6. Evaluation of the meanfield integrals

An important subproblem in the model reductions presented earlier (MCTDHF, TDDFT) is the evaluation of nonlocal (integral) operators, referred to as "meanfield terms" in the MCTDH(F) literature, and "Hartree terms" in TDDFT,

$$\langle \phi_1(x) | V(x,y) | \phi_2(x) \rangle \phi_3(y) = \int_{\mathbb{R}^3} \overline{\phi}_1(x) \frac{1}{|x-y|} \phi_2(x)\, dx\, \phi_3(y). \quad (1)$$

Due to the phenomenon called "correlation", many of these terms have to be evaluated, and due to the unbounded domain, quadrature is expensive. ⇒ This is the computationally most expensive part of the numerical algorithms described earlier. The problem is tackled by the technique of "hierarchical matrices" ($\mathcal{H}$-matrices [44]).

Discretize (1) on 99 on a finite-dimensional space of compactly supported functions,

$$\mathcal{B} = \{ i = i(r) \, , \, i = 1, \dots, L \},$$

$$V \approx V_{app} = RVR$$

R ... orthogonal projection onto $\mathcal{B}$.

Then, with the "<u>ket notation</u>"

$$V_{app}(r, r') = \sum_{i,j,i',j'=1}^{L} |i(r)\rangle Q^{-1}_{ii'} \tilde{V}_{i'j'} Q^{-1}_{j'j} \langle j(r')| ,$$

$$V_{app}(r, r') \phi(r') = \sum_{i,j,i',j'=1}^{L} i(r) Q^{-1}_{ii'} \tilde{V}_{i'j'} Q^{-1}_{j'j} \langle j | \phi \rangle ,$$

where

$$\tilde{V}_{ij} = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \bar{i}(r) V(r, r') j(r') \, dr \, dr' .$$

We seek to find an approximation for $\tilde{V}$ such that $\tilde{V}\phi$ is cheap to evaluate for any vector ϕ. A method which is known to scale "<u>almost linearly</u>", i.e. with computational complexity $\sim L \log L$ (L ... matrix dimension, size of basis) is provided by "<u>hierarchical matrices</u>" described in the following.

6.1 Hierarchical Matrices [44]

Let $\mathcal{I} = \{1, \dots, L\}$ be an index set. The elements of $\mathcal{I}$ are called "degrees of freedom". Associate with each index i a point $x_i \in \mathbb{R}^L$. Non-empty subsets $\sigma \subseteq \mathcal{I}$ are referred to as "clusters" and associated with a bounded domain $U\sigma$. The latter is assumed to be contained in an axis oriented "bounding box" B_σ of minimal size.

Definition: $\mathcal{T}$ is a "cluster tree" for the index set $\mathcal{I}$, if for a parameter C there holds

(1) $\mathcal{I}$ is the root of $\mathcal{T}$.

(2) Each node $\sigma \in \mathcal{T}$ is a subset of $\mathcal{I}$.

(3) If $\sigma \in \mathcal{T}$ is a "leaf", then $|\sigma| \leq C$.

(4) If $\sigma \in \mathcal{T}$ is not a leaf, then there are two unique non-empty clusters σ', σ'' satisfying $\sigma' \cup \sigma'' = \sigma$, $\sigma' \cap \sigma'' = \emptyset$, called "sons".

One way to construct a cluster tree from purely geometric information is as follows:

1) Start with $I = \mathcal{I}$
2) Split I in two by halving B_I along the longest edge and partitioning I according to the new geometric information.
3) Unless $|I| \leq C$, continue with 2).

From the cluster tree, select "admissible blocks" (σ, τ) by the criterion

$$\max(\operatorname{diam}(B_\sigma), \operatorname{diam}(B_\tau)) < \eta \operatorname{dist}(B_\sigma, B_\tau)$$

(diam ... diameter of bounding box, euclid. dist.)

Remark: Alternatively, more general admissibility criteria are also conceivable;

Define function $\operatorname{Adm}: \mathcal{P}(\mathbb{R}^d) \times \mathcal{P}(\mathbb{R}^d) \to \{\text{true}, \text{false}\}$

power set

s.t. $\begin{cases} X \subseteq X' \wedge Y \subseteq Y' \wedge \operatorname{Adm}(X', Y') = \text{true} \Rightarrow \\ \operatorname{Adm}(X, Y) = \text{true} \end{cases}$

(monotonicity).

Important example: Cluster tree from cardinality of index set.

The important feature of $\mathcal{H}$-matrices is that both storage requirements and computational complexity scale <u>almost linearly</u> with the matrix size L, i.e. $\sim L \log(L)$ [44].

Hierarchical matrices can be employed successfully for a computationally efficient approximation of the Hartree terms appearing for example in MCTDHF or TDDFT computations,

$$\langle \phi_1(x) | \frac{1}{|x-y|} | \phi_2(x) \rangle \phi_3(y) =$$

$$= \int \frac{1}{|x-y|} \overline{\phi_1(x)}\, \phi_2(x)\, dx\, \phi_3(y).$$

These nonlocal (integral) operators constitute the computational bottleneck of these methods.

A procedure based on discretization by finite elements and low rank approximation is described and analyzed in

http://www.othmar-koch.org/slides_hm.pdf.