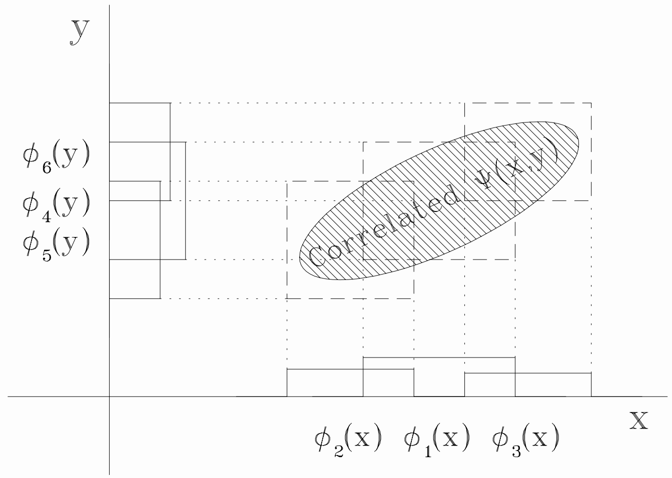
Evaluation of the Hartree terms

Evaluation of $\overline{V}_{l,k} = \langle \psi_l | V | \psi_k \rangle$:

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

Nonlocality in space, ‘correlation’:
Numerical evaluation — computational bottleneck!



From: Caillat et al. 2005.

Discretization

Choose basis functions $|i\rangle = i(x)$ defined on subgrid of spatial grid, $i = 1, \dots L$.

$Q_{i,j} := \langle i|j\rangle$ . . . symmetric, nonsingular

Projection $R := \sum_{i,j=1}^{L} |i\rangle (Q^{-1})_{i,j} \langle j|$

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

$$\tilde{V}_{j,j'} = \int\int \frac{1}{|x-y|} j(x) j'(y)\, dy\, dx.$$

Discretization (2)

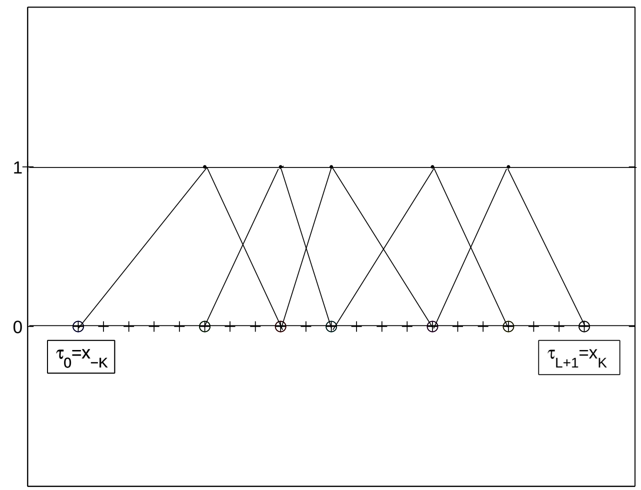
Consider conforming (H^1) finite elements ('FE'), polynomials of degree $\leq m-1$:

- Suitable subdivision $\{\mathcal{T}_j : \; j = 1, \dots, N\}$ of domain (tetrahedra, cubes,. . .)
- $\mathrm{supp}(|i\rangle) = \mathcal{T}_{j(i)}$
- Define suitable interpolation nodes τ_{j_k} in $\mathcal{T}_j$
- $\{|i\rangle\}$ . . . nodal basis,
  $i(\tau_{j_k(i)}) = 1, \; i(\tau_{j_k}) = 0$ otherwise

Discretization (3)

Example: 1D linear FE.

Nodal basis: ‘hat functions’



Quasi-uniform mesh:

$$\tilde{\kappa} h \leq \tau_{i+1} - \tau_i \leq \kappa h, \; i = 0, \dots, L, \quad h = x_{j+1} - x_j.$$

Discretization Error

Recall: $R \ldots$ orthog. proj. to FE space, $V_{\text{app}} = RVR$.

$$\begin{aligned}
&\|\langle\phi_1|V - V_{\text{app}}|\phi_2\rangle\phi_3\|_{L^2} \\
&\quad \le \|\langle\phi_1|V - V_{\text{app}}|\phi_2\rangle\|_{L^\infty}\,\|\phi_3\|_{L^2} \\
&\quad \le \|\langle\phi_1|V|\phi_2 - R\phi_2\rangle\|_{L^\infty} + \|\langle\phi_1 - R\phi_1|V|R\phi_2\rangle\|_{L^\infty}\,\|\phi_3\|_{L^2} \\
&\quad \le \text{const.}(\|\phi_1\|_{H^1}\|\phi_2 - R\phi_2\|_{L^2} + \|\phi_1 - R\phi_1\|_{L^2}\|R\phi_2\|_{H^1})\|\phi_3\|_{L^2}
\end{aligned}$$

(Hardy's inequality).

$\|\phi - R\phi\|_{L^2} \le$ interpolation error $= O(h^m)$ for $\phi \in H^m$

$\|R\phi\|_{H^1} = O(1/h)$ for $\phi \in L^2$

$\Longrightarrow$ discretization error $= O(h^{m-1})$ for $\phi_i, \phi_j \in H^m$

Global Low Rank Approximation

Let

$$S_{i,j} := \int i(x)g(x)j(x)\,dx, \quad g > 0.$$

S ... symmetric, positive definite

Consider generalized eigenvalue problem

$$\tilde{V}u = \lambda S u.$$

Cholesky

$$S = \tilde{Q}^T \tilde{Q}, \quad \tilde{u} := \tilde{Q}u$$

$\Rightarrow$ exists orthogonal basis of eigenvectors $\tilde{U}$ of

$$(\tilde{Q}^T)^{-1}\tilde{V}\tilde{Q}^{-1}\tilde{u} = \lambda\tilde{u}.$$

Balanced SVD

$\hat{U} := S\tilde{Q}^{-1}\tilde{U} \Rightarrow$

$\tilde{V} = \hat{U}\Lambda\hat{U}^T, \quad \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_L)$

$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_L > 0, \quad \lambda_i < \varepsilon$ for $i > M \rightsquigarrow$

$$\begin{aligned} V_{\mathrm{app}} &\approx \sum_{i,j=1}^{L} |i\rangle \sum_{\mu=1}^{M} [Q^{-1}\hat{U}]_{i,\mu} \lambda_\mu [\hat{U}^T Q^{-1}]_{\mu,j} \langle j| \\ &= \sum_{\mu=1}^{M} P_\mu(x) P_\mu(y). \end{aligned}$$

Approximation Error

Approximation error

$$\leq \text{const.}\varepsilon h^2 L \|Q^{-1}\hat{U}\|_2^2 \leq \text{const.}\varepsilon h^2 L \|Q^{-1}\|_2^2 \|S\|_2 \leq \text{const.}\varepsilon$$

$$Q = O(h) \begin{pmatrix} 1 & 1/2 & & & \\ 1/4 & 1 & 1/4 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \end{pmatrix},$$

$\|Q^{-1}\|_2 = O(1/h)$,

$\|S\|_2 = O(h)$.

Hierarchical Matrices

- $\mathcal{H}$-matrices replace the global low rank approximation by 'local' approximations of matrix subblocks.
- The index set $\mathcal{I}$ is endowed with a tree structure — recursive splitting into subsets; based on geometrical interpretation, or on cardinality, ...
- Admissible subsets of $\mathcal{I} \times \mathcal{I}$ are defined: Admissibility reflects smoothness of $\frac{1}{|x-y|}$ for $x \neq y$ $\Rightarrow$ possibility of low rank approximation of corresponding subblock of mass matrix.
- Both storage requirements for and standard matrix operations with a hierarchical matrix $A_{\mathcal{H}} \in \mathbb{R}^{N \times N}$ scale *almost linearly*, that is $\sim N \log(N)$.

Approximation Result

Theorem: Let a matrix $A \in \mathbb{R}^{N \times N}$ be approximated by a hierarchical matrix $A_{\mathcal{H}}$, where on each admissible block $A_{\mathcal{J} \times \mathcal{K}}$,

$$\|A_{\mathcal{J} \times \mathcal{K}} - A_{\mathcal{H}, \mathcal{J} \times \mathcal{K}}\|_2 \leq \varepsilon$$

holds with an error margin ε which can be freely chosen. Then, the spectral norm of the approximation error satisfies

$$\|A - A_{\mathcal{H}}\|_2 \leq \mathrm{const.} \ln(N) \varepsilon.$$

Proof: Hackbusch 2008.

Hartree Terms

- On each admissible subblock, compute truncated SVD of

$$(\tilde{Q}^T)^{-1}_{\mathcal{I}\times\mathcal{I}}\tilde{V}_{\mathcal{I}\times\mathcal{J}}\tilde{Q}^{-1}_{\mathcal{J}\times J}$$

to compute low rank approximation with error ε.

- By the approximation result,

$$\tilde{V}-\tilde{V}_{\mathcal{H},\varepsilon}=\hat{U}\Lambda\hat{U}^T,$$

$\hat{U}$ unitary, $\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_L)$, $\lambda_j=|\ln(N)|O(\varepsilon h)$.

- Approximation error $\leq \mathrm{const.}|\ln(N)|\varepsilon.$
- Significant increase in performance.
- Also applicable to Hartree terms in TDDFT computations!

Test Results

Test results indicate significant gain in performance!

- Test runs for the helium atom (with laser pulse).
- MCTDHF with $N = 4,\ f = 2$, $t \in [-1, -0.9]$ with 110321 steps.
- Spatial discretization by 192×96 quadratic finite elements, cylindrical coordinates.
- $\mathcal{H}$-matrices with accuracy ε, minimal blocksize 10.

ε	time global	time $\mathcal{H}$	energy global	energy $\mathcal{H}$
1e−4	475418 sec.	407808 sec.	-2.87843584	-2.87842838
1e−5	627251 sec.	471203 sec.	-2.87831975	-2.87831817
1e−6	981078 sec.	590412 sec.	-2.87831766	-2.87831758