Fully guaranteed and computable bounds for eigenvalue problems

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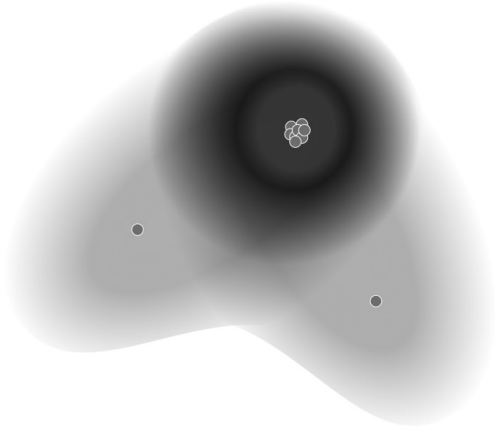
Motivation : Kohn–Sham model (1965)

Compute the **electronic density** of a molecular system.



Mathematical problem : M **nonlinear eigenvalue** equations in 3D

Find M orthonormal eigenfunctions

$$\Phi^0 = (\phi_1^0, \dots, \phi_M^0) \in X = \left\{ \Phi = (\phi_1, \dots, \phi_M) \in \left[H^1(\Omega) \right]^M \middle| \int_\Omega \phi_i \phi_j = 1 \right\}$$

with corresponding lowest eigenvalues $\lambda_1^0, \dots, \lambda_M^0$, such that

$$\left(-\frac{1}{2}\Delta + V^{KS}_{\mathbf{R_k}, \rho_{[\Phi^0]}} \right) \phi_i^0 = \lambda_i^0 \phi_i^0, \quad i = 1, \dots, M, \quad \text{with} \quad \rho_{[\Phi^0]} = 2 \sum_{i=1}^{M} |\phi_i^0|^2.$$

Difficulties : Several eigenvalues to compute, possibly degenerate, nonlinearity. In practice, approximate solutions.

How to estimate the errors ?

Different levels of approximations

Input $\{\mathbf{R}_k\}$
(atomic positions)
$\downarrow$
Reference model
$\downarrow$
Approximate
model

1- Model error

Error of the mathematical model with respect to a reference model.

In our case :

- Simplification of the Schrödinger equation
- Dimension reduction
- Introduction of a nonlinear eigenvalue problem (DFT)
- K-point sampling
- Pseudopotentials

Different levels of approximations

Input $\{\mathbf{R}_k\}$
(atomic positions)
$\downarrow$
Reference model
$\downarrow$
Approximate
model
$\downarrow$
Discretization

1- Model error

2- Discretization error

Error between the solution in the whole space X and the solution in the approximate space X_h

Different discretization methods :

- Finite elements
- Planewaves
- Wavelets
- Gaussians

Different levels of approximations

Input $\{\mathbf{R}_k\}$
(atomic positions)
$\downarrow$
Reference model
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Approximate model
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Discretization
$\downarrow$
Numerical scheme

1- Model error

2- Discretization error

3- Algorithmic error

Error between the solution on the discrete space X_h and the solution computed with the chosen algorithm

Example :

- Use of an iterative process to solve the problem (finite number of iterations)

Different levels of approximations

Input $\{\mathbf{R}_k\}$
(atomic positions)
↓
Reference model
↓
Approximate
model
↓
Discretization
↓
Numerical scheme
↓
Computer code
↓
Computed output

1- Model error

2- Discretization error

3- Algorithmic error

4- Numerical error

- Numerical integration errors
- Roundoff errors
- Errors caused by possible defects in computer codes (bugs or random hardware failures)

Toward certified and optimized molecular simulations

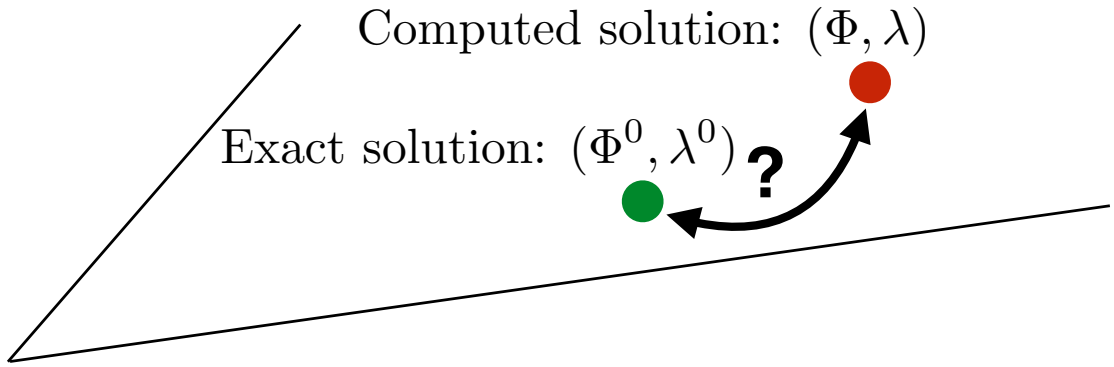
A lot of approximations

- **How large is the total error ?**
- **How large is each error component ?**

Two main goals :

1. **Certify** the precision of the results.
2. **Optimize** the computational ressources : minimize the computational cost to obtain a desired accuracy.

Wish-list for a good error bound



The goal is to derive an inequality of the type :

$$\|(\Phi^0, \lambda^0) - (\Phi, \lambda)\|_? \leq \eta(\textit{disc.}, \textit{algo.}, \ldots) = \text{ Error bound}$$

Properties of the error bound :

1. Computable upper bound of the error
2. Valid under checkable assumptions
3. Efficient (close to the error)
4. Cheap to compute
5. Allow adaptivity

Outline

Error estimation for a boundary value problem

Error estimation for nonlinear problems

Fully guaranteed bounds

Error balance between several parameters

Error estimation for a boundary value problem

Problem : solve $Au = f$.
Residual $Res(v) = Av - f$.
There holds $Res(u) = 0$ but in general $Res(u_N) \neq 0$.

Measure on the error with respect to the equation.

Galerkin method : Solve

$$\langle Au, v \rangle = \langle f, v \rangle \quad \forall v \in V.$$

Discrete problem :

$$\langle Au_N, v \rangle = \langle f, v \rangle \quad \forall v \in V_N.$$

Error estimation :

$$\begin{aligned} \langle Res(u_N), v \rangle &= \langle Au_N - f, v \rangle \quad \forall v \in V \\ &= \langle A(u_N - u), v \rangle \quad \forall v \in V \end{aligned}$$

We obtain

$$\|A^{1/2}(u_N - u)\| \leq \|A^{-1/2} Res(u_N)\|.$$

($A^{1/2}$ norm corresponds to energy norm)

Bauer–Fikke error bound for eigenvalue problems

Problem : Solve $Au = \lambda u$.

Approximate solution (u_N, λ_N) : $Res_N = Au_N - \lambda_N u_N$.

Theorem **(Bauer-Fike)**
Assumption : A is a diagonalizable matrix.
Let X be the matrix that transforms it into diagonal form. Then, there exists an eigenvalue λ of A such that

$$|\lambda - \lambda_N| \leq \text{Cond}(X)\|Res_N\|_2$$

Hermitian case : If A is hermitian, then

$$|\lambda - \lambda_N| \leq \|Res_N\|_2.$$

Proof

Assume that λ_N is not an eigenvalue of A.
Diagonalization of A : $A = XDX^{-1}$.
$Res_N = Au_N - \lambda_N u_N$.

$$\begin{aligned} u_N &= (A - \lambda_N)^{-1} Res_N \\ &= X(D - \lambda_N)^{-1} X^{-1} Res_N \end{aligned}$$

Therefore,

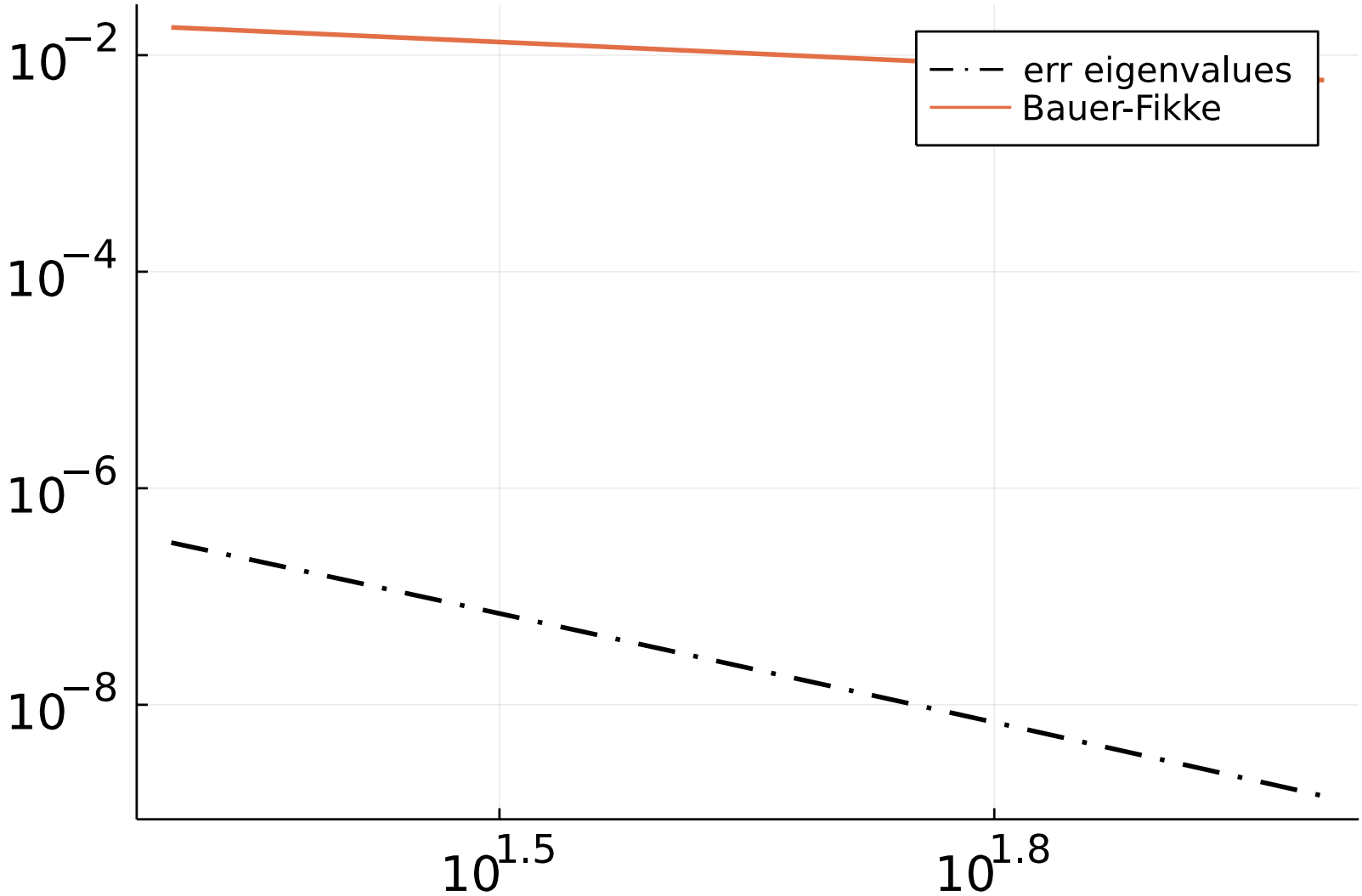
$$\begin{aligned} 1 &= X(D - \lambda_N)^{-1} X^{-1} Res_N \\ &\leq \|X\|_2 \|(D - \lambda_N)^{-1}\|_2 \|X^{-1}\|_2 \|Res_N\|_2. \end{aligned}$$

Hence

$$1 \leq \mathrm{Cond}(X) \|Res_N\|_2 \max_{\lambda_i \in \Lambda(A)} |\lambda_i - \lambda_N|^{-1}.$$

(See Saad 1992)

Numerical illustration



Kato–Temple error bounds for eigenvalue problems

Theorem **(Kato–Temple)** Let u_N be an approximate eigenvector of A and $\lambda_N = \langle Au_N, u_N \rangle$. Let λ be the eigenvalue closest to λ_N and δ the distance from λ_N to the rest of the spectrum

$$\delta = \min_i \{|\lambda_i - \lambda_N|, \quad \lambda_i \neq \lambda\}$$

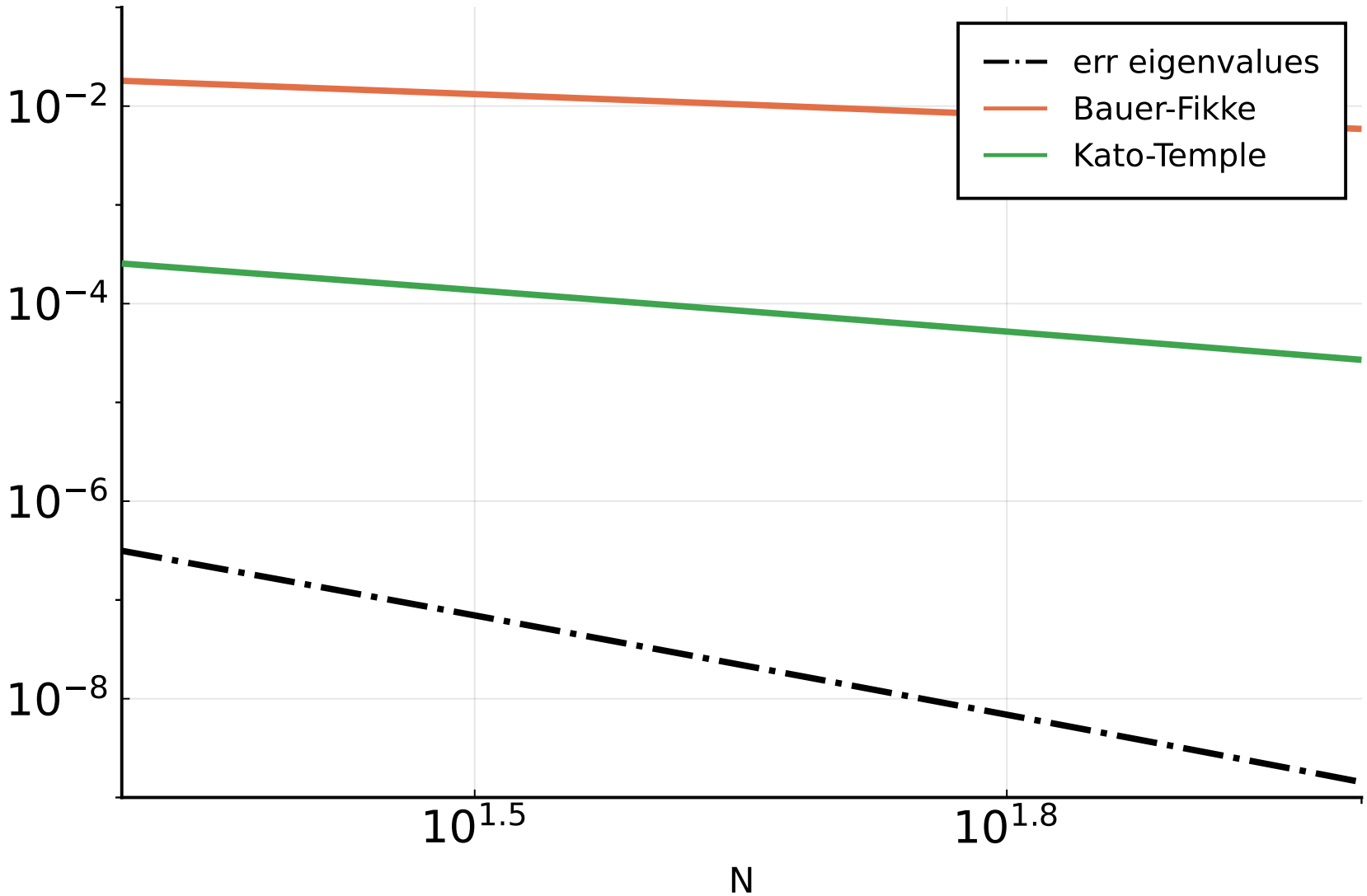
Then

$$\lambda_N - \lambda \leq \frac{\|Res_N\|_2^2}{\delta}.$$

Proof : First show that $(\beta - \lambda_N)(\lambda_N - \alpha) \leq \|Res_N\|_2^2$, where (α, β) contains λ_N and no eigenvalue of A.

See Cances, Herbst, Levitt, Faraday Discussions, 2020.

Numerical illustration



An asymptotically optimal bound

Theorem **(Cances, D., Maday, Stamm, Vohralik)**

First bound :

$$|\lambda_N - \lambda| \leq \|A^{-1/2} Res_N\|_2^2 + (\lambda + \lambda_N)\|u - u_N\|_2^2$$

Second bound :

$$|\lambda_N - \lambda| \leq C_N^{-1} \|A^{-1/2} Res_N\|_2^2$$

where $C_N = \min \left\{ \left(1 - \frac{\lambda_N}{\lambda_{i-1}}\right)^2, \left(1 - \frac{\lambda_N}{\lambda_{i+1}}\right)^2 \right\}$

See Cances, Dusson, Maday, Stamm, Vohralik, Math. Comput. 89, 2563-2611 (2020).

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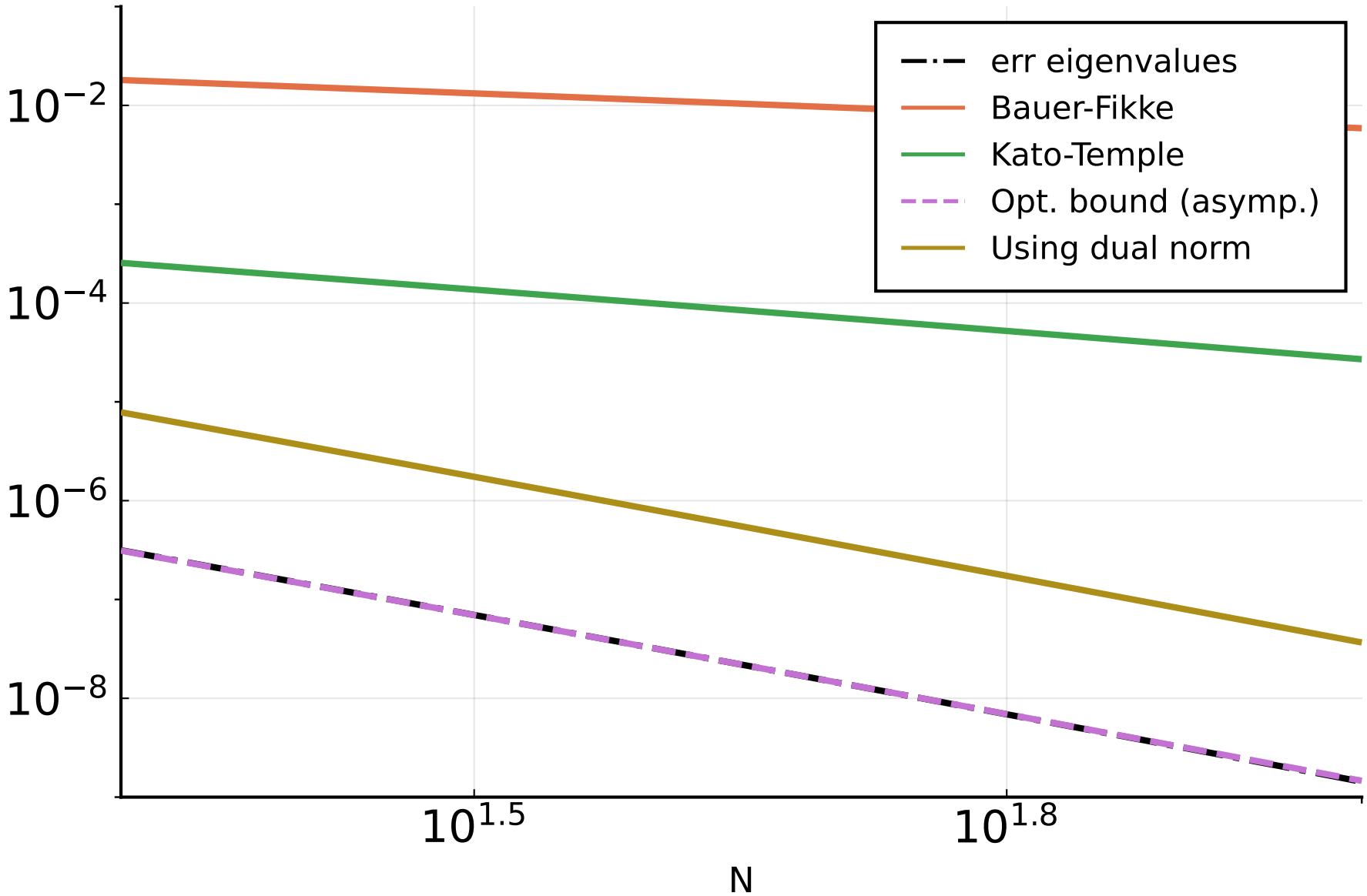

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Abstract formulation

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Example : $x = (\Phi, \lambda)$.

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Taylor expansion close to a solution x_* :

$$R(x) \simeq DR(x)(x - x_*).$$

Hence,

$$x - x_* \simeq [DR(x)]^{-1} R(x).$$

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Quantity of interest : A

$$I(x) - I(x_*) \simeq [DI(x)][DR(x)]^{-1} R(x).$$

To estimate the error, one needs to estimate $[DI(x)][DR(x)]^{-1} R(x)$.

Possible bound : $\|[DI(x)]\| \|[DR(x)]^{-1}\| \|R(x)\|$.

Guaranteed bounds

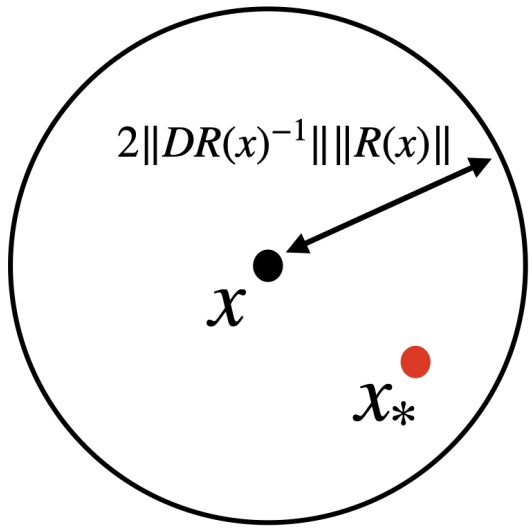
Solve $R(x) = 0$ with $R : Y \to Z$.

Inverse function theorem - Newton–Kantorovitch [1]

Two conditions to be satisfied :

- $DR(x) \in \mathcal{L}(Y; Z)$ is an isomorphism
- $2\|DR(x)^{-1}\|_{Z,Y'} L(2\|DR(x)^{-1}\|_{Z,Y'}\|R(x)\|_{Z'}) \leq 1$

  with $\quad L(\alpha) = \sup_{y \in \bar{B}(x,\alpha)} \|DR(x) - DR(y)\|_{Y,Z'}.$



Then the problem $R(x) = 0$ has a unique solution x_* in the ball $\bar{B}(x, 2\|DR(x)^{-1}\|_{Z,Y'}\|R(x)\|_{Z'})$.

Moreover, $\boxed{\|x - x_*\|_Y \leq 2\|DR(x)^{-1}\|_{Z,Y'}\|R(x)\|_{Z'}.}$

- Possible to obtain guaranteed bounds
- Requires control over first and second order derivatives
- Result on existence of solution

1. Caloz, Rappaz : Numerical analysis for nonlinear and bifurcation problems. Handb. Numer. Anal. 5, 487-637 (1997).

Main difficulties for applications to DFT

- Structure of the problem not too easy to write in this form - constraints and degeneracies
- Computation of the inverse of the Jacobian very costly
- Choice of the norm in

$$\|x - x_*\|_Y \leq 2\|DF(x)^{-1}\|_{Z,Y'}\|F(x)\|_{Z'}.$$

- Inequalities may be suboptimal

Practical error bounds for DFT problems [2]

2. Cances, D., Kemlin, Levitt : Practical error bounds for properties in plane-wave electronic structure calculations, http ://arxiv.org/abs/2111.01470, (2021)

Outline

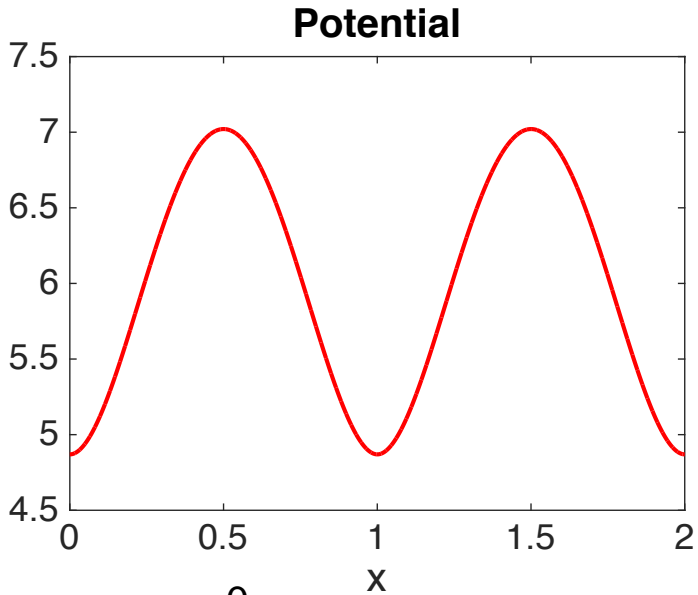
Problem presentation : the Gross-Pitaevskii equation

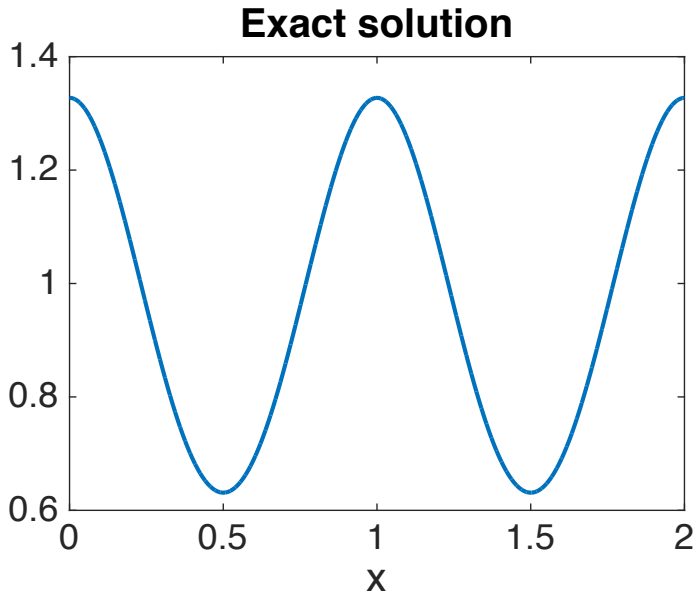
Physical problem : Ground state of a system of bosons at very low temperature.

Nonlinear eigenvalue problem : Find $(\phi^0, \lambda^0) \in H^1_\#(\Omega)$ such that $\|\phi^0\|_{L^2} = 1$ and

$$\Big(-\Delta + V + (\phi^0)^2 \Big)\phi^0 = \lambda^0 \phi^0.$$

Setting : 1-Dimensional, Periodic Setting.





Remark : λ^0 is the lowest eigenvalue and is **simple**.

Exact solution : (ϕ^0, λ^0)
Resolution with planewave discretization and iterative algorithm

A posteriori analysis–Approach

How to find a guaranteed, computable and guaranteed upper bound of the error $\|\phi^0 - \phi_N^k\|_{H^1}$?

Residual-based a posteriori analysis :

$$\mathrm{Res}(\phi_N^k, \lambda_N^k) = (-\Delta + V + (\phi_N^k)^2)\phi_N^k - \lambda_N^k \phi_N^k.$$

First-order development of the residual :

$$0 = \mathrm{Res}(\phi^0, \lambda^0) \simeq \mathrm{Res}(\phi_N^k, \lambda_N^k) + D\mathrm{Res}_{(\phi_N^k, \lambda_N^k)}(\phi^0 - \phi_N^k)$$

$$\phi^0 - \phi_N^k \simeq -D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)} \left(\mathrm{Res}(\phi_N^k, \lambda_N^k)\right)$$

- A first **coarse** bound based on **inverse function theorem**, writing

  $$\|\phi^0 - \phi_N^k\|_{H^1} \leq 2\|D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)}\|_{H^{-1},H^1} \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}}.$$

- A second **precise** bound valid only in the asymptotic regime, writing

  $-D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)} \left(\mathrm{Res}(\phi_N^k, \lambda_N^k)\right) = -\Delta^{-1}\mathrm{Res}(\phi_N^k, \lambda_N^k) +$ superconvergent terms.

Ref : Dusson, Maday 2017.

First a posteriori bound

To characterize the error bound :

- Determine **computable** conditions on N and k s.t. $D\mathrm{Res}_{(\phi_N^k, \lambda_N^k)}$ **is an isomorphism**
- Find a **computable** bound for $\|D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)}\|_{H^{-1}, H^1}$

Extra-computation : Resolution of a discrete linear eigenvalue problem.

Theorems (D., Maday) :

- **Guaranteed bound :** Under the previous conditions, there exists a unique (ϕ, λ) such that $\mathrm{Res}(\phi, \lambda) = 0$ and

$$\|\phi - \phi_N^k\|_{H^1} + |\lambda - \lambda_N^k| \leq 2\gamma \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}} \tag{1}$$

- **Ground state :** There exists a computable condition depending on $\|\phi - \phi_N^k\|_{H^1}$, $|\lambda - \lambda_N^k|$, ϕ_N^k, $\lambda_N^k, \mu_N^1, \mu_N^2$ guaranteeing that (ϕ, λ) is the ground state (ϕ^0, λ^0) of our problem.

A **coarse** a posteriori error bound valid under computable conditions.

Second a posteriori bound

Theorem [Asymptotic error bound] (D., Maday) :
If $\|\phi^0 - \phi_N^k\|_{H^1}$ and $|\lambda^0 - \lambda_N^k|$ are small enough, then we can show that

$$\left(1 - \varepsilon(\phi^0 - \phi_N^k, \lambda^0 - \lambda_N^k)\right) \|\phi^0 - \phi_N^k\|_{H^1} \leq \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}} + F(\phi_N^k, \lambda_N^k, \mu_N^1, \mu_N^2),$$

where

- $\varepsilon(\phi^0 - \phi_N^k, \lambda^0 - \lambda_N^k) \xrightarrow[\|\phi^0 - \phi_N^k\|_{H^1} \to 0]{} 0$ can be estimated with the first bound
- $F(\phi_N^k, \lambda_N^k, \mu_N^1, \mu_N^2)$ is asymptotically small, and equal to 0 if $\|(V + 3(\phi_N^k)^2 - \lambda_N^k - 1)_-\|_{L^\infty} = 0$.

Asymptotically,

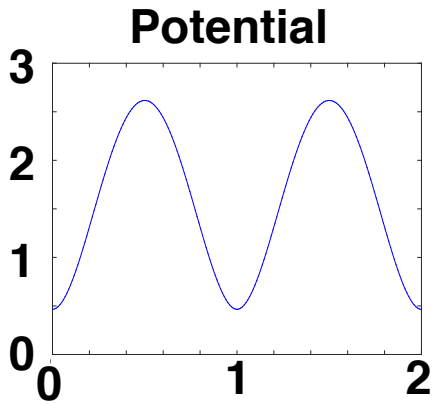
$$\|\phi^0 - \phi_N^k\|_{H^1} \leq \alpha_N^k \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}},$$

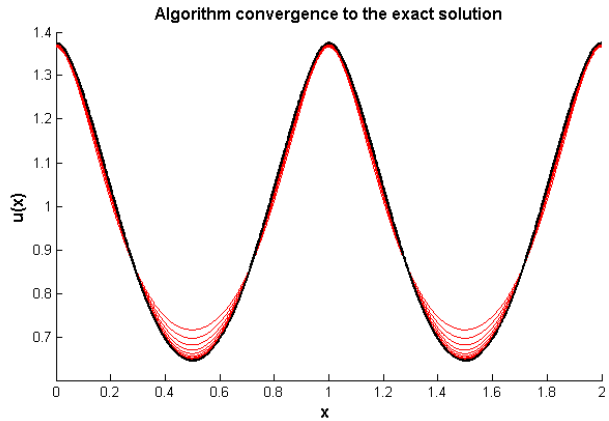
with α_N^k computable and as close to 1 as we wish.

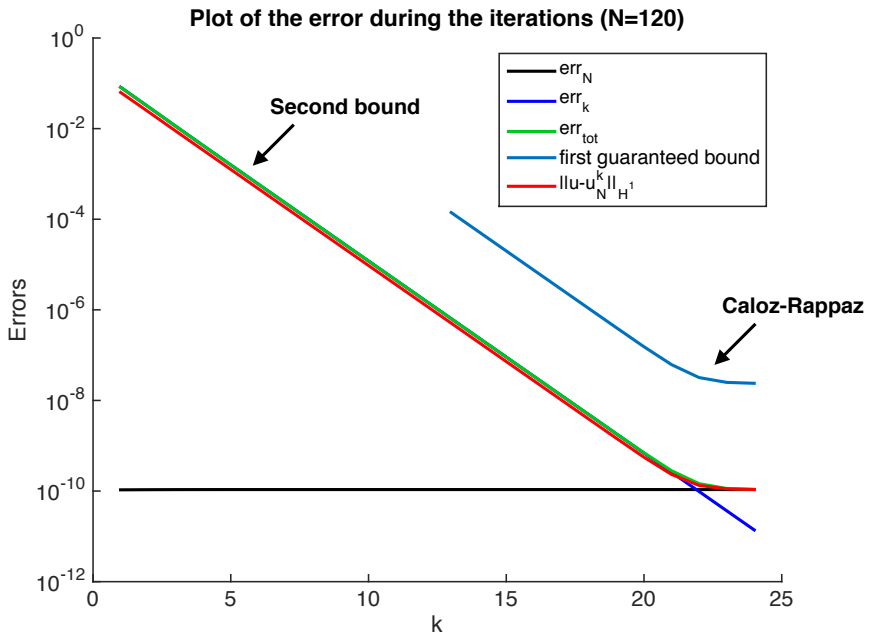
Better bound...but guaranteed only if the error is small enough.

Numerical simulations

- Fourier coefficients of the potential V are given by $\widehat{V}_k = -\frac{1}{\sqrt{2\pi}} \frac{1}{|k|^4 - \frac{1}{4}}$.
- Reference solution computed in a discrete space with N=500.







Outline

Error balance for efficient simulation

How to perform **efficient simulations** using error bounds ?

Example : Error estimation comes from different sources 1, 2, 3.

$$\mathrm{Err}_{\mathrm{tot}} \simeq \mathrm{Err}_1 + \mathrm{Err}_2 + \mathrm{Err}_3.$$

Efficient scheme : try to **balance the errors**

$$\mathrm{Err}_1 \simeq \mathrm{Err}_2 \simeq \mathrm{Err}_3.$$

In that direction :

- Discretization and SCF iterations [D., Maday, IMA J. Numer. Anal. (2017)]
- Discretization and eigenvalue solver [Cances, D., Maday, Stamm, Vohralik, Numer. Math. (2018)]

Example of error balance

D., Maday, IMA J. Numer. Anal. (2017) : **Gross-Pitaevskii**-type eigenvalue problem (in 1d).

Two sources of error : discretization (dimension $2N+1$), iterations (k).

How to get the **best compromise** between the discretization and the number of iterations ?

1. Decompose the residual into **two parts :**

$$H_{\rho_N^k}\phi_N^k - \lambda_N^k\phi_N^k = \mathrm{Res}_{N,k} = \mathrm{Res}_N + \mathrm{Res}_k,$$

with

$$\mathrm{Res}_N = H_{\rho_N^{k-1}}\phi_N^k - \lambda_N^{k-1}\phi_N^{k-1},$$

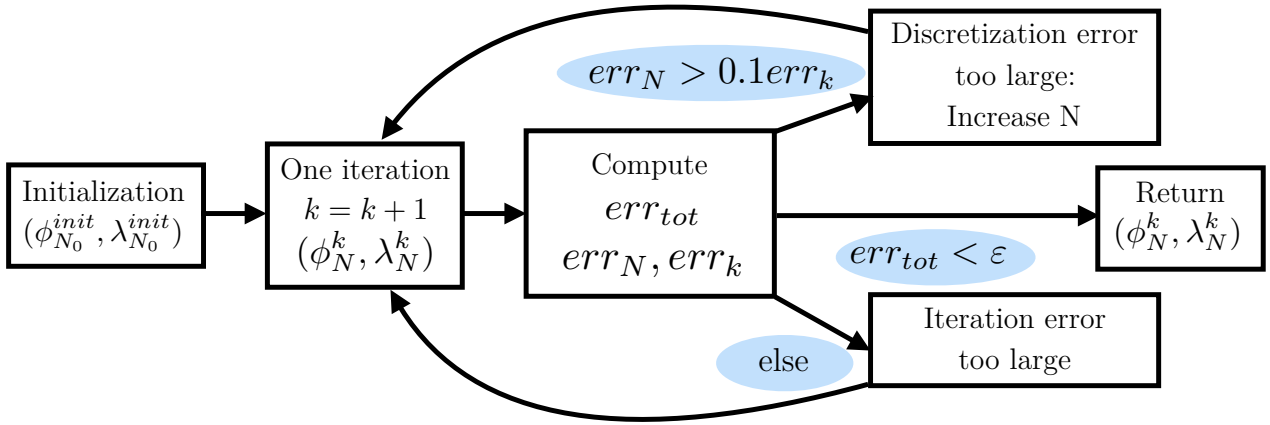
$$\mathrm{Res}_k = H_{\rho_N^k}\phi_N^k - H_{\rho_N^{k-1}}\phi_N^k - \lambda_N^k\phi_N^k + \lambda_N^{k-1}\phi_N^{k-1}.$$

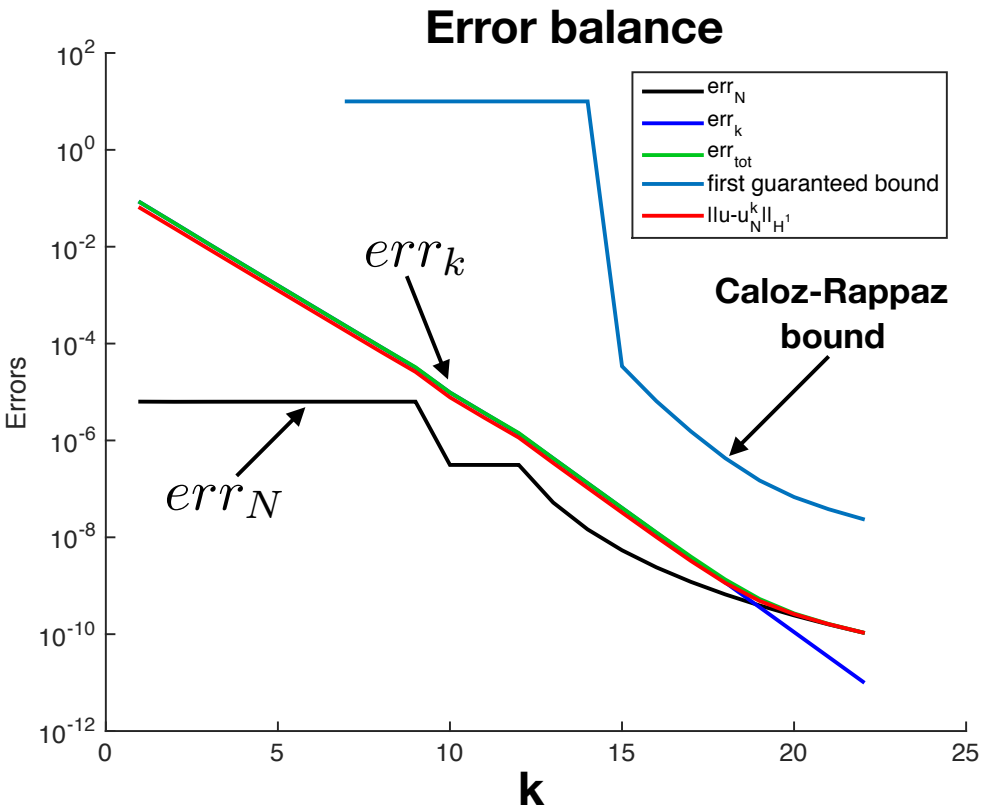
2. Decompose the error bound : essentially,

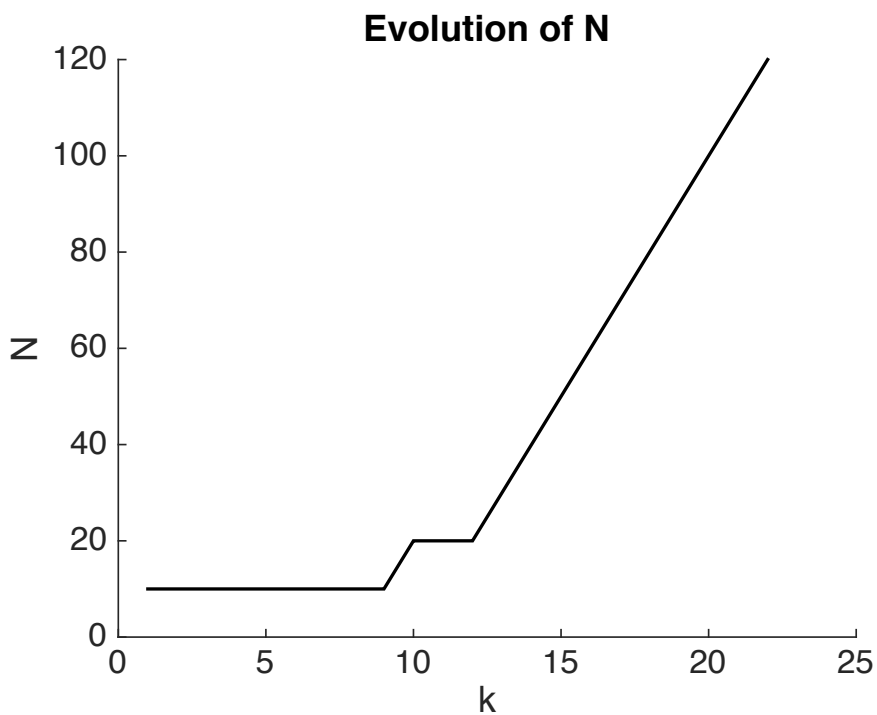
$$\|\phi^0 - \phi_N^k\|_{H^1} \leq \alpha_N^k \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}} \leq \alpha_N^k \left(\|\mathrm{Res}_N\|_{H^{-1}} + \|\mathrm{Res}_k\|_{H^{-1}}\right)$$

3. Compute each of these terms for **adaptative refinement**.

Error balance results



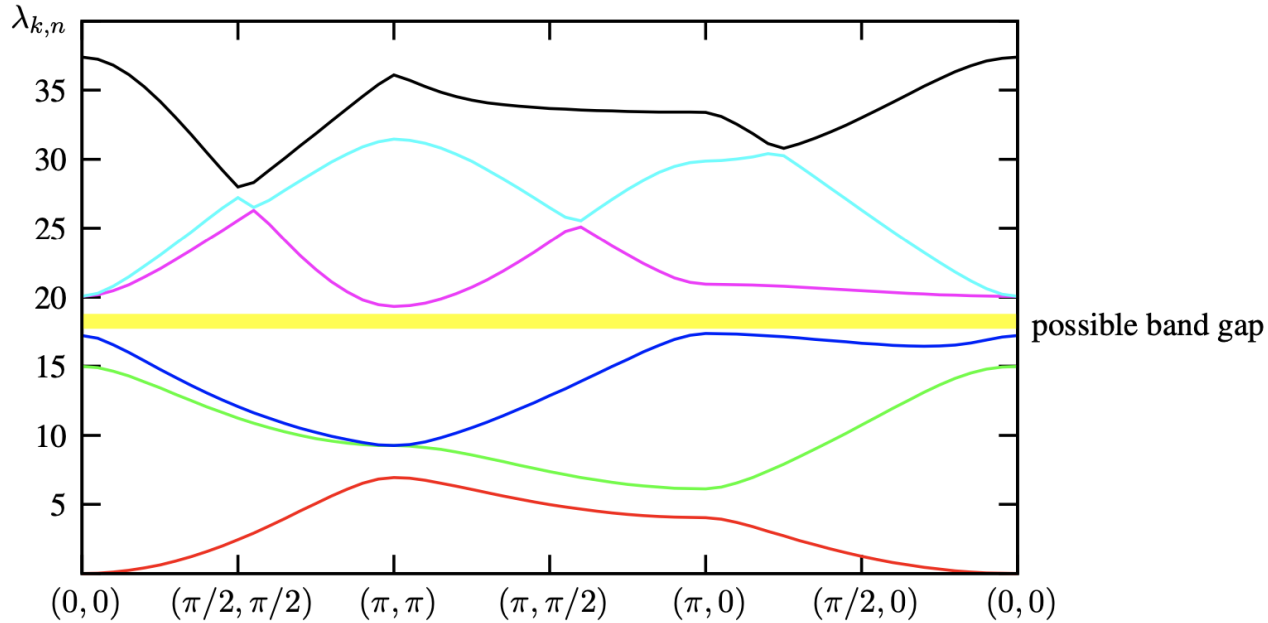




Combining several sources of errors

In that direction :

- SCF error and basis set error [Maday, D. 2014]
- Inexact solver : error balance between iteration and discretization error [3]
- Error bounds on the whole band structure [4]



3. Cances, D., Maday, Stamm, Vohralik : Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors : a unified framework. Numer. Math. 140, 1033-1079 (2018)

4. Hoang, Plum, Wieners : A computer-assisted proof for photonic band gaps. Z. Angew. Math. Phys. 60, 1035 (2009).

Conclusion

- Error bounds for **clusters** of eigenvalues, density matrices and quantities of interest
- **Computable bounds** available if dual norms of the residual can be estimated/computed
- Balance to find between computational cost and accuracy of error bound

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Thank you for your attention.