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Optimal Design & Numerics

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Variational Characterization of Diagonalization Operators & Eigenvalues

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- Joint work with Stéphane Mischler

Today's talk

Origin of the problem
A global approach
A global approach: infinite dimension
Remarks

Origin of the problem

Origin of the problem

- We were interested in the determination of a system of orthonormal functions $\psi := (\psi_m)_{m\geq 1}$ satisfying

$$(1.1)\qquad \begin{cases} \mathrm{i}\partial_t \psi_m - \Delta\psi_m + (V + \widetilde{V})\,\psi_m = 0 & \text{in } (0,T)\times\Omega \\ -\Delta V = \displaystyle\sum_{m=1}^{\infty} \alpha_m |\psi_m(x,t)|^2 & \text{in } (0,T)\times\Omega \\ \psi_m(0,x) = \psi_{0m}(x) & \text{in } \Omega \\ \psi_m(t,\sigma) = 0 & \text{on } [0,T]\times\partial\Omega \end{cases}$$

- A *standing wave solution* is an orthonormal system of functions $(\varphi_m)_{m\geq 1}$ such that the family defined by

$$\psi_m(t,x) = \mathrm{e}^{\mathrm{i}\lambda_m t}\varphi_m(x)$$

satisfies **(1.1)**.

- For instance $(\psi_{0m})_{m\geq 0}$ may be a Hilbert basis of $L^2(\Omega)$ with each $\psi_{0m} \in H^1_0(\Omega)$.

Origin of the problem

- The Schrödinger–Poisson system becomes: find a system of orthonormal functions $\varphi := (\varphi_m)_{m\geq 1}$ and a sequence of real eigenvalues $(\lambda_m)_{m\geq 1}$ satisfying

$$(1.2)\qquad \begin{cases} -\Delta\varphi_m + (V + \widetilde{V})\,\varphi_m = \lambda_m\varphi_m & \text{in } \Omega \\ -\Delta V = \displaystyle\sum_{m=1}^{\infty} \alpha_m|\varphi_m(x)|^2 & \text{in } \Omega \\ \varphi_m(\sigma) = 0 & \text{on } \partial\Omega \end{cases}$$

- The coefficients α_m are assumed to satisfy

$$\alpha_m > 0, \qquad \sum_{m=1}^{\infty} \alpha_m < \infty.$$

- Various types of domains Ω and boundary conditions may be considered.
- The potential $\widetilde{V}$ is given and may be singular.

A global approach

A global approach

- Even the linear case (that is dropping the second equation in **(1.2)** and setting $V \equiv 0$) deserves a new approach... also in the finite dimensional case
- **In other words:** can one characterize the whole eigensystem of a linear operator through **one** variational problem?
- Consider a selfadjoint positive definite matrix $A : H \longrightarrow H$ where H is an n-dimensional Hilbert space
- The eigenvalues of A can be found through the critical values of the Rayleigh quotient

$$\frac{(Au|u)}{(u|u)} \tag{2.1}$$

A global approach

- Namely, for $1 \leq k \leq n-1$,

  (2.2) $$\lambda_1 = \inf_{u \in H} \frac{(Au|u)}{(u|u)}, \qquad \lambda_{k+1} = \inf \left\{ \frac{(Au|u)}{(u|u)} \; ; \; u \in \mathrm{span}\{e_1, \dots, e_k\}^\perp \right\}$$

  where $e_1, \dots, e_k$ are eigenvectors for $\lambda_1, \dots, \lambda_k$.

- In practice, one finds n critical values (or critical points), each depending on the previous ones.

- When H_0 is a separable, infinite dimensional Hilbert space and $(A, D(A))$ is an unbounded positive self-adjoint operator such that the imbedding $H := D(A^{1/2}) \subset H_0$ is compact, then the above procedure **(2.2)** yields all the eigenvalues of A.

A global approach: finite dimensional space

- Finding $(\lambda_j)_j$ is equivalent to find a Hilbert basis $(\widetilde{u}_j)_j$ such that $A\widetilde{u}_j = \lambda_j \widetilde{u}_j$
- Fix $(e_j)_{1\leq j\leq n}$, a Hilbert basis of H
  Denoting by U the matrix such that $Ue_j = \widetilde{u}_j$, the problem is thus to find a unitary operator U such that

$$AUe_j = \lambda_j Ue_j \iff U^* AUe_j = \lambda_j e_j.$$

- For simplicity, assume A positive definite, and denote

$$\mathbb{S} := \{U : H \longrightarrow H \,;\, U^* U = I\}.$$

  and choose n numbers $\alpha_j > 0$, with $\alpha_j \neq \alpha_k$ for $j \neq k$, and denote $D := \mathrm{diag}(\alpha_j)$
- Let $J : S \longrightarrow \mathbb{R}$ be defined by

$$J(U) := \mathrm{tr}(DU^* AU) = \sum_{j=1}^{n} \alpha_j (U^* AUe_j | e_j). \tag{2.3}$$

A global approach: finite dimensional space

- We show the following

  Theorem. *The functional J is smooth and achieves its minimum on $\mathbb{S}$, at some $U_0 \in \mathbb{S}$. Moreover if $u_j := U_0 e_j$, then $(u_j)_{1 \le j \le n}$ is the eigensystem of A.*

Finite dimension: Idea of proof

- Let M be skew-adjoint, that is $M^* = -M$. Then for all $t \in \mathbb{R}$ we have

$$U(t) := \exp(tM)U_0 \in \mathbb{S}.$$

- Thus for all $t \in \mathbb{R}$ we have $J(U_0) \leq J(U(t))$
- We conclude that

$$\left(\frac{d}{dt} J(U(t))\right)_{|t=0} = 0.$$

- This means that for all M such that $M^* = -M$

$$\operatorname{tr}(DU_0^* MAU_0) = \operatorname{tr}(DU_0^* AMU_0).$$

- Setting $B := U_0 D U_0^*$, we have that for all M such that $M^* = -M$,

$$\operatorname{tr}(M(AB - BA)) = 0$$

Finite dimension: Idea of proof

- This implies that $BA = AB$, that is

$$U_0 D U_0^* A = A U_0 D U_0^*.$$

- Set $u_j := U_0 e_j$, and apply the above operators to u_j

$$(U_0 D U_0^*) A u_j = A U_0 D U_0^* u_j = A U_0 D e_j = \alpha_j A U_0 e_j = \alpha_j A u_j,$$

- Thus $U_0 D U_0^* A u_j = \alpha_j A u_j$, and

$$D(U_0^* A u_j) = \alpha_j (U_0^* A u_j).$$

- Since α_j is a simple eigenvalue of D, with a corresponding eigenvector e_j, and since $A u_j \neq 0$ we conclude that

$$U_0^* A u_j = \lambda_j e_j \iff A u_j = \lambda_j u_j.$$

and finally $U_0^* A U_0 = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$.

♡

A global approach: infinite dimension

A global approach: infinite dimension

- **Assumptions:** H infinite dimensional, separable, complex Hilbert space, scalar product $(\cdot|\cdot)$, norm $\|\cdot\|$.
- $(A, D(A))$ operator H, with $D(A) \subset H$ dense and compact, $A^* = A \geq 0$.
- $(e_j)_{j\geq 1}$ a Hilbert basis of H, such that $e_j \in D(A^{1/2})$ for each $j \geq 1$.
- $(\alpha_j)_{j\geq 1}$, with $\alpha_j > 0$, such that

  (3.1) $$\sum_{j\geq 1} \alpha_j \|e_j\|^2_{D(A^{1/2})} < \infty,$$

  and we denote by D the diagonal operator defined by $De_j := \alpha_j e_j$ for $j \geq 1$ (note that $\alpha_j \to 0$ and D is compact).
- Consider $U : H \longrightarrow H$ such that

  (3.2) $$U^*U = UU^* = I, \quad Ue_j \in D(A^{1/2}) \text{ for } j \geq 1, \quad \sum_{j\geq 1} \alpha_j (U^*AUe_j|e_j) < \infty.$$

A global approach: infinite dimension

- Define the set $\mathbb{S}$ by

$$\mathbb{S} := \Big\{ U : H \longrightarrow H \;;\; U \text{ satisfies } \textbf{(3.2)} \Big\}.$$

$\mathbb{S} \neq \emptyset$ is non trivial: for $\lambda > 0$, one has $\mathrm{e}^{\mathrm{i}\lambda A} \in \mathbb{S}$ and $U_\lambda := (I + \mathrm{i}\lambda A)(I - \mathrm{i}\lambda A)^{-1} \in \mathbb{S}$

- For $U \in \mathbb{S}$ define $J_0(U)$ by

$$J_0(U) := \operatorname{tr}(DU^* AU) := \sum_{j \geq 1} \alpha_j (U^* AU e_j | e_j) \tag{3.3}$$

Theorem. *J_0 achieves its minimum on $\mathbb{S}$. There exists $\widehat{U}_0 \in \mathbb{S}$ such that*

$$J_0(\widehat{U}_0) = \min_{U \in \mathbb{S}} J_0(U),$$

and $\widehat{U}_0$ is a diagonalization operator for A; more precisely, for each $j \geq 1$, the vector $\varphi_j := \widehat{U}_0 e_j$ is an eigenvector of A corresponding to the eigenvalue $\lambda_j := (A\varphi_j | \varphi_j)$.

Infinite dimension: idea of proof

- Consider $b := \inf_{U \in \mathbb{S}} J_0(U) \geq 0$.
- Let $(U_n)_{n \geq 1} \in \mathbb{S}$ be such that $b \leq J(U_n) \leq b + 1/n \leq b + 1$.
- For fixed $j \geq 1$, setting $u_j^n := U_n e_j$, we have for all $n \geq 1$

$$\|u_j^n\|^2_{D(A^{1/2})} = 1 + (Au_j^n | u_j^n) \leq 1 + \frac{b+1}{\alpha_j}.$$

- By Cantor's diagonal scheme, one finds a subsequence (denoted by) $(u_j^n)_n$ such that there exists a family $(u_j)_j$ such that for $j \geq 1$ fixed

$$u_j^n \rightharpoonup u_j =: U_0 e_j \quad \text{weakly in } D(A^{1/2}), \qquad u_j^n \to u_j =: U_0 e_j \quad \text{strongly in } H.$$

- U_0 can be extended to H, and ${U_0}^* U_0 = I$.
- Finally, one shows that $J_0(U_0) < \infty$ and $U_0 \in \mathbb{S}$ and that $J_0(U_0) = b$.

Infinite dimension: idea of proof

- Let $M : H \longrightarrow H$ be bounded, skew-adjoint, that is $M^* = -M$, and moreover $M : D(A^{1/2}) \longrightarrow D(A^{1/2})$ continuous. Then for all $t \in \mathbb{R}$ we have

$$U(t) := \exp(tM)U_0 \in \mathbb{S}.$$

- Thus for all $t \in \mathbb{R}$ we have $J(U_0) \leq J(U(t)) =: g_0(t)$. We conclude that $g_0'(0) = \mathrm{tr}(DU_0{}^*MAU_0) - \mathrm{tr}(DU_0{}^*AMU_0) = 0$.

- Since $\mathrm{tr}(DU_0{}^*MAU_0) = -\sum_j \alpha_j(Au_j|Mu_j)$ and $\mathrm{tr}(DU_0{}^*AMU_0) = \sum_j \alpha_j(Mu_j|Au_j)$ this means

$$\mathrm{Re} \sum_{j\geq 1} \alpha_j(Au_j|Mu_j) = 0. \tag{3.4}$$

- Choosing $M := \mathrm{i}L$ with $L^* = L$, one gets

$$\mathrm{Im} \sum_{j\geq 1} \alpha_j(Au_j|Lu_j) = 0. \tag{3.5}$$

Infinite dimension: idea of proof

- Let $n \neq k$ and let the operators M and L be defined by:

$$Mu_k := u_n, \quad Mu_n := -u_k, \quad Lu_k := u_n, \quad Lu_n := u_k, \quad Lu_j = Mu_j = 0 \text{ if } j \notin \{k, n\}.$$

- Using **(3.4)** and **(3.5)**, we conclude that

$$(\alpha_n - \alpha_k)(Au_n|u_k) = 0.$$

- Thus if $\alpha_n \neq \alpha_k$, we have

$$0 = (Au_n|u_k) = ({U_0}^* A U_0 e_n|e_k).$$

- Assume for instance for all $n \neq k$ one has $\alpha_n \neq \alpha_k$. Then the above means that

$${U_0}^* A U_0 e_n \in \operatorname{span}\{e_n\} \iff \exists\, \lambda_n \in \mathbb{R}, \quad Au_n = \lambda_n u_n.$$

♡

Remarks

Remarks

- When in **(2.3)** one chooses $\alpha_j > \alpha_{j+1}$ for all $j \geq 1$, then one can check that the eigenvalues λ_j are ordered in a non decreasing order.
- In the infinite dimenional case, a typical example of application is the case

$$Au := -\Delta u + Vu, \qquad \text{for } u \in D(A),$$

with

$$D(A) := \left\{ u \in H_0^1(\Omega) \; ; \; -\Delta u + Vu \in L^2(\Omega) \right\}.$$

- Here $\Omega \subset \mathbb{R}^N$ is bounded, and $V^+ \in L^1_{\mathrm{loc}}(\Omega)$ while $V^- \in L^p(\Omega)$ for some $p > N/2$.
- In the case of $\Omega = \mathbb{R}^N$, one can adapt the above method if one assumes that there exists a sequence $(e_j)_{j\geq 1}$ which is total in $L^2(\mathbb{R}^N)$ and such that

$$\int_{\mathbb{R}^N} e_j(x)\overline{e_k}(x)dx = \delta_{kj}, \quad \text{and for all } j \geq 1, \quad \int_{\mathbb{R}^N} \left(|\nabla e_j|^2 + V|e_j(x)|^2 \right) dx < 0.$$

Remarks

- Bob Kohn mentioned to us a result due to J. von Neumann which states that for two $n \times n$ matrices A and B

$$|\mathrm{tr}(AB)| \leq \sum_{j=1}^{n} \sigma_j(A)\sigma_j(B)$$

  where $(\sigma_j(A))_{1\leq j\leq n}$ and $(\sigma_j(B))_{1\leq j\leq n}$ denote the decreasing singular values of A and B respectively.

- From this L. Mirsky (1975) points out that one can conclude another result due to J. von Neumann, stating that:

$$\sup_{U,V} |\mathrm{tr}(BUAV)| = \sum_{j=1}^{n} \sigma_j(A)\sigma_j(B).$$

- Our result, which is specialized to self-adjoint matrices, can be interpreted as another proof of the above result in that particular case, and also characterizes the diagonalization matrice by a variational method.