Perturbation of nonlinear eigenvalue problems

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Joint works with ...

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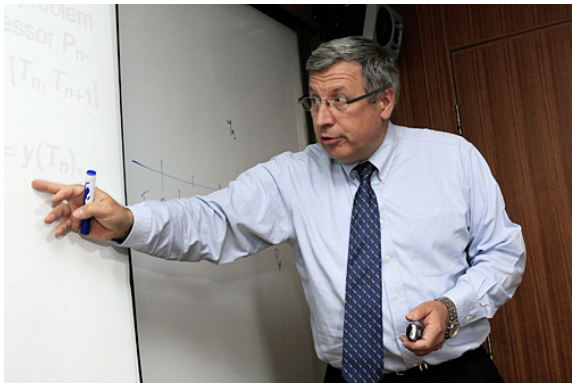

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1. Regular perturbation theory for linear self-adjoint operators

2. Numerical analysis of linear Schrödinger equations

3. Numerical analysis of nonlinear Schrödinger (NLS) equations

4. Density Functional Theory

Density Functional Theory is used by thousands of physicists, chemists, biologists, materials scientists, nanoscientists on a daily basis:

- **over 15,000 papers a year and growing;**
- **about 15% of the resources available in scientific computing centers;**
- **Kohn was awarded the 1998 Nobel prize in Chemistry for his contributions to Density Functional Theory**
- **Karplus, Levitt and Warshel were awarded the 2013 Nobel prize in Chemistry for their contributions to multiscale modeling of (bio)molecules.**

Numbers of hits (2015) for "Density Functional Theory"

- **in google scholar: 1,250,000 (559,000 for "Navier-Stokes")**
- **in mathscinet: 251 (17,357 for "Navier-Stokes")**

1 - Regular perturbation theory for linear self-adjoint operators

The main mathematical problem in quantum physics is the computation of eigenvalues (and eigenvectors) of self-adjoint operators:

$$H\Psi = E\Psi$$

Example: hydrogen atom

$$-\frac{\hbar^2}{2m_e}\Delta\Psi(x) - \frac{e^2}{4\pi\varepsilon_0|x|}\Psi(x) = E\Psi(x), \qquad \Psi \in L^2(\mathbb{R}^3;\mathbb{C}^2), \qquad E \in \mathbb{R}$$

$$E_n = -\frac{E_{\mathrm{H}}}{2n^2}, \quad n \in \mathbb{N}^*, \quad E_{\mathrm{H}} = m_e\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2, \quad \lambda_{m\to n} = \frac{4\pi\hbar c}{E_{\mathrm{H}}}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)^{-1}$$

Balmer series (nm): $\lambda_{6\to2} = 410.07$, $\lambda_{5\to2} = 433.94$, $\lambda_{4\to2} = 486.01$, $\lambda_{3\to2} = 656.11$
$\lambda^{\mathrm{exp}}_{6\to2} = 410.17$, $\lambda^{\mathrm{exp}}_{5\to2} = 434.05$, $\lambda^{\mathrm{exp}}_{4\to2} = 486.13$, $\lambda^{\mathrm{exp}}_{3\to2} = 656.28$

The main mathematical problem in quantum physics is the computation of eigenvalues (and eigenvectors) of self-adjoint operators:

$$H\Psi = E\Psi$$

Perturbation theory aims at answering the following question: consider a reference (unperturbed) self-adjoint operator H_0 on a Hilbert space $\mathcal{H}$ and E_0 a discrete eigenvalue of H_0 of multiplicity m.

What happens to E_0 (and to the associated eigenvectors) when H_0 is replaced by

$$H = H_0 + W$$

with W symmetric and "small"?

Consider

- **a Hilbert space $\mathcal{H}$;**
- **is a self-adjoint operator H_0 on $\mathcal{H}$ with domain $D(H_0)$;**
- **a H_0-bounded symmetric operator W on $\mathcal{H}$ (regular perturbation);**
- **a discrete eigenvalue E_0 of H_0 with multiplicity m.**

For $\beta \in \mathbb{C}$, we consider the operator $H(\beta) = H_0 + \beta W : D(H_0) \to \mathcal{H}$.

Theorem (Kato-Rellich). There exists $\eta > 0$ and $\varepsilon > 0$ such that

1. **for all $\beta \in (-\eta, \eta)$, the operator $H(\beta)$ is self-adjoint on $\mathcal{H}$;**
2. **there exist m (non-necessarily distinct) single-valued analytic functions**

$$\mathbb{C} \supset B(0,\eta) \ni \beta \mapsto E^{(j)}(\beta) \in B(E_0,\varepsilon) \subset \mathbb{C}, \qquad 1 \leq j \leq m,$$

which provide all the eigenvalues of $H(\beta)$ in the disk $B(E_0,\varepsilon) \subset \mathbb{C}$.

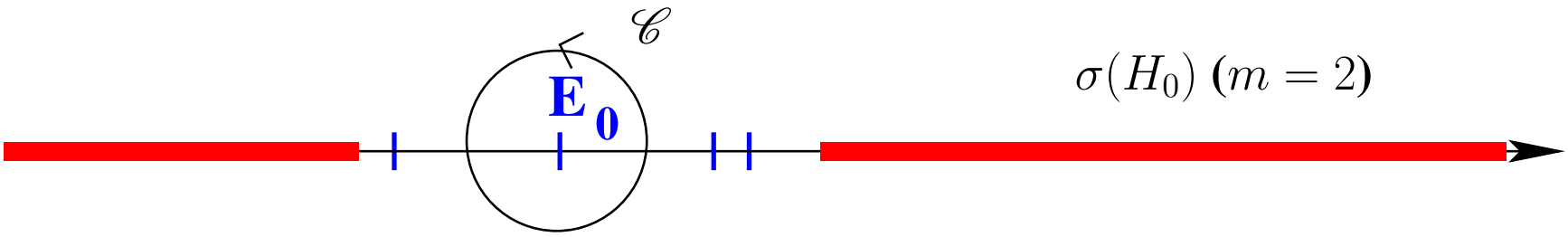
Sketch of the proof (see e.g. Reed and Simon, Vol. 4)

1. **Well-known result for matrices (Rellich '37): expansion of the roots of the secular equation in Puiseux series + real eigenvalues are for β real.**

2. **In infinite dimensional Hilbert spaces, use Cauchy residue theorem and functional calculus for self-adjoint operators:**

$$P(0) = \frac{1}{2i\pi} \oint_{\mathscr{C}} (z - H_0)^{-1}\, dz = \textbf{ orthogonal projector on Ker}(H_0 - E_0)$$

$$\forall z \in \mathscr{C}, \quad z - H(\beta) = z - H_0 - \beta W = (1 - \beta W (z - H_0)^{-1})(z - H_0)$$



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$$= \frac{1}{2i\pi} \oint_{\mathscr{C}} \left((1 - \beta W(z - H_0)^{-1})(z - H_0)\right)^{-1} dz$$

$$= \frac{1}{2i\pi} \oint_{\mathscr{C}} (z - H_0)^{-1} \left(1 - \beta W(z - H_0)^{-1}\right)^{-1} dz$$

$$= \sum_{k=0}^{+\infty} \beta^k \left(\frac{1}{2i\pi} \oint_{\mathscr{C}} (z - H_0)^{-1} \left(W(z - H_0)^{-1}\right)^k dz \right)$$

Dyson expansion

Sketch of the proof (see e.g. Reed and Simon, Vol. 4)

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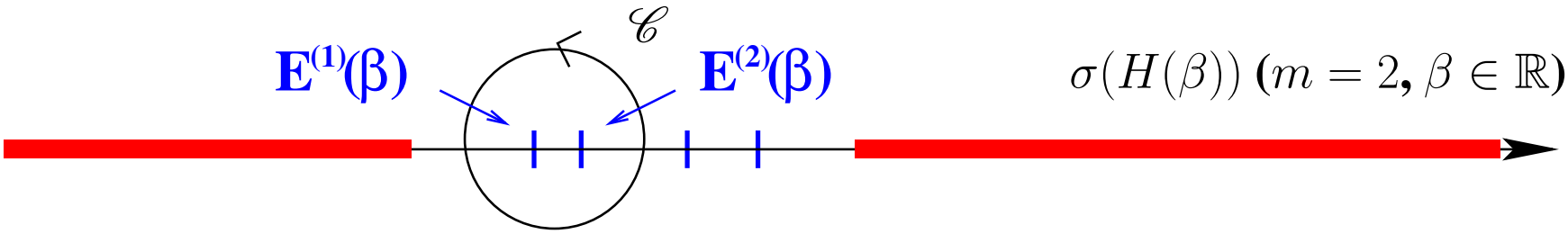
analytic rank-m projector on the vector space spanned by the eigenfunctions of $H(\beta)$ located in $B(E_0, \varepsilon)$.



Theorem (non-degenerate perturbation). **Let E_0 be a simple discrete eigenvalue of H_0 and let ψ_0 be an associated normalized eigenvector. There exist single-valued analytic functions**

$$\mathbb{C} \supset B(0,\eta) \ni \beta \mapsto E(\beta) \in \mathbb{C}, \qquad \mathbb{C} \supset B(0,\eta) \ni \beta \mapsto \psi(\beta) \in D(H_0)$$

such that

$$E(0) = E_0,\ \psi(0) = \psi_0, \quad \forall \beta \in B(0,\eta),\ (H_0 + \beta W)\psi(\beta) = E(\beta)\psi(\beta),\ \|\psi(\beta)\| = 1.$$

The coefficients E_k and ψ_k in the Taylor expansions

$$E(\beta) = \sum_{k=0}^{+\infty} \beta^k E_k, \qquad \psi(\beta) = \sum_{k=0}^{+\infty} \beta^k \psi_k,$$

are obtained by solving the triangular system (real Hilbert space case)

$$\forall k \in \mathbb{N}^*, \qquad \begin{cases} (H_0 - E_0)\psi_k = f_k + E_k\psi_0, \\ (\psi_0, \psi_k) = \alpha_k, \end{cases}$$

where

$$f_k = -W\psi_{k-1} + \sum_{j=1}^{k-1} E_j \psi_{k-j} \qquad \textbf{et} \qquad \alpha_k = -\frac{1}{2}\sum_{j=1}^{k-1} (\psi_j, \psi_{k-j}).$$

2 - Numerical analysis of linear Schrödinger equations

Notation: $\Omega = [0, 2\pi)^d \subset \mathbb{R}^d$**,**

$$L^2_\#(\Omega) := \left\{ v \in L^2_{\rm loc}(\mathbb{R}^d),\ v \textbf{ real-valued},\ v\ 2\pi\mathbb{Z}^d\textbf{-periodic} \right\},$$

$$C^k_\#(\Omega) := \left\{ v \in C^k(\mathbb{R}^d),\ v \textbf{ real-valued},\ v\ 2\pi\mathbb{Z}^d\textbf{-periodic} \right\},$$

$$\forall s \in \mathbb{R}, \quad H^s_\#(\Omega) := \left\{ v \in H^s_{\rm loc}(\mathbb{R}^d),\ v \textbf{ real-valued},\ v\ 2\pi\mathbb{Z}^d\textbf{-periodic} \right\}.$$

Caracterization of periodic Sobolev spaces:

$$H^s_\#(\Omega) := \left\{ v = \sum_{\mathbf{k}\in\mathbb{Z}^d} \widehat{v}_{\mathbf{k}} e_{\mathbf{k}},\ v \textbf{ real valued},\ \|v\|^2_{H^s_\#} := \sum_{\mathbf{k}\in\mathbb{Z}^d} \left(1+|\mathbf{k}|^2\right)^s |\widehat{v}_{\mathbf{k}}|^2 < \infty \right\},$$

where $e_{\mathbf{k}}(\mathbf{r}) = \dfrac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{d/2}}, \quad \mathbf{k} \in \mathbb{Z}^d$**.**

Truncation operator Π_n**: for all** $n \in \mathbb{N}$**,** Π_n **is defined on** $\mathcal{S}'_\#(\Omega)$ **by**

$$\Pi_n \left(\sum_{\mathbf{k}\in\mathbb{Z}^d} \widehat{v}_{\mathbf{k}} e_{\mathbf{k}} \right) = \sum_{|\mathbf{k}|\le n} \widehat{v}_{\mathbf{k}} e_{\mathbf{k}}.$$

Π_n **is the orthogonal projector from** $H^s_\#(\Omega)$ **onto** X_n **for all** $s \in \mathbb{R}$**.**

Schrödinger operators with periodic boundary conditions

$$W \in C^0_\#(\Omega), \qquad H = -\Delta + W \quad \textbf{on } L^2_\#(\Omega).$$

H is a bounded below self-adjoint operator on $L^2_\#(\Omega)$ with domain $H^2_\#(\Omega)$, form domain $H^1_\#(\Omega)$, and compact resolvent.

Computation of the lowest N eigenvalues and associated eigenvectors

$$\begin{cases} \textbf{seek } (\lambda, u) \in \mathbb{R} \times H^2_\#(\Omega) \textbf{ such that } \|u\| = 1 \textbf{ and} \\ -\Delta u + Wu = \lambda u \end{cases}$$

$$\Leftrightarrow \qquad \begin{cases} \textbf{seek } (\lambda, u) \in \mathbb{R} \times H^1_\#(\Omega) \textbf{ such that } \|u\| = 1 \textbf{ and} \\ \forall v \in H^1_\#(\Omega), \quad \displaystyle\int_\Omega \nabla u \cdot \nabla v + \int_\Omega Wuv = \lambda \int_\Omega uv. \end{cases}$$

Variational approximation: X_n finite-dim. subspace of $H^1_\#(\Omega)$ s.t. dim$(X_n) \geq N$

$$\begin{cases} \textbf{seek } (\lambda_n, u_n) \in \mathbb{R} \times X_n \textbf{ such that } \|u_n\| = 1 \textbf{ and} \\ \forall v_n \in X_n, \quad \displaystyle\int_\Omega \nabla u_n \cdot \nabla v_n + \int_\Omega W u_n v_n = \lambda_n \int_\Omega u_n v_n. \end{cases} \tag{1}$$

Suitable approximation space: **for all** $n \in \mathbb{N}$**,**

$$X_n = \left\{ v_n = \sum_{|\mathbf{k}| \leq n} \widehat{v}_{\mathbf{k}} e_{\mathbf{k}},\ v_n \textbf{ real valued} \right\} \subset H^s_{\#}(\Omega), \quad \forall s \in \mathbb{R}.$$

Key properties:

1. Since $X_n \subset H^2_{\#}(\Omega)$**,**

$$\textbf{(1)} \quad \Leftrightarrow \quad \begin{cases} \textbf{seek } (\lambda_n, u_n) \in \mathbb{R} \times X_n \textbf{ such that } \|u_n\| = 1 \textbf{ and} \\ \\ \Pi_n H \Pi_n u_n = \lambda_n u_n, \end{cases}$$

where Π_n **is the orthogonal projector on** X_n **(for any** $H^s_{\#}$ **inner product).**

2. Π_n **commutes with** $-\Delta$ **so that**

$$\Pi_n H \Pi_n u_n = -\Delta u_n + \Pi_n W \Pi_n u_n.$$

The exact and approx. solutions (λ, u) and (λ_n, u_n) to the eigenvalue pb satisfy

$$\begin{cases} H_n u_n = \lambda_n u_n, \\ \|u_n\|_{L^2_\#} = 1, \end{cases} \quad \textbf{and} \quad \begin{cases} (H_n + W_n)u = \lambda u, \\ \|u\|_{L^2_\#} = 1, \end{cases}$$

with

$$H_n = -\Delta + \Pi_n W \Pi_n \qquad \textbf{and} \qquad W_n = W - \Pi_n W \Pi_n$$

Rayleigh-Schrödinger perturbation expansion:

$$u = u_n + u_n^1 + R_n \qquad \textbf{with} \qquad u_n^1 = -(H_n - \lambda_n)|^{-1}_{u_n^\perp} \Pi_{u_n^\perp}(W_n u_n)$$

Is $\widetilde{u}_n = u_n + u_n^1$ a better approximation of u (compared to u_n)?

How costly is the computation of (an approximation of) u_n^1?

Theorem (E.C., Dusson, Maday, Stamm, Vohralík '14).

Let $W \in H^s_\#(\Omega)$ for some $s > d/2$.

For all $n \in \mathbb{N}$ such that $n^2 > \lambda_n$, the function

$$u_n^1 = -(H_n - \lambda_n)|_{u_n^\perp}^{-1} \Pi_{u_n^\perp}(W_n u_n)$$

is well defined, and the post-treated solutions

$$\widetilde{u}_n = u_n + u_n^1 \qquad \textbf{and} \qquad \widetilde{\lambda}_n = \lambda_n + (u_n^1, W u_n)_{L^2_\#}$$

are such that

$$\boxed{\|u - \widetilde{u}_n\|_{H^1_\#} \leq C n^{-2} \|u - u_n\|_{H^1_\#} \quad \textbf{and} \quad |\lambda - \widetilde{\lambda}_n| \leq C n^{-2} |\lambda - \lambda_n|}$$

for a constant $C > 0$ independent of n.

Proof: Dyson expansion + the operators $W_n(z - H_n)^{-1}$ go to zero in Hilbert-Schmidt norm as n^{-2}, uniformly in $z \in \mathscr{C}$ + Aubin-Nitsche argument.

Practical calculation of the perturbation u_n^1

$$L^2_{\#}(\Omega) = X_n \oplus X_n^{\perp}, \qquad u_n = \begin{pmatrix} u_n \\ 0 \end{pmatrix}, \qquad H_n = \left(\begin{array}{c|c} -\Delta|_{X_n} + \Pi_n W \Pi_n & 0 \\ \hline 0 & -\Delta_{X_n^{\perp}} \end{array}\right)$$

$$W_n = \left(\begin{array}{c|c} 0 & \Pi_n W \Pi_n^{\perp} \\ \hline \Pi_n^{\perp} W \Pi_n & \Pi_n^{\perp} W \Pi_n^{\perp} \end{array}\right)$$

$$u_n^1 = -(H_n - \lambda_n)|^{-1}_{u_n^{\perp}} \Pi_{u_n^{\perp}}(W_n u_n)$$

$$W_n u_n = \Pi_n^{\perp} W \Pi_n u_n = \Pi_n^{\perp} W u_n \in X_n^{\perp}$$

Therefore,

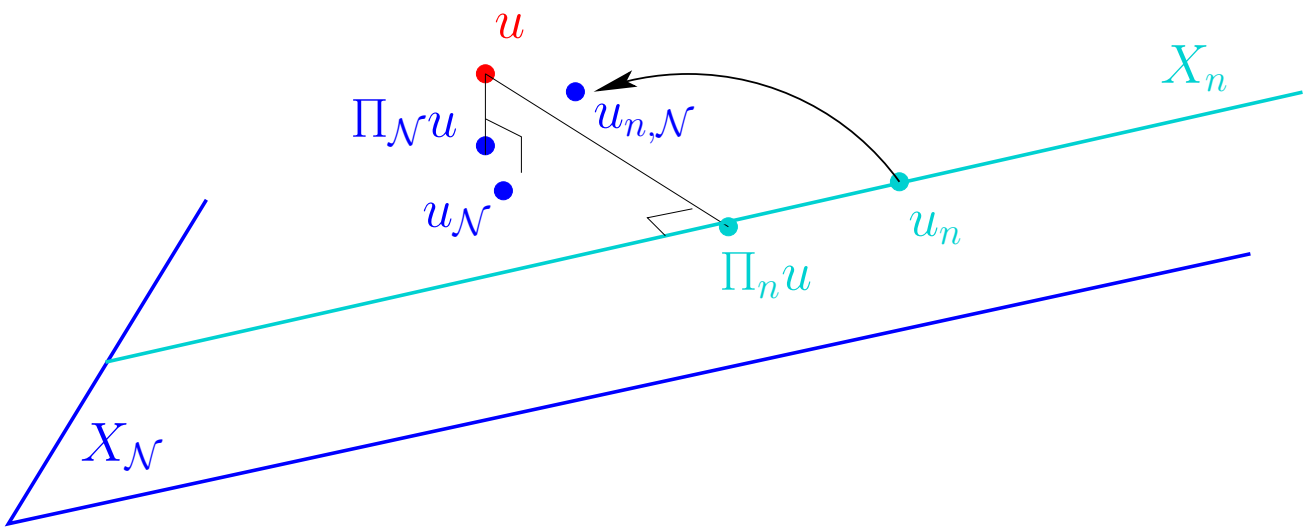
$$\boxed{u_n^1 = -(-\Delta|_{X_n^{\perp}} - \lambda_n)^{-1} r_n \quad \textbf{with} \quad r_n := \Pi_n^{\perp} W u_n.}$$

Note that

$$r_n = \Pi_n^{\perp} W u_n = \Pi_n^{\perp}\left(-\Delta u_n + W u_n - \lambda_n u_n\right) = -\Delta u_n + W u_n - \lambda_n u_n \in X_n^{\perp}$$

$\longrightarrow$ **residual of the eigenvalue problem.**

CPU time reduction by post-treatment



Solving the pb in a fine approximation space $X_{\mathcal{N}}$ is costly ($\sim \mathcal{K}\mathcal{N}^d \ln \mathcal{N}$ op.).
Alternative:

1. **solve the pb on a coarser approximation space X_n, $n \ll \mathcal{N}$ ($\sim \mathcal{K} n^d \ln n$ op.);**
2. **set $u_{n,\mathcal{N}} = u_n + u^1_{n,\mathcal{N}}$, with $u^1_{n,\mathcal{N}}$: approx. of u^1_n in $X_{\mathcal{N}}$ ($\sim \mathcal{N}^d \ln \mathcal{N}$ op.).**

3 - Numerical analysis of nonlinear Schrödinger (NLS) equations

Periodic Gross-Pitaevskii model

- **used to simulate Bose-Einstein condensates;**
- **simplified version of the Kohn-Sham model for condensed matter.**

$$I = \inf \left\{ E(v),\ v \in H^1_{\#}(\Omega),\ \int_\Omega |v|^2 = 1 \right\} \tag{2}$$

where $\Omega = (0, 2\pi)^d$ **(**$d = 1$**,** 2 **or** 3**) and where**

$$E(v) = \int_\Omega |\nabla v|^2 + \int_\Omega V|v|^2 + \frac{\mu}{2}\int_\Omega |v|^4,$$

V **being a** $2\pi\mathbb{Z}^d$**-periodic real-valued continuous function and** $\mu > 0$**.**

- **(2) has exactly two minimizers** u **(with** $u > 0$ **in** Ω**) and** $-u$**;**
- $\exists ! \lambda \in \mathbb{R}$ **such that** (λ, u) **satisfies the nonlinear Schrödinger equation**

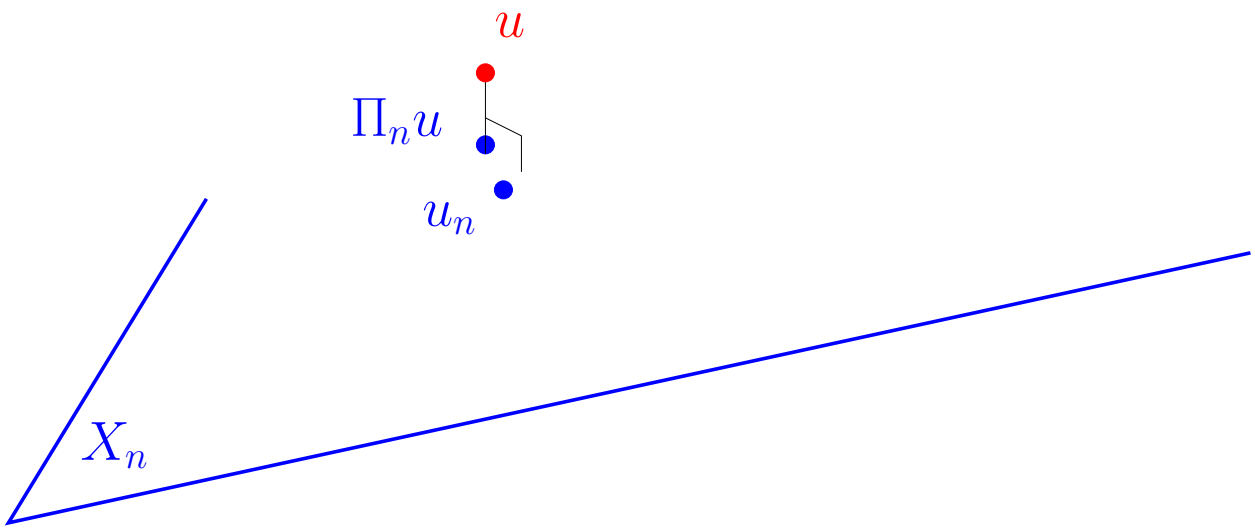
$$-\Delta u + Vu + \mu u^3 = \lambda u, \qquad \|u\|_{L^2_{\#}} = 1;$$

- λ **is the lowest eigenvalue of the self-adjoint operator** $-\Delta + V + \mu u^2$**.**

Galerkin approximation

Find a minimizer u_n to the finite-dimensional variational problem

$$I_n = \inf \left\{ E(v_n),\ v \in X_n,\ \int_\Omega |v_n|^2 = 1 \right\} \qquad (u_n, 1)_{L^2_\#} \geq 0.$$



If $V \in H^\sigma_\#(\Omega)$ for some $\sigma \geq 0$, then $u \in H^{\sigma+2}_\#(\Omega)$ and

$$\forall s < \sigma + 2, \quad \|u - \Pi_n u\|_{H^s_\#} = \left(\sum_{|\mathbf{k}|>n} \left(1 + |\mathbf{k}|^2\right)^s |\widehat{v}_\mathbf{k}|^2 \right)^{1/2} \leq \frac{\|u\|_{H^{\sigma+2}_\#}}{n^{\sigma+2-s}}.$$

Theorem (E.C., Chakir, Maday '10)

There exists $0 < c \leq C < \infty$ **such that for all** $n \in \mathbb{N}$**,**

$$\|u - \Pi_n u\|_{H^1_\#} \leq \|u - u_n\|_{H^1_\#} \leq C\|u - \Pi_n u\|_{H^1_\#} \underset{n\to 0}{\longrightarrow} 0$$

$$c\|u - u_n\|^2_{H^1_\#} \leq I_n - I = E(u_n) - E(u) \leq C\|u - u_n\|^2_{H^1_\#}.$$

Assume that $V \in H^\sigma_\#(\Omega)$ **for some** $\sigma > d/2$**. Then**

- $(u_n)_{n\in\mathbb{N}}$ **converges to** u **in** $H^{\sigma+2}_\#(\Omega)$**;**
- **there exists positive constants** C **and** C_s **such that**

$$\forall -\sigma \leq s < \sigma + 2, \quad \|u - u_n\|_{H^s_\#} \leq \frac{C_s}{n^{\sigma+2-s}}, \qquad |\lambda - \lambda_n| \leq \frac{C}{n^{2(\sigma+1)}}.$$

Remark: **these** *a priori* **convergence rates are optimal.**

Post-treatment of approximate solutions by the perturbation method

The exact and approx. solutions (λ, u) **and** (λ_n, u_n) **to the GP equation satisfy**

$$\begin{cases} H_n u_n = \lambda_n u_n, \\ \\ \|u_n\|_{L^2_\#} = 1, \end{cases} \quad \textbf{and} \quad \begin{cases} (H_n + \mathcal{V}_n + \mathcal{W}_n)u = \lambda u, \\ \\ \|u\|_{L^2_\#} = 1, \end{cases}$$

with

$$H_n = -\Delta + \Pi_n(V + \mu u_n^2)\Pi_n$$

$$\mathcal{V}_n = V + \mu u_n^2 - \Pi_n(V + \mu u_n^2)\Pi_n, \qquad \mathcal{W}_n = \mu(u^2 - u_n^2).$$

Rayleigh-Schrödinger perturbation expansion:

$$u = u_n \underbrace{-(H_n - \lambda_n)|^{-1}_{u_n^\perp}\Pi_{u_n^\perp}(\mathcal{V}_n u_n)}_{u_n^{1,1}} \underbrace{-(H_n - \lambda_n)|^{-1}_{u_n^\perp}\Pi_{u_n^\perp}(\mathcal{W}_n u_n)}_{u_n^{1,2}} + R_n$$

First-order perturbation of the eigenvector

$$u = u_n + u_n^{1,1} + u_n^{1,2} + R_n$$

where

$$u_n^{1,1} = -(-\Delta|_{X_n^\perp} - \lambda_n)^{-1} r_n$$

with

$r_n = -\Delta u_n + V u_n + \mu u_n^3 - \lambda_n u_n \in X_n^\perp$ **residual of the GP equation.**

An approximation $u_{n,\mathcal{N}}^{1,1}$ **of** $u_n^{1,1}$ **in** $X_\mathcal{N}$ **is easily obtained by FFT (**$\sim \mathcal{N}^d \ln \mathcal{N}$ **op.).** $u_n^{1,2}$ **and** R_n **are small in** H^1**-norm (***a priori* **estimates).**

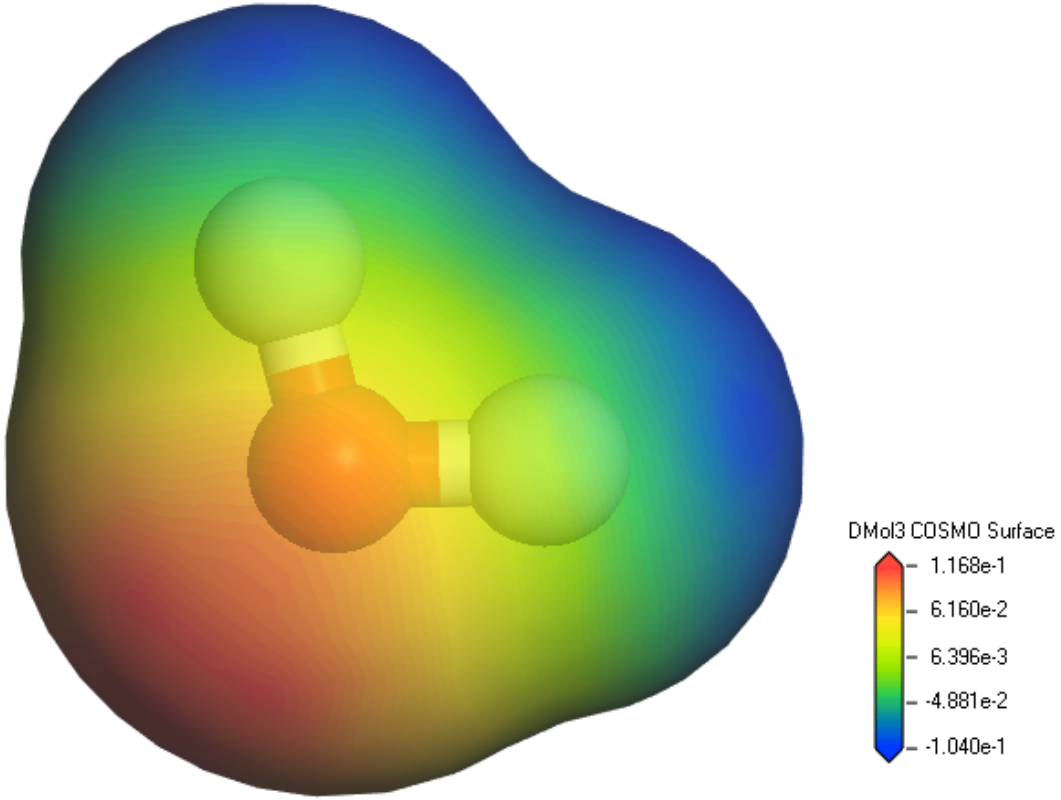
Theorem (E.C., Dusson, Maday, Stamm, Vohralík '14).

Let $V \in H^\sigma_\#(\Omega)$ **for some** $\sigma > d/2$ **and** $u_{n,\mathcal{N}} = u_n + u_{n,\mathcal{N}}^{1,1}$**.**

There exists $C \in \mathbb{R}_+$ **such that for all** $n \in \mathbb{N}$ **such that** $n^2 > \lambda_n$**,**

$$\|u - u_{n,\mathcal{N}}\|_{H^1_\#} \leq C \left(n^{-(\sigma+3)} + \mathcal{N}^{-(\sigma+1)} \right).$$

4 - Density Functional Perturbation Theory (DFPT)



Atomic units: $\hbar = 1, \quad m_e = 1, \quad e = 1, \quad \varepsilon_0 = (4\pi)^{-1}.$

Nuclear charges $\{z_k\}_{1 \leq k \leq M} \in (\mathbb{N}^*)^M$**.**

Nuclear configuration $\{\mathbf{R}_k\}_{1 \leq k \leq M} \in (\mathbb{R}^3)^M$**.**

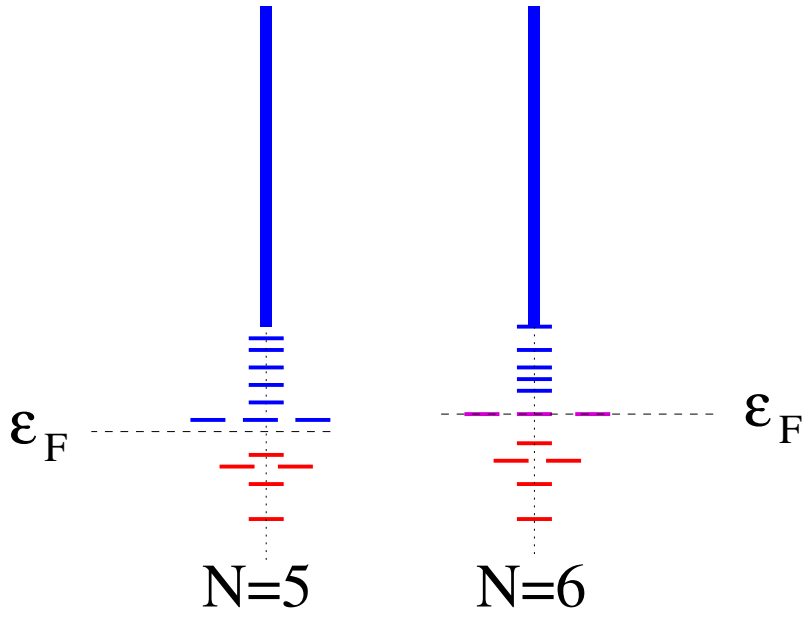
Extended Kohn-Sham equations

$$\rho_0(\mathbf{r}) = \sum_i \nu_i |\phi_i(\mathbf{r})|^2$$

$$\begin{cases} H^{\mathrm{KS}}_{\rho_0}\,\phi_i = \varepsilon_i \phi_i \\ \displaystyle\int_{\mathbb{R}^3} \phi_i \phi_j = \delta_{ij} \end{cases} \quad \textbf{and} \quad \left| \begin{array}{l} \nu_i = 1 \textbf{ if } \varepsilon_i < \varepsilon_{\mathrm{F}}, \\ 0 \leq \nu_i \leq 1 \textbf{ if } \varepsilon_i = \varepsilon_{\mathrm{F}}, \\ \nu_i = 0 \textbf{ if } \varepsilon_i > \varepsilon_{\mathrm{F}}, \end{array} \right. \quad \sum_i \nu_i = N$$

$$H^{\mathrm{KS}}_{\rho_0} = -\frac{1}{2}\Delta + V + \rho_0 \star |\cdot|^{-1} + v^{\mathrm{xc}}_{\rho_0}$$

$$V(\mathbf{r}) = -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r} - \mathbf{R}_k|}$$



Non-degenerate case (**$\varepsilon_{\mathrm{F}} < 0$ and ε_{F} is not an eigenvalue of $H^{\mathrm{KS}}_{\rho_0}$**).

- **Regular perturbation theory applies**
  - **– to the reduced Hartree-Fock model in the whole space or with PBC**
  - **– to the Kohn-Sham LDA model with PBC**

  under the assumption that the ground state density matrix is unique (E.C., Mourad '14);

- **The ground state density matrix of atoms is unique in the rHF model (E.C., Mourad '14);**

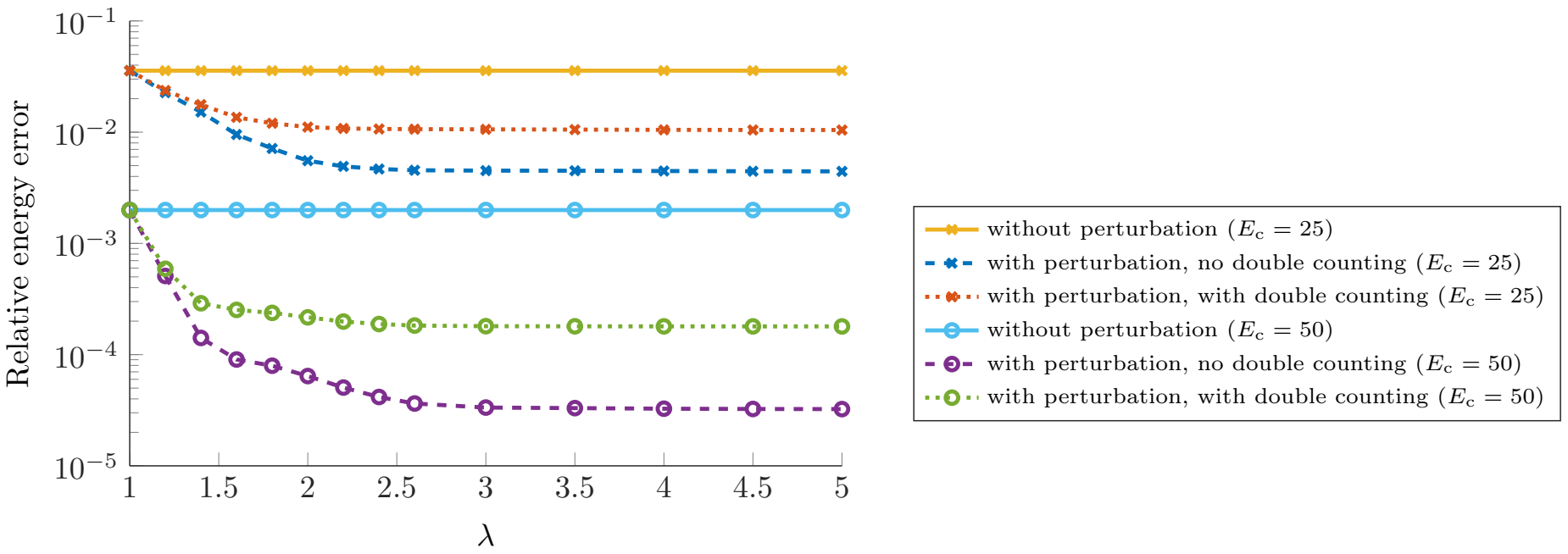
- **DFPT can then be used for post-treatment of numerical approximations (E.C., Dusson, Maday, Stamm, Vohralík '15).**

Post-treatment of numerical approximations using DFPT

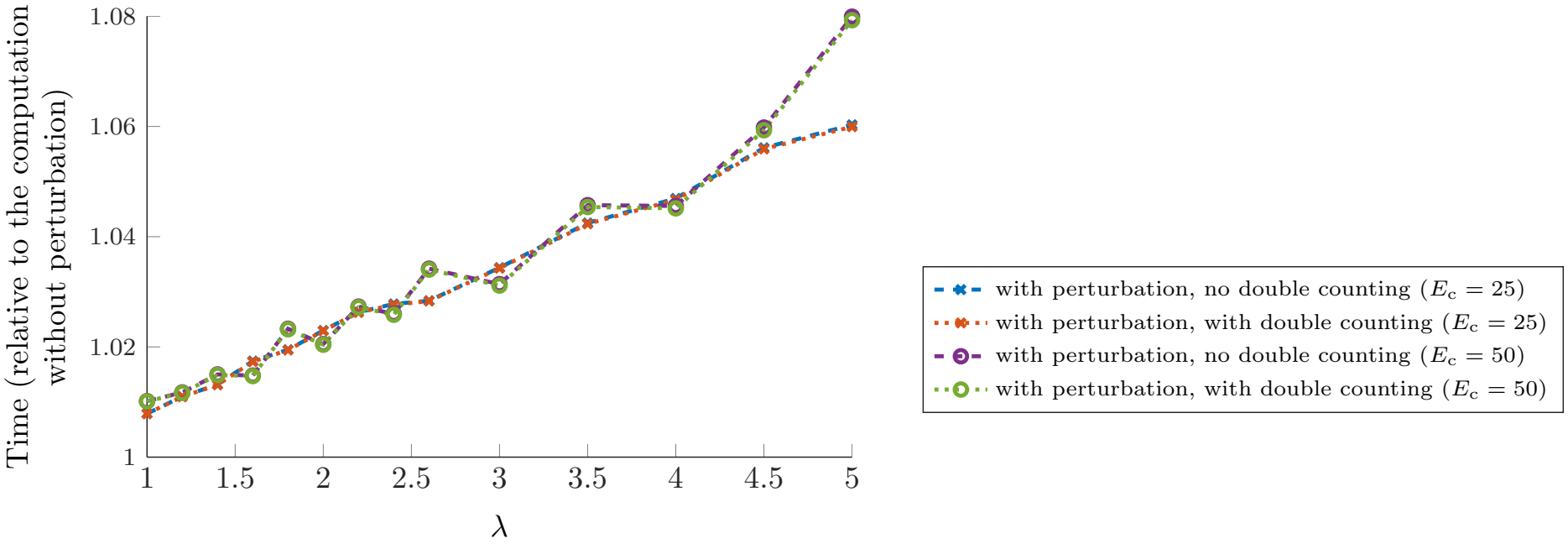
Kohn-Sham LDA simulations of the CO_2 molecule with KSSOLV (Berkeley).

Relative energy errors computed for $E_{\mathrm{c}}^{\mathcal{N}} = \lambda^2 E_{\mathrm{c}}^{n}$ as a function of λ, with $E_{\mathrm{c}}^{n} = 25$ eV and $E_{\mathrm{c}}^{n} = 50$ eV.

Reference calculation: $E_{\mathrm{c}}^{\infty} = 800$ eV (382,323 basis functions).



Post-treatment of numerical approximations using DFPT



Degenerate case ($\varepsilon_{\rm F} < 0$ **and** $\varepsilon_{\rm F}$ **is an eigenvalue of** $H^{\rm KS}_{\rho_0}$**).**

- **Regular perturbation theory applies**
  - **– to the reduced Hartree-Fock model in the whole space or with PBC**
  - **– to the Kohn-Sham LDA model with PBC**

  under the assumption that the ground state density matrix is unique and that the occupation numbers at the Fermi level all are positive

  (E.C., Mourad '14);

- **there is no energy level splitting at the Fermi level;**

- **Wigner's (2n+1)-rule still applies: knowing the perturbed eigenstates at order** n **allows one to compute the perturbed energy at order (2n+1).**

Conclusion

Linear perturbation theory has been a fundamental tool in quantum physics since the very first days of the quantum theory.

In a recent paper

E. Cancès and N. Mourad, *A mathematical perspective on density functional perturbation theory*, Nonlinearity 27 (2014) 1999-2033,

we put nonlinear perturbation theory for Density Functional Theory and the Kohn-Sham model (DFPT) on sound mathematical ground, even in the degenerate case (see also the contributions by J. Angyan for the non-degenerate case).

Nonlinear perturbation theory can be used in numerical simulation to improve the quality of the numerical approximation at a low computational cost.