV. Arrays of Gaussians

Polynomial completeness to a higher order

- **Induction**

$$0 \approx C^{(n)}(x) = \sum_{l,m} C_{l,m} x^m \sum_j j^l g_j(x).$$

$$C_{l,0} \sum_j j^n g_j(x) \approx - \sum_{l<n,m} C_{l,m} x^m P_l(x).$$



IV. Arrays of Gaussians

Weakness of grid of Gaussians as a basis…

Let;

Overlap matrix = $S(j,k)$

- $$S(j,k) = f(j-k) = < g_j | g_k >$$

How to have a orthogonal basis?

Let q be a transformation

$$q(j-k) \equiv S^{-1/2}(j,k)$$

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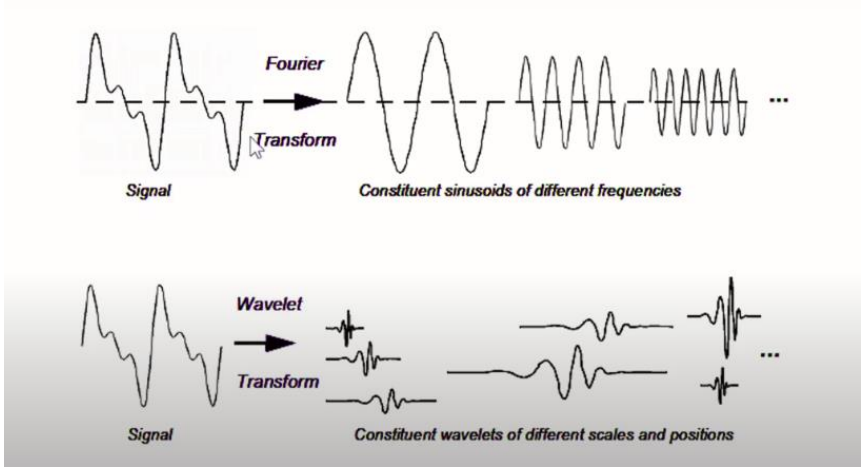
- Diagonal Approximation

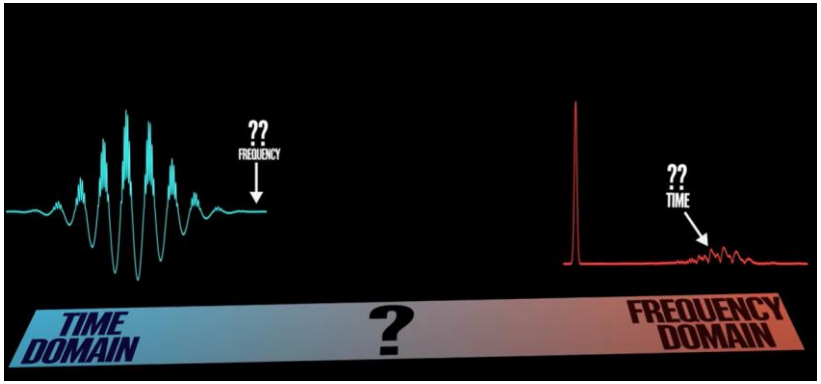
V. Ternary Wavelet Transformations

- **Side talk**
  - **Wavelets**
  - **Wavelets transformations**

Wavelets

- Importance
- Fourier Transformation
- Wavelets
- Properties

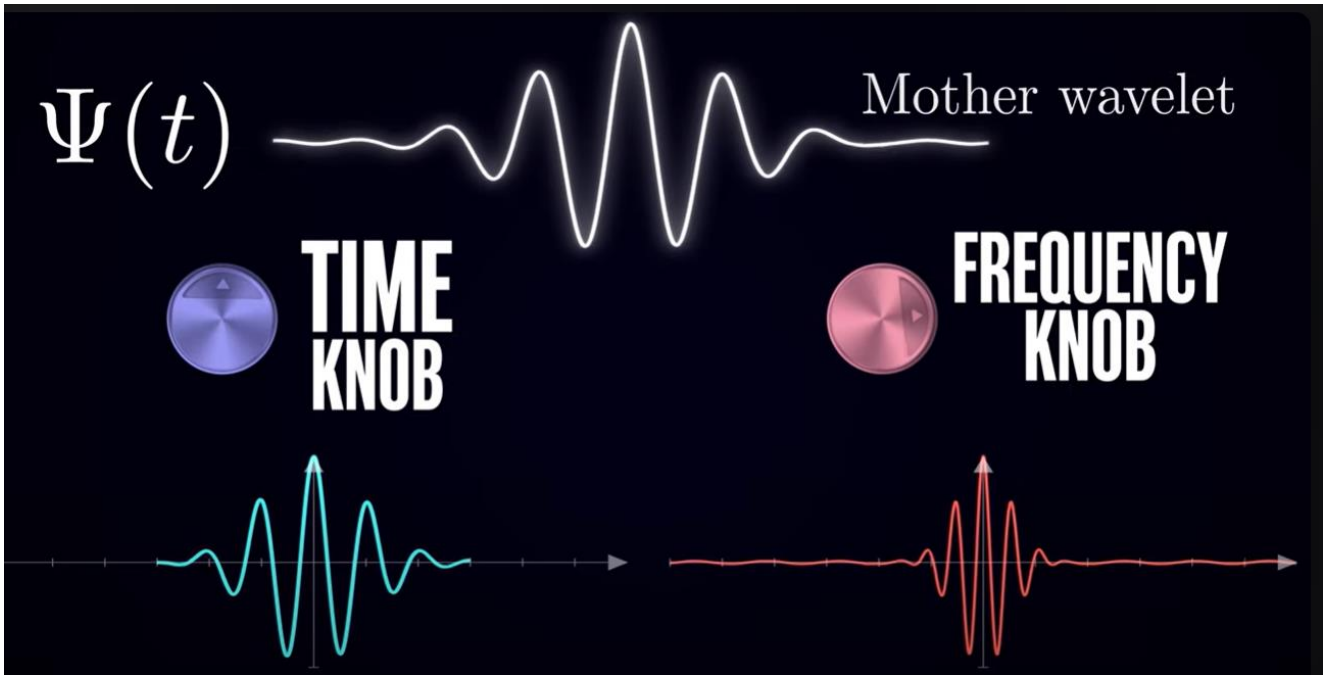




V. Ternary Wavelet Transformations

Wavelet Transformation

- Time knob and Frequency Knob
- Translation and scaling



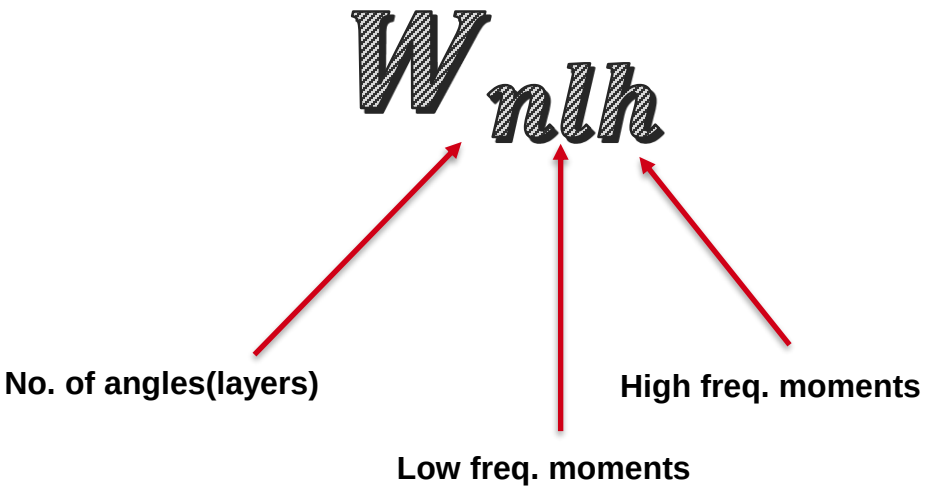
V. Ternary Wavelet Transformations

- **From there;**
  - **Statement on scaling 3 instead of 2 and why it is a better candidate?**
  - **E&W WTs**

E&W WTs

- Correspondence to quantum circuit theory
- The way they choose it is a key, why?
- W_{nlh}
- Properties

- **Applying on Gaussian arrays**
  - **Choose W_{432}, W_{652}, W_{872}, and W_{1092}**



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VI. Diagonal Approximations

- **What is the Goal?**
- **Before deal with two-electron coulomb integral first let us consider**

One-electron case.

Note: Our basis is now Gausslets

- **Let us start with $U(x)$**: One-electron potential term.

VI. Diagonal Approximations

Let $\boldsymbol{U(x)}$ acts on continues wavefunction to give another wave function

$$\phi(x) = U(x)\psi(x)$$

Consider the coefficients expansion;

$$\phi_i = \int dx\ \mathcal{G}_i(x)\phi(x) = \sum_j \psi_j \int dx\ \mathcal{G}_i(x)U(x)\mathcal{G}_j(x).$$

Matrix element U_{ij} is in the convention of non-diagonal

Lets make it diagonal…

VI. Diagonal Approximations

To put this in diagonal form; Assume each G_i integrates like a Weighted delta function, with location $\mathbf{x}_i$

$$\int dx\ \mathcal{G}_i(x) f(x) = f(x_i) w_i$$

For any smooth function $f(x)$ with;

$$w_i \equiv \int dx\ \mathcal{G}_i(x).$$

Then;

$$\phi_i = \phi(x_i) w_i = U(x_i)\psi(x_i) w_i = U(x_i)\psi_i.$$

VI. Diagonal Approximations

Now we have diagonal approximation of U

$$U_{ij} \to \delta_{ij} U(x_i).$$

Two other close diag. approximations;

- **Integral**
- **Summed**

1. Lets move to something which is not approximating things;

$$U_{ij} \to \delta_{ij} \int dx \; \mathcal{G}_i(x) U(x) / w_i.$$

VI. Diagonal Approximations

2. Assume $\{G_i\}$ can exactly represent a constant function over the range of interest;

- Then w_k is the expansion coefficient for G_k to represent the identity function;

$$1 = \sum_k w_k \mathcal{G}_k(x).$$

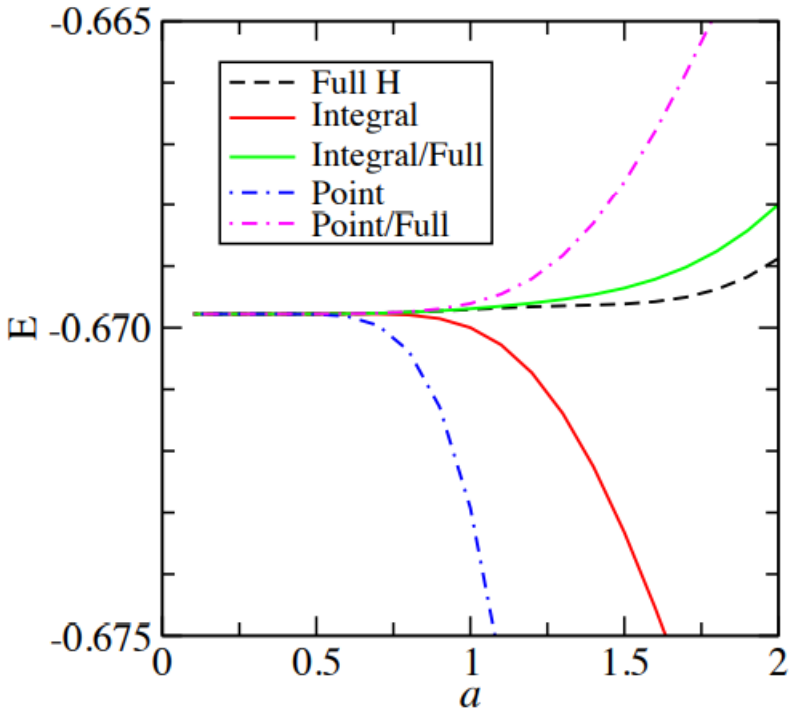
To integral diag. approximation;

$$U_{ij} \to \delta_{ij} \sum_k U_{ik} w_k / w_i.$$

VI. Diagonal Approximations

Test for diagonal approximations:

Energy solving the soft Coulomb potential



VI. Diagonal Approximations

Now we have the base. Lets move on to 2-electron case

Let us transform approximation to 2-electron case;

- **Point wise**

$$V_{ijkl} \rightarrow \delta_{il}\delta_{jk}V(x_i, x_j).$$

- **Integral**

$$V(x_i, x_j) \rightarrow \int dx\ dx'\ \mathcal{G}_i(x)V(x, x')\mathcal{G}_j(x')/(w_i w_j).$$

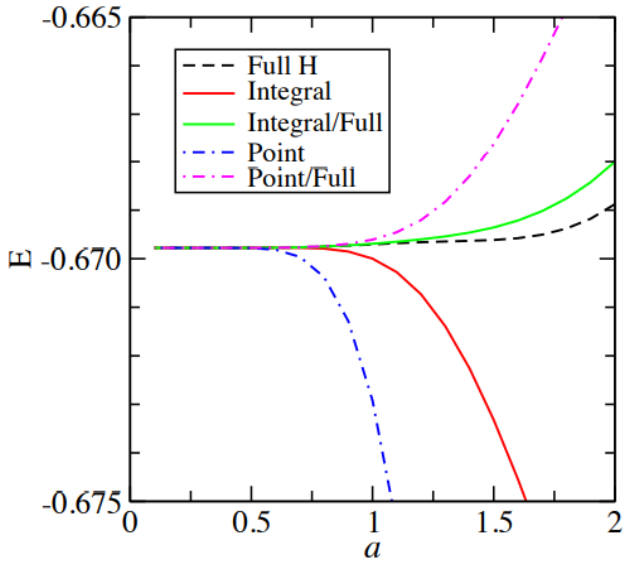
- **Summed**

$$V(x_i, x_j) \rightarrow \sum_{kl} V_{ijkl} w_l w_k/(w_i w_j)$$

VI. Diagonal Approximations

Scaling difference for 1-electron case and 2-electron case, how we approach?

Continuing from observation from the graph:- the approach…



ANY QUESTIONS!!!

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