h-P discontinuous Galerkin finite element method for electronic structure calculations

Carlo Marcati
joint work with Yvon Maday

Laboratoire Jacques-Louis Lions, UPMC, France

Advanced numerical methods: recent developments, analysis, and applications
IHP quarter on Numerical Methods for PDEs
Paris, France

h-P discontinuous finite elements for electronic structure calculations

We combine results from

- Numerical approximation of elliptic problems in non smooth domains
- Approximation of non linear eigenvalue problems

and apply them to the models used in quantum chemistry.

Outline of the presentation:

1. Motivation: models for electronic structure calculations
2. Analysis on a model problem: convergence, regularity
3. Asymptotics of the solution and design of an optimal h-P space from a priori estimates.

h-P discontinuous finite elements for electronic structure calculations

We combine results from

- Numerical approximation of elliptic problems in non smooth domains
- Approximation of non linear eigenvalue problems

and apply them to the models used in quantum chemistry.

Outline of the presentation:

1. Motivation: models for electronic structure calculations
2. Analysis on a model problem: convergence, regularity
3. Asymptotics of the solution and design of an optimal h-P space from a priori estimates.

h-P discontinuous finite elements for electronic structure calculations

We combine results from

- Numerical approximation of elliptic problems in non smooth domains
- Approximation of non linear eigenvalue problems

and apply them to the models used in quantum chemistry.

Outline of the presentation:

1. Motivation: models for electronic structure calculations
2. Analysis on a model problem: convergence, regularity
3. Asymptotics of the solution and design of an optimal h-P space from a priori estimates.

h-P discontinuous finite elements for electronic structure calculations

We combine results from

- Numerical approximation of elliptic problems in non smooth domains
- Approximation of non linear eigenvalue problems

and apply them to the models used in quantum chemistry.

Outline of the presentation:

1. Motivation: models for electronic structure calculations
2. Analysis on a model problem: convergence, regularity
3. Asymptotics of the solution and design of an optimal h-P space from a priori estimates.

Motivation: the Schrödinger equation

Ground, stationary state of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Ψ is a function of $1 + 3(N + M)$ variables (N electrons, M nuclei).

Born-Oppenheimer approximation: $3(N + M)$ to $3N$

Full-electron: the potential V has a singularity at the nuclear positions

Non linear models for electron exchange and correlation: from $3N$ to 3. For example,

- Hartree-Fock (and post Hartree-Fock) methods,
- methods based on density functional theory.

Motivation: the Schrödinger equation

Ground, stationary state of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Ψ is a function of $1 + 3(N + M)$ variables (N electrons, M nuclei).

Born-Oppenheimer approximation: $3(N + M)$ to $3N$

Full-electron: the potential V has a singularity at the nuclear positions

Non linear models for electron exchange and correlation: from $3N$ to 3. For example,

- Hartree-Fock (and post Hartree-Fock) methods,
- methods based on density functional theory.

Motivation: the Schrödinger equation

Ground, stationary state of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Ψ is a function of $1 + 3(N + M)$ variables (N electrons, M nuclei).

Born-Oppenheimer approximation: $3(N + M)$ to $3N$

Full-electron: the potential V has a singularity at the nuclear positions

Non linear models for electron exchange and correlation: from $3N$ to 3. For example,

- Hartree-Fock (and post Hartree-Fock) methods,
- methods based on density functional theory.

Motivation: the Schrödinger equation

Ground, stationary state of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Ψ is a function of $1 + 3(N + M)$ variables (N electrons, M nuclei).

Born-Oppenheimer approximation: $3(N + M)$ to $3N$

Full-electron: the potential V has a singularity at the nuclear positions

Non linear models for electron exchange and correlation: from $3N$ to 3. For example,

- Hartree-Fock (and post Hartree-Fock) methods,
- methods based on density functional theory.

Motivation: the Hartree-Fock approximation

Hartree-Fock: $\mathcal{F}$ the self adjoint operator

$$\mathcal{F}\psi = -\frac{1}{2}\Delta\psi + V\psi + \left(\rho_\Phi \star \frac{1}{|x|}\right)\psi - \int_{\mathbb{R}^3} \frac{\tau_\Phi(x,y)}{|x-y|}\psi(y)dy.$$

of the eigenvalue problem

$$\mathcal{F}\varphi_i = \varepsilon_i\varphi_i \qquad i = 1, \dots, N$$

[Flad et al., 2008] showed that around the nuclei the solutions belong to (a subset of) the countably normed spaces

$$\mathcal{K}^\infty_\gamma(\Omega) = \left\{u \in \mathcal{D}'(\Omega) : \; r_c^{|\alpha|-\gamma}\partial^\alpha u \in L^2(\Omega),\; |\alpha| = s,\; \forall s \in \mathbb{N}\right\}.$$

with r_c giving the distance to the nearest nucleus.

Classical finite element and spectral approximations

The eigenfunctions are thus not regular in the Sobolev spaces $H^k(\Omega) = W^{k,2}(\Omega)$.

The convergence rate of "classical" finite element and spectral methods is bounded by the regularity of the solution in Sobolev spaces.

Classical finite element and spectral methods

If $u \in H^{s+1}(\Omega)$, the following approximation results hold:

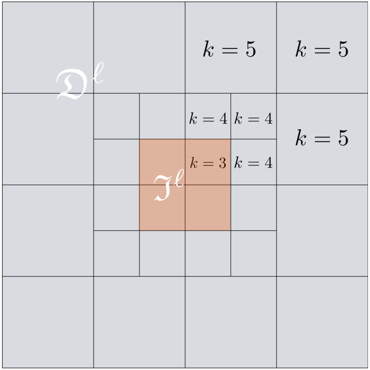
- for finite element methods of degree r and element size h:

$$\|u - u_h\|_{H^1(\Omega)} \lesssim h^{\min(r,s)} |u|_{H^{r+1}(\Omega)};$$

- for spectral methods of degree p:

$$\|u - u_\delta\|_{H^1(\Omega)} \lesssim p^{-s} \|u\|_{H^{s+1}(\Omega)};$$

The discontinuous h-P finite elements method



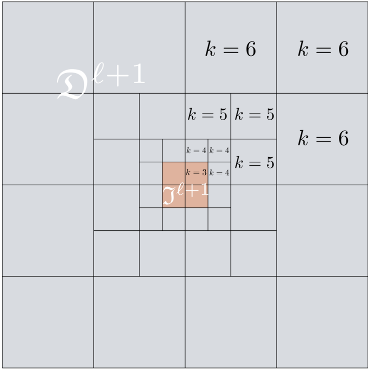
Finite element space:

$$X_\delta = \{v \in L^2(\Omega) : v_{|S} \in \mathbb{Q}_{k_S}(S), \forall S \in \mathcal{T}\}.$$

The mesh is geometrically refined by a factor σ towards the center (where the singularity lies), while the polynomial degree usually decreases with a slope s.

Graded mesh, uniform slope:
At the refinement step ℓ, the elements in $\mathcal{I}^\ell$ will have edges of length σ^ℓ, while in the outermost element the polynomial degree will be $k_0 + \lfloor s\ell \rfloor$

The discontinuous h-P finite elements method



Finite element space:

$$X_\delta = \{v \in L^2(\Omega) : v_{|S} \in \mathbb{Q}_{k_S}(S), \forall S \in \mathcal{T}\}.$$

The mesh is geometrically refined by a factor σ towards the center (where the singularity lies), while the polynomial degree usually decreases with a slope s.

Graded mesh, uniform slope:
At the refinement step ℓ, the elements in $\mathcal{I}^\ell$ will have edges of length σ^ℓ, while in the outermost element the polynomial degree will be $k_0 + \lfloor s\ell \rfloor$

The discontinuous approach

The bilinear form associated with the Laplace operator

$$d(u,v) = (\nabla u, \nabla v)_\Omega,$$

is replaced by

$$d_\delta(u_\delta, v_\delta) = \sum_{S\in\mathcal{T}} (\nabla u_\delta, \nabla v_\delta)_S - \underbrace{\sum_{e\in\mathcal{E}} (\{\!\{\nabla u_\delta\}\!\}, [\![v_\delta]\!])_e}_{\text{consistency}} - \underbrace{\sum_{e\in\mathcal{E}} (\{\!\{\nabla v_\delta\}\!\}, [\![u_\delta]\!])_e}_{\text{adjoint consistency}}$$

$$+ \underbrace{\sum_{e\in\mathcal{E}} \alpha \frac{k_e^2}{h_e} ([\![u_\delta]\!], [\![v_\delta]\!])_e}_{\text{stability}} .$$

- The set $\mathcal{E}$ is the set of all $d-1$ dimensional inter-element boundaries
- $\{\!\{\cdot\}\!\}$ and $[\![\cdot]\!]$ are average and jump operators respectively.

Approximation results in the discontinuous h-P space

Mesh dependent norms:

$$\|u\|_{\mathrm{DG}}^2 = \sum_{S\in\mathcal{T}} \|u\|_{H^1(S)}^2 + \sum_{e\in\mathcal{E}} \frac{k_e^2}{h_e} \|[\![u]\!]\|_e^2$$

$$|\!|\!|u|\!|\!|_{\mathrm{DG}}^2 = \|u\|_{\mathrm{DG}}^2 + \sum_{K\in\mathfrak{D}^\ell} \sum_{e\in\mathcal{E}_K} \frac{h_e}{k_e^2} \|\nabla u\|_e^2 + \sum_{K\in\mathfrak{I}^\ell} \sum_{e\in\mathcal{E}_K} k_e^2 |e|^{-1} h_e \|\nabla u\|_{L^1(e)}^2$$

"Weighted analytic" space

$$\mathcal{A}_\gamma = \left\{ v \in X,\ |v|_{\mathcal{K}_\gamma^k} \leq C A^k k! \right\}$$

with $|v|_{\mathcal{K}_\gamma^k}^2 = \sum_{|\alpha|=k} \|r_c^{k-\gamma} \partial^\alpha v\|^2$, r_c distance from the nearest singularity in $\mathcal{C}$.

Exponentially convergent approximation

[Schötzau et al., 2013] showed that for a function $u \in \mathcal{A}_\gamma$ and a space X_δ with N degrees of freedom,

$$\inf_{v_\delta \in X_\delta} |\!|\!|u - v_\delta|\!|\!|_{\mathrm{DG}} \lesssim \exp(-bN^{1/(d+1)}).$$

The Gross-Pitaevskii (aka nonlinear Schrödinger) equation

In a periodic domain $\Omega = (\mathbb{R}/L)^d$ we consider the problem of minimizing the energy

$$E(v) = \underbrace{\frac{1}{2}\int_\Omega |\nabla v|^2}_{d(v,v)} + \frac{1}{2}\int_\Omega V v^2 + \frac{1}{2}\int_\Omega F(v^2)$$

under the constraint $\|v\| = 1$. The unique minimizer u satisfies for $\lambda \in \mathbb{R}$

$$_{X'}\langle A^u u - \lambda u, v\rangle_X = 0 \quad \forall v \in X$$

where

$$_{X'}\langle A^u v, w\rangle_X = d(u,v) + \int_\Omega V uv + \int_\Omega F'(u^2)vw.$$

The discrete counterparts are

$$\langle A_\delta^{u_\delta} u_\delta - \lambda_\delta u_\delta, v_\delta\rangle = 0 \quad \forall v_\delta \in X_\delta$$

$$\langle A_\delta^{u_\delta} v_\delta, w_\delta\rangle = d_\delta(v_\delta, w_\delta) + \int_\Omega V v_\delta w_\delta + \int_\Omega F'(u_\delta^2) v_\delta w_\delta.$$

Non homogeneous weighted Sobolev spaces

Non homogeneous weighted Sobolev space $\mathcal{J}^s_\gamma(\Omega)$

Normed by

$$\|u\|^2_{\mathcal{J}^s_\gamma(\Omega)} = \sum_{|\alpha|\leq s} \|r^{s-\gamma}\partial^\alpha u\|^2_{L^2(\Omega)}$$

equivalent to the "step-weighted" norm: $\rho \in (-d/2, s-\gamma]$, $s > \gamma - d/2$

$$\|u\|^2_{\mathcal{J}^s_\gamma(\Omega)} = \sum_{|\alpha|\leq s} \|r^{\max(|\alpha|-\gamma,\rho)}\partial^\alpha u\|^2_{L^2(\Omega)}$$

In our case,

$$\|u\|^2_{\mathcal{J}^s_\gamma(\Omega)} = \|u\|^2_{H^1(\Omega)} + \sum_{2\leq|\alpha|\leq s} \|r^{\max(|\alpha|-\gamma,\rho)}\partial^\alpha u\|^2_{L^2(\Omega)}$$

such that $J^{m+1}_\gamma(\Omega) \subset J^m_\gamma(\Omega)$ and

$$\mathcal{B}_\gamma(\Omega, \mathcal{C}) = \left\{ v \in H^1(\Omega),\ |u|_{\mathcal{K}^k_\gamma} \leq C A^k k! \text{ for } k \geq 2 \right\}.$$

Regularity

For the nonlinear Schrödinger equation:

Regularity of the solution

If $u \in X$ is the solution to the eigenvalue problem for a potential $V \in \mathcal{A}^{\infty}_{-2+\varepsilon}(\Omega, \mathcal{C})$ and under some hypotheses on the nonlinear term,

$$u \in \mathcal{B}_{\gamma}(\Omega, \mathcal{C}),$$

with $\gamma = 3/2 + \varepsilon$.

Note that singular potentials are allowed, and those give rise to solutions with cusp-like singularities.

Sketch of the proof:

- $\|r^{|\alpha|+2}\partial^{\alpha+\beta}u\| \leq \|r^{|\alpha|+2}\partial^{\alpha}\Delta u\| + \|\left[r^{|\alpha|+2}, \Delta\right]\partial^{\alpha}u\| + \|\left[\partial^{\beta}, r^{|\alpha|+2}\right]\partial^{\alpha}u\|$, with $|\beta| = 2$.
- Equation on the first term, then bounds on the three terms.
- Decomposition in singular part and regular part for the nonlinear term. □

Regularity

For the nonlinear Schrödinger equation:

Regularity of the solution

If $u \in X$ is the solution to the eigenvalue problem for a potential $V \in \mathcal{A}^{\infty}_{-2+\varepsilon}(\Omega, \mathcal{C})$ and under some hypotheses on the nonlinear term,

$$u \in \mathcal{B}_{\gamma}(\Omega, \mathcal{C}),$$

with $\gamma = 3/2 + \varepsilon$.

Note that singular potentials are allowed, and those give rise to solutions with cusp-like singularities.

Sketch of the proof:

- $\|r^{|\alpha|+2}\partial^{\alpha+\beta}u\| \leq \|r^{|\alpha|+2}\partial^{\alpha}\Delta u\| + \|\left[r^{|\alpha|+2}, \Delta\right]\partial^{\alpha}u\| + \|\left[\partial^{\beta}, r^{|\alpha|+2}\right]\partial^{\alpha}u\|$, with $|\beta| = 2$.
- Equation on the first term, then bounds on the three terms.
- Decomposition in singular part and regular part for the nonlinear term. □

Convergence

Convergence of the approximation

Let (u, λ) be the solution to the eigenvalue problem and let $(u_\delta, \lambda_\delta)$ be the h-P discontinuous approximations. Then, under proper hypotheses on F,

$$\|u - u_\delta\|_{\mathrm{DG}} \leq C \inf_{v_\delta \in X_\delta} \|u - v_\delta\|_{\mathrm{DG}}$$

and

$$|\lambda_\delta - \lambda| \leq C \left(\|u - u_\delta\|_{\mathrm{DG}}^2 + \|u - u_\delta\|_{L^2} \right).$$

Similar results in [Cancès et al., 2010] in the simpler case of a continuous approximation.

In this case the approximation is not conforming, i.e., $X_\delta \not\subset X$, thus $\lambda_\delta \not\geq \lambda$.

Convergence

Convergence of the approximation

Let (u, λ) be the solution to the eigenvalue problem and let $(u_\delta, \lambda_\delta)$ be the h-P discontinuous approximations. Then, under proper hypotheses on F,

$$\|u - u_\delta\|_{\mathrm{DG}} \leq C \inf_{v_\delta \in X_\delta} \|\|u - v_\delta\|\|_{\mathrm{DG}}$$

and

$$|\lambda_\delta - \lambda| \leq C \left(\|u - u_\delta\|_{\mathrm{DG}}^2 + \|u - u_\delta\|_{L^2} \right).$$

Similar results in [Cancès et al., 2010] in the simpler case of a continuous approximation.

In this case the approximation is not conforming, i.e., $X_\delta \not\subset X$, thus $\lambda_\delta \not\geq \lambda$.

Sketch of the proof: "coercivity", "stability" and convergence

To prove the convergence result, we introduce the solution $(u_\delta^*, \lambda_\delta^*)$ to the linear problem

$$\langle A_\delta^u u_\delta^* - \lambda_\delta^* u_\delta^*, v_\delta \rangle = 0 \quad \forall v_\delta \in X_\delta.$$

The convergence of these eigenvalue and eigenspace towards the exact one has been proven in [Antonietti et al., 2006]. It is then possible to prove the inequalities

$$\begin{aligned}
\langle (A_\delta^u - \lambda_\delta^*) v_\delta, v_\delta \rangle &\geq 0 && \forall v_\delta \in X_\delta \\
|\langle (A_\delta^u - \lambda_\delta^*) v, v_\delta \rangle| &\lesssim \|v\|_{\mathrm{DG}} \|v_\delta\|_{\mathrm{DG}} && \forall v \in X(\delta), v_\delta \in X_\delta \\
\langle (A_\delta^u - \lambda_\delta^*) (u_\delta - u_\delta^*), (u_\delta - u_\delta^*) \rangle &\gtrsim \|u_\delta - u_\delta^*\|_{\mathrm{DG}}^2 && \\
\langle (E_\delta''(u) - \lambda_\delta^*) v_\delta, v_\delta \rangle &\gtrsim \|v_\delta\|_{\mathrm{DG}}^2 && \forall v_\delta \in X_\delta \\
|\langle (E_\delta''(u) - \lambda_\delta^*) v, v_\delta \rangle| &\lesssim \|v\|_{\mathrm{DG}} \|v_\delta\|_{\mathrm{DG}} && \forall v \in X(\delta), v_\delta \in X_\delta.
\end{aligned}$$

which then lead to the proof of convergence.

Sketch of the proof: "coercivity", "stability" and convergence

To prove the convergence result, we introduce the solution $(u_\delta^*, \lambda_\delta^*)$ to the linear problem

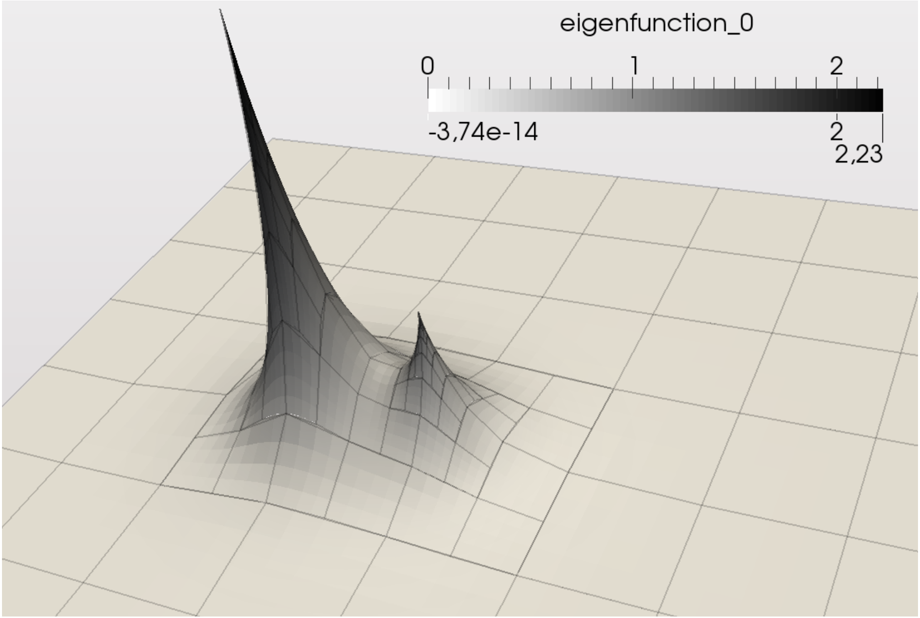
$$\langle A_\delta^u u_\delta^* - \lambda_\delta^* u_\delta^*, v_\delta \rangle = 0 \quad \forall v_\delta \in X_\delta .$$

The convergence of these eigenvalue and eigenspace towards the exact one has been proven in [Antonietti et al., 2006]. It is then possible to prove the inequalities

$$\begin{aligned}
\langle (A_\delta^u - \lambda_\delta^*) v_\delta, v_\delta \rangle &\geq 0 && \forall v_\delta \in X_\delta \\
|\langle (A_\delta^u - \lambda_\delta^*) v, v_\delta \rangle| &\lesssim \|\!|v|\!\|_{\mathrm{DG}} \|v_\delta\|_{\mathrm{DG}} && \forall v \in X(\delta), v_\delta \in X_\delta \\
\langle (A_\delta^u - \lambda_\delta^*)(u_\delta - u_\delta^*), (u_\delta - u_\delta^*) \rangle &\gtrsim \|u_\delta - u_\delta^*\|_{\mathrm{DG}}^2 && \\
\langle (E_\delta''(u) - \lambda_\delta^*) v_\delta, v_\delta \rangle &\gtrsim \|v_\delta\|_{\mathrm{DG}}^2 && \forall v_\delta \in X_\delta \\
|\langle (E_\delta''(u) - \lambda_\delta^*) v, v_\delta \rangle| &\lesssim \|\!|v|\!\|_{\mathrm{DG}} \|v_\delta\|_{\mathrm{DG}} && \forall v \in X(\delta), v_\delta \in X_\delta .
\end{aligned}$$

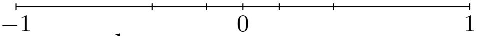
which then lead to the proof of convergence.

Results visualized

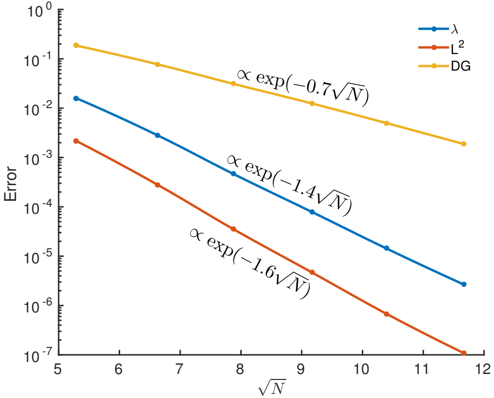


Numerical experiments

In the one dimensional case, with periodic domain $\Omega = [-1, 1]/2\mathbb{Z}$ and the singularity at the center, with potential $V(x) = -|x|^{-3/4}$,



we get the convergence results



Asymptotics of the solution: iterative scheme

Iterative scheme:

$$-\Delta u_{n+1} - \frac{1}{|x|^{2-\varepsilon}} u_{n+1} + u_n^2 u_{n+1} - bP_{u_n} u_{n+1} = \lambda_{n+1} u_{n+1}$$

where

- $\varepsilon > 0$,
- P_{u_n} is the projector on u_n,
- $b > 0$ is a shift parameter that enforces convergence.

Then

- $\|u_n\|_{H^1(\Omega)}$ is bounded, and
- $\sum_{n \in \mathbf{N}} \|u_{n+1} - u_n\|$ is bounded.

u_n converges towards a solution of the nonlinear Gross-Pitaevskii equation, with $f(u^2) = u^2$.

Asymptotics of the solution: Mellin transform

Iterative scheme:

$$-\Delta u_{n+1} - \frac{1}{|x|^{2-\varepsilon}} u_{n+1} + u_n^2 u_{n+1} - bP_{u_n} u_{n+1} = \lambda_{n+1} u_{n+1}.$$

Using the Mellin transform

$$\hat{u}(z) = (\mathcal{M}u)(z) = \int_0^\infty r^{z-1} u(r) dr \qquad \left(\mathcal{M}^{-1}\hat{u}\right)(r) = \int_{\Re z = \beta} r^{-z} \hat{u}(z) dz$$

and an hypothesis on u_n, we get

$$z(z+1)\hat{u}(z) \simeq \hat{u}(z+\varepsilon) + \lambda \hat{u}(z+2) + \sum_{j\in\mathbf{N}} \sum_{k=0}^{\lfloor j/2 \rfloor} a_{jk} \hat{u}(z+2+j-k\gamma).$$

The opposites of the poles of the Mellin transform are the exponents of the asymptotic expansion: for $r \to 0$ and $\omega \in S_{n-1}$,

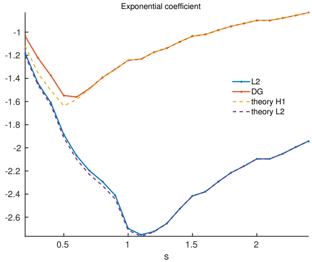
$$u(r,\omega) \sim \left(C + r^{\varepsilon} + \dots\right) Y_{\ell,m}(\omega)$$

One dimensional error analysis

[Gui and Babuška, 1986] showed that for $u \sim x^\alpha$ $(x \to 0)$, with scaling factor σ and polynomial increase s

$$\|u - \Pi(u)\| \simeq C(\sigma) \left(\sum_{i=2}^{m} \frac{\sigma^{(2\alpha-1)(1-i)} r^{2(1+s(i-1))}}{(1+s(i-1))^{2\alpha}} \right)^{1/2},$$

where one part is bigger in the element at the singularity and the other tends to be bigger in outer elements.



$u'(x) \sim x^{\alpha-1}$: maximal rate of convergence for different spaces.

Slope optimization: different potentials

Behaviour for different values of γ in

$$-\Delta u - \frac{1}{|x|^\gamma} u + u^3 = \lambda u.$$

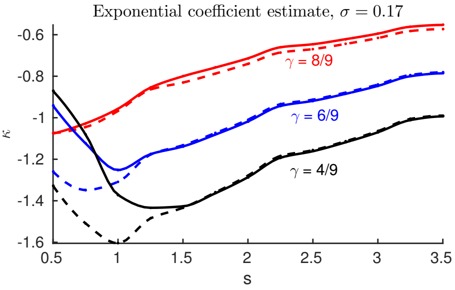


Figure: κ for the DG norm of the error. Dashed line: “theory”; continuous line: numerical results.

As long as the error is concentrated near the singularity, we have a good estimator for the rate of convergence.

Conclusions and perspectives

- The approximate eigenfunctions and eigenvalues converge with exponential rate to the exact solution.

- The analysis may be applied to the Gross-Pitaevskii and the Thomas-Fermi-von Weizsäcker models, but should be extended to more complex models.

- Given the asymptotics of the solution to the problem considered, the mesh and finite dimensional space can be optimized *a priori* and estimates for the convergence rate can be derived, mainly where the error near the singularity is bigger.

Conclusions and perspectives

- The approximate eigenfunctions and eigenvalues converge with exponential rate to the exact solution.
- The analysis may be applied to the Gross-Pitaevskii and the Thomas-Fermi-von Weizsäcker models, but should be extended to more complex models.
- Given the asymptotics of the solution to the problem considered, the mesh and finite dimensional space can be optimized *a priori* and estimates for the convergence rate can be derived, mainly where the error near the singularity is bigger.

Conclusions and perspectives

- The approximate eigenfunctions and eigenvalues converge with exponential rate to the exact solution.

- The analysis may be applied to the Gross-Pitaevskii and the Thomas-Fermi-von Weizsäcker models, but should be extended to more complex models.

- Given the asymptotics of the solution to the problem considered, the mesh and finite dimensional space can be optimized *a priori* and estimates for the convergence rate can be derived, mainly where the error near the singularity is bigger.

Thank you for your attention

Essential bibliography I

Antonietti, P. F., Buffa, A., and Perugia, I. (2006).
Discontinuous Galerkin approximation of the Laplace eigenproblem.
Computer Methods in Applied Mechanics and Engineering, 195(25-28):3483–3503.

Cancès, E., Chakir, R., and Maday, Y. (2010).
Numerical Analysis of Nonlinear Eigenvalue Problems.
Journal of Scientific Computing, 45(1-3):90–117.

Flad, H., Schneider, R., and Schulze, B.-W. (2008).
Asymptotic regularity of solutions to Hartree–Fock equations with Coulomb potential.
Mathematical Methods in the applied sciences, (June):2172–2201.

Gui, W. and Babuška, I. (1986).
The h, p and h-p versions of the finite element method in 1 dimension.
Numerische Mathematik, 49(6):613–657.

Essential bibliography II

Maday, Y. (2014).
h-P finite element approximation for full-potential electronic structure calculations.
In *Partial differential equations: theory, control and approximation*, pages 349–377. Springer, Dordrecht.

Schötzau, D., Schwab, C., and Wihler, T. P. (2013).
hp-DGFEM for Second Order Elliptic Problems in Polyhedra II: Exponential Convergence.
SIAM Journal on Numerical Analysis, 51(4):2005–2035.