# Numerical aspects of relative Krein spectral shift function in acoustic scattering and Casimir energy computation

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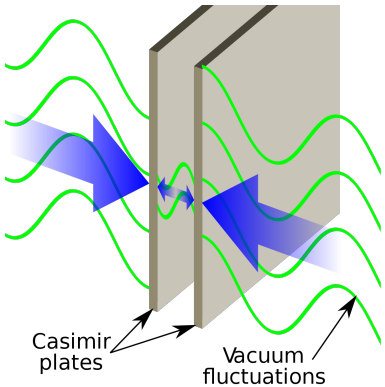
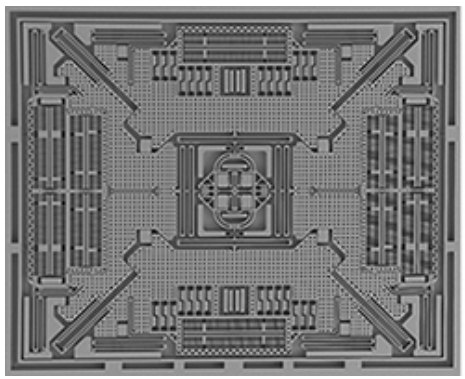
# Introduction: Definition and application

- Sum of zero-point energy

$$\mathcal{E}(a) = \frac{1}{2}\sum_n \hbar\omega_n(a),$$




- MEMS (Micro-Electro-Mechanical Systems)

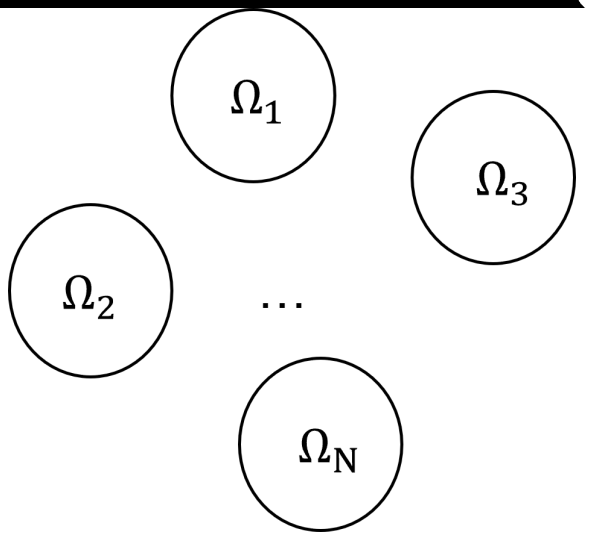


# Outline

- Introduce the Krein spectral shift function (KSSF)
- Derive the formula of Casimir energy via the KSSF
- Speed up Casimir computations for large-scale practical problems
- Numerical experiments

# Krein spectral shift function (KSSF)

$$\xi(k) = \frac{1}{2\pi \mathrm{i}} \log\left(\frac{\det(S_k)}{\det(S_{1,k}) \cdots \det(S_{N,k})}\right)$$




- $k$ is the wavenumber
- $S_{i,k} = I + 2T_{i,k}$ is the scattering matrix associated with the $i$th object
- $T_{i,k}$ is the $T$-matrix associated with the $i$th object

**Birman-Krein Formula**

$$\mathrm{Tr}\left(f(\Delta^{\frac{1}{2}}) - f(\Delta_0^{\frac{1}{2}}) - \left(\sum_{j=1}^{N}[f(\Delta_j^{\frac{1}{2}}) - f(\Delta_0^{\frac{1}{2}})]\right)\right) = \int_0^{\infty} f'(k)\xi(k)dk$$

# Derive the Casimir energy via KSSF

**Birman-Krein Formula**

$$\mathrm{Tr}\left(f(\Delta^{\frac{1}{2}}) - f(\Delta_0^{\frac{1}{2}}) - \left(\sum_{j=1}^{N}[f(\Delta_j^{\frac{1}{2}}) - f(\Delta_0^{\frac{1}{2}})]\right)\right) = \int_0^{\infty} f'(k)\xi(k)dk$$

When $f(x) = x$:

$$Tr\left(\Delta^{\frac{1}{2}} + (N-1)\Delta_0^{\frac{1}{2}} - \sum_{i=1}^{N}\Delta_j^{\frac{1}{2}}\right) = \int_0^{\infty}\xi(k)dk$$

**Casimir energy formula[a] — Scattering matrix method**

$$\mathcal{E}_{\mathbf{sca}} = \frac{\hbar c}{2}\int_0^{\infty}\xi(k)dk$$

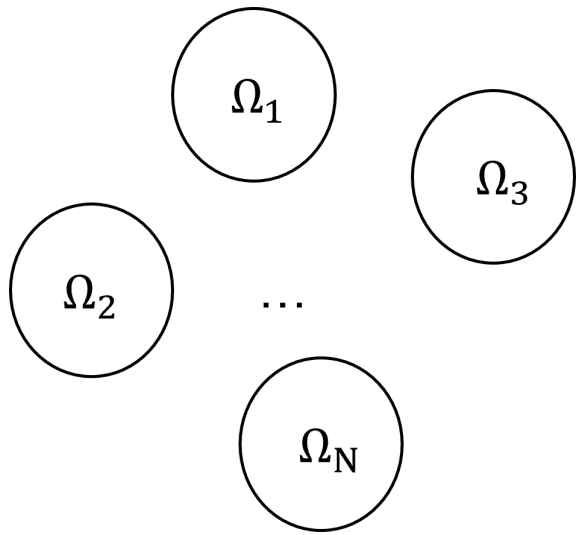
[a] Hanisch F, Strohmaier A, Waters A. A relative trace formula for obstacle scattering[J]. arXiv preprint arXiv:2002.07291, 2020.

# Derive the Casimir energy via KSSF

- $\Omega$: a domain assembling from individual objects $\Omega_i$
- $V_k$: the single-layer boundary operator defined on the boundary $\partial\Omega = \bigcup_{i=1}^{N} \partial\Omega_i$
- $\tilde{V}_k$: the "diagonal part" of $V_k$ by restricting the integral kernel to the subset $\bigcup_{i=1}^{N} \partial\Omega_i \times \partial\Omega_i \subset \partial\Omega \times \partial\Omega$

Define:

$$\Xi(k) = \log\det\left(V_k \tilde{V}_k^{-1}\right)$$




**Relation between the single-layer operator and KSSF**
For $k > 0$,

$$-\frac{1}{\pi}\mathrm{Im}\Xi(k) = \frac{\mathrm{i}}{2\pi}(\Xi(k) - \Xi(-k)) = \xi(k)$$

# Derive the Casimir energy via KSSF

**Relation between the single-layer operator and KSSF**

For $k > 0$,

$$-\frac{1}{\pi}\mathrm{Im}\Xi(k) = \frac{\mathrm{i}}{2\pi}(\Xi(k) - \Xi(-k)) = \xi(k)$$

This relation can help to derive:

**Casimir energy formula[a] — Single-layer operator method**

$$\mathcal{E}_{\mathbf{slp}} = -\frac{\hbar c}{2\pi}\int_0^\infty \Xi(\mathrm{i}k)dk$$

[a] Hanisch F, Strohmaier A, Waters A. A relative trace formula for obstacle scattering[J]. arXiv preprint arXiv:2002.07291, 2020.

# Compute the Casimir energy

**Casimir energy formula — Single-layer operator method**

$$\mathcal{E}_{\mathbf{slp}} = -\frac{\hbar c}{2\pi}\int_0^\infty \Xi(\mathrm{i}k)dk = -\frac{\hbar c}{2\pi}\int_0^\infty \log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right)dk$$

- Task 1: Compute the integrand $\log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right)$ by using the Galerkin discretization form of operators
- Task 2: Evaluate the integral $\int_0^\infty \log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right)dk$ via the trapezoidal rule

# Compute the Casimir energy

**Task 1**: Compute the integrand $\log\det\left(V_{ik}\tilde{V}_{ik}^{-1}\right)$ by using the Galerkin discretization form of operators

**Single-layer boundary operator:**

$$(V_k\mu)(\boldsymbol{x}) := \int_\Gamma g_k(\boldsymbol{x},\boldsymbol{y})\psi(\boldsymbol{y})dS_{\boldsymbol{y}}, \qquad \text{for } \mu \in H^{-\frac{1}{2}}(\Gamma) \text{ and } \boldsymbol{x} \in \Gamma,$$

where

$$g_k(\boldsymbol{x},\boldsymbol{y}) = \begin{cases} \frac{\mathrm{i}}{4}H_0^{(1)}(k|\boldsymbol{x}-\boldsymbol{y}|), & \text{for } d=2 \\ \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}, & \text{for } d=3. \end{cases}$$

To discretize it, we define the continuous piecewise linear basis functions:

$$P_h^1(\Gamma) := \operatorname{span}\{\phi_j\} \subset H^{-\frac{1}{2}}(\Gamma)$$

with

$$\phi_j(\boldsymbol{x}_j) = \begin{cases} 1, & i=j, \\ 0, & i\neq j. \end{cases}$$

# Compute the Casimir energy

**Task 1**: Compute the integrand $\log\det\left(V_{ik}\,\tilde{V}_{ik}^{-1}\right)$ by using the Galerkin discretization form of operators

**Matrix representation of Galerkin discretised single-layer boundary operator:**

$$\mathrm{V}_k = \begin{bmatrix} \mathrm{V}_{11}(k) & \cdots & \mathrm{V}_{1N}(k) \\ \vdots & \ddots & \vdots \\ \mathrm{V}_{N1}(k) & \cdots & \mathrm{V}_{NN}(k) \end{bmatrix}, \quad \tilde{\mathrm{V}}_k = \begin{bmatrix} \mathrm{V}_{11}(k) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathrm{V}_{NN}(k) \end{bmatrix},$$

where

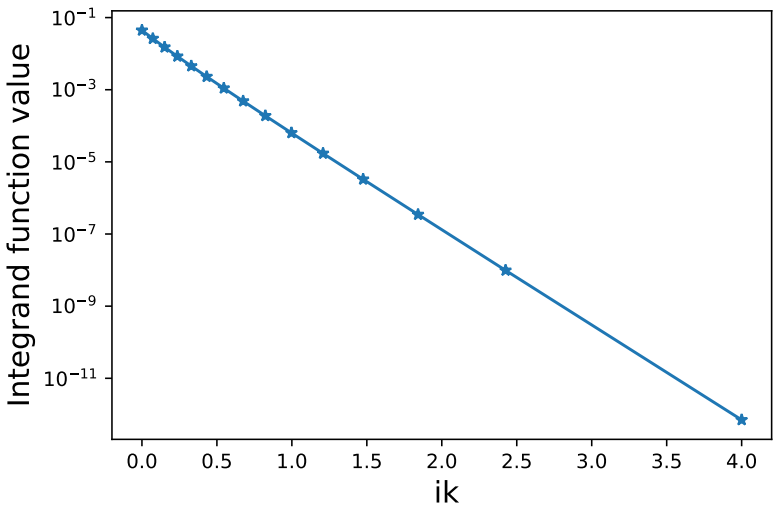
$$\mathrm{V}_{ij}^{(m,n)}(k) = \langle V_{ij}(k)\phi_m^{(i)}, \phi_n^{(j)} \rangle = \int_\Gamma \overline{\phi_n^{(j)}}(\boldsymbol{x}) \int_\Gamma g_k(\boldsymbol{x},\boldsymbol{y})\phi_m^{(i)}(\boldsymbol{y}) dS_{\boldsymbol{y}} dS_{\boldsymbol{x}}$$

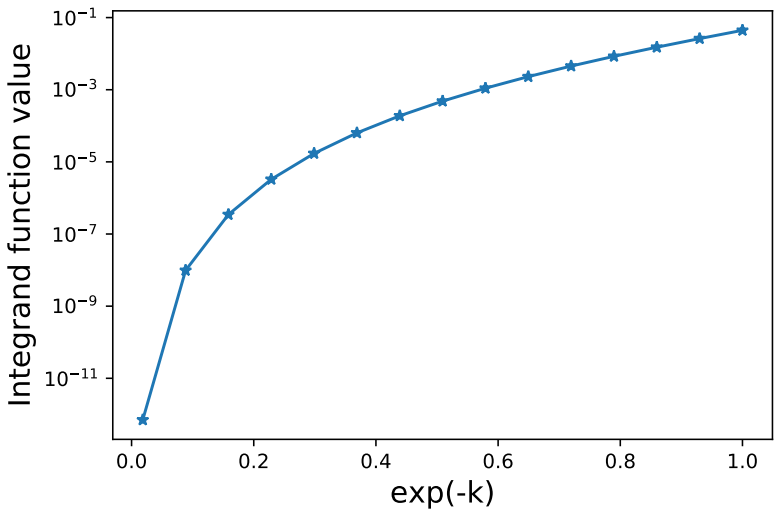
and $\phi^{(i)} = \begin{bmatrix} \phi_1^{(i)} & \phi_2^{(i)} & \dots & \phi_N^{(i)} \end{bmatrix} \subset P_h^1(\Gamma)$ is the set of basis functions defined on the $i$th object.

# Compute the Casimir energy

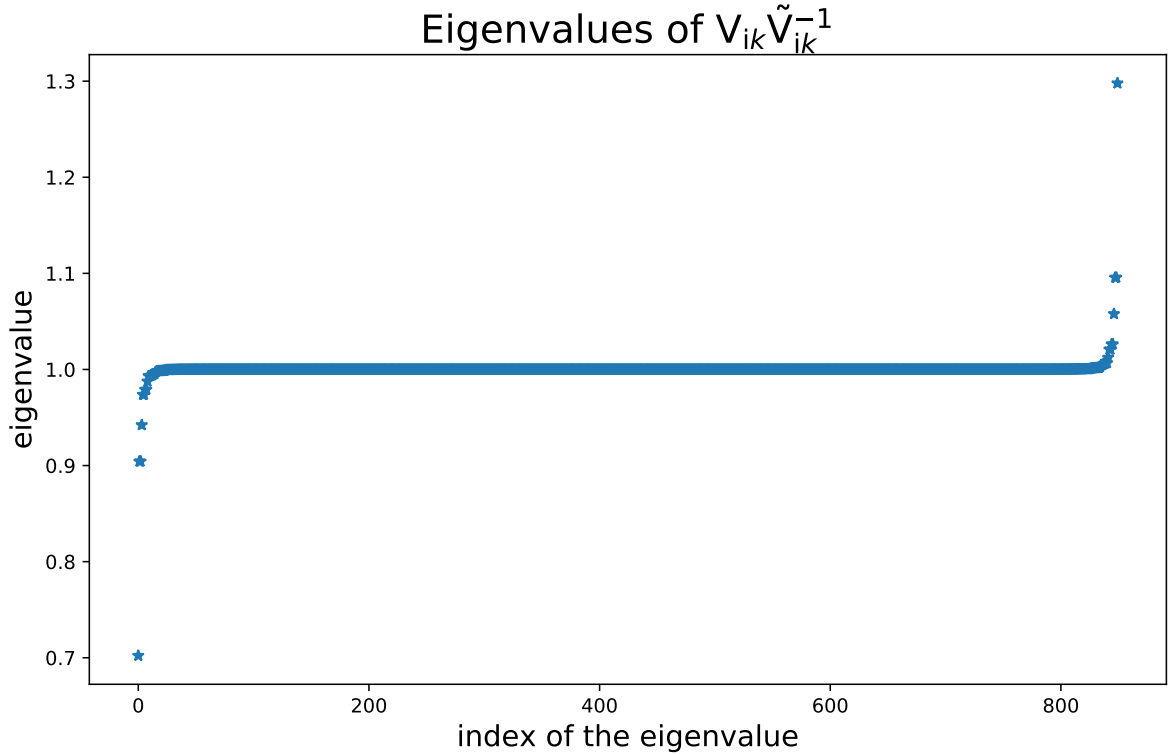
**Task 2**: Evaluate the integral $\int_0^\infty \log\det\left(V_{ik}\,\tilde{V}_{ik}^{-1}\right) dk$ via the trapezoidal rule

- (Left) The integrand value $\log\det\left(V_{ik}\,\tilde{V}_{ik}^{-1}\right)$ exponentially decay with the increasing $k$.
- (Right) By changing the variable from $k$ to $k = -\log(y)$, we can apply the normal trapezoidal rule to compute the integral.



Most of the eigenvalues of $V_{\mathrm{i}k}\,\tilde{V}_{\mathrm{i}k}^{-1}$ are around 1, which contribute nothing on the log determinant.




The eigenvalues of the matrix $V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}$ when $\mathrm{i}k = 0.8\mathrm{i}$.

**Method I:** Inverse-free Krylov subspace method for computing $p$ smallest (or largest) eigenvalues of $\mathrm{V}_{ik}\tilde{\boldsymbol{x}} = \lambda\tilde{\mathrm{V}}_{ik}\tilde{\boldsymbol{x}}$.

Input: Symmetric $A \in \mathbb{R}^{n\times n}$, s.p.d $B \in \mathbb{R}^{n\times n}$ and $X^{(1)} \in \mathbb{R}^{n\times p}$ with $X^{(1)*}BX = I_p$ and $m \geq 1$
Output: The approximated $p$ smallest eigenvalues of $A\boldsymbol{x} = \lambda B\boldsymbol{x}$

1: Set $\Theta^{(1)} = \mathrm{diag}(X^{(1)*}AX^{(1)})$
2: **for** $k = 1, 2, \ldots$ **do**
3:  **for** $i = 1, 2, \ldots, p$ **do**
4:  Construct a basis $\hat{Z}_i$ of the $i$th Krylov subspace $K_m(A - \theta_i^{(k)}B, x_i^{(k)})$ with dimension $m$
5:  Orthonormalize $\left[\hat{Z}_1 \cdots \hat{Z}_p\right]$ to obtain $Z$
6:  Project $A$ and $B$ on $Z$: $A_m = Z^*AZ$, $B_m = Z^*BZ$
7:  Compute $p$ smallest eigenpairs $(\theta_i, u_i)$, $1 \leq i \leq p$ of the matrix pencil $(A_m, B_m)$
8:  $\Theta^{(k+1)} = \mathrm{diag}(\theta_1, \ldots, \theta_p)$; $X^{(k+1)} = ZU$, $U = (u_1 \cdots u_p)$
9:  **end for**
10: **end for**

**Method II:** LU decomposition for inverting the matrix.

$$\tilde{\mathrm{V}}_{\mathrm{i}k}^{-1} = \begin{bmatrix} \mathrm{V}_{11}^{-1}(\mathrm{i}k) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathrm{V}_{NN}^{-1}(\mathrm{i}k) \end{bmatrix}$$

For each block $\mathrm{V}_{ii} = \mathrm{V}_{ii}(\mathrm{i}k)$, for $i = 1, 2, \ldots, N$:

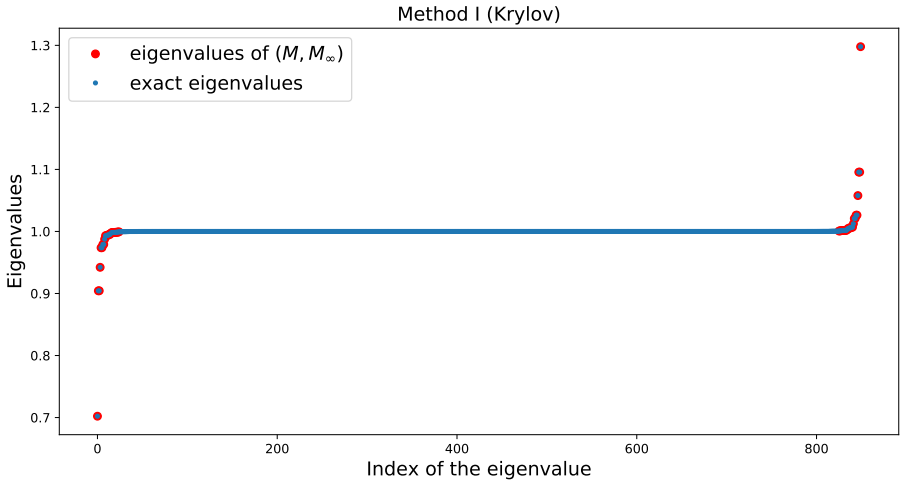
- Compute its LU decomposition $\mathrm{V}_{ii} = \mathrm{L}_{ii}\mathrm{U}_{ii}$
- Solve the linear system $\mathrm{L}_{ii}\mathrm{U}_{ii}\boldsymbol{x_j} = \boldsymbol{e}_j$, for $j = 1, 2, \ldots, N_{\mathrm{V}_{ii}}$
- $\mathrm{V}_{ii}^{-1} = \begin{bmatrix} \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_{N_{\mathrm{V}_{ii}}} \end{bmatrix}$

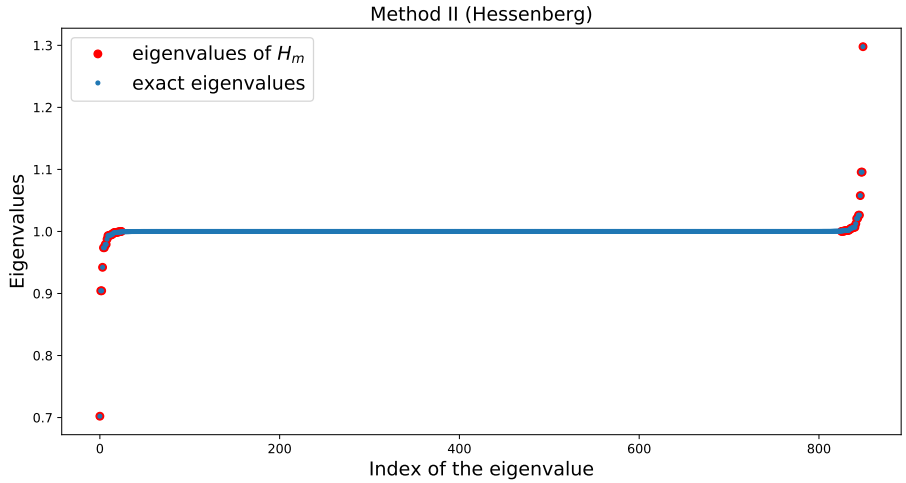
**Method II:** LU decomposition for inverting the matrix.

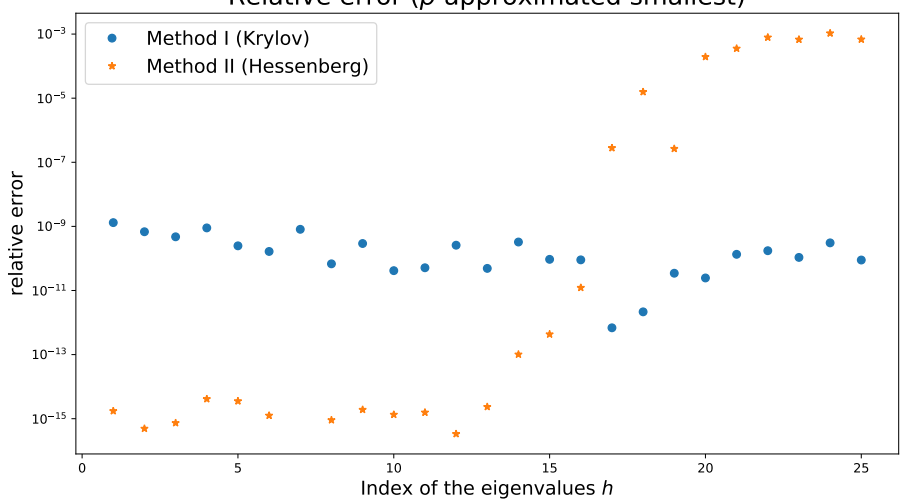
- Define the inverse of the matrix $\tilde{\mathrm{V}}_{ik}$ computed by the inverse-free *LU* decomposition method as $\tilde{\mathrm{V}}_{ik}^{-1,\mathrm{LU}}$.
- Compute the basis of the Krylov subspace $K_m(\mathrm{V}_{ik}\tilde{\mathrm{V}}_{ik}^{-1,\mathrm{LU}}, \boldsymbol{b})$ and project via the Arnoldi iterations and project $\mathrm{V}_{ik}\tilde{\mathrm{V}}_{ik}^{-1,\mathrm{LU}}$ onto it to obtain the Hessenberg matrix $H_m$.
- The eigenvalues of Hessenberg matrix can be used to approximate extreme eigenvalues of $\mathrm{V}_{ik}\tilde{\mathrm{V}}_{ik}^{-1,\mathrm{LU}}$

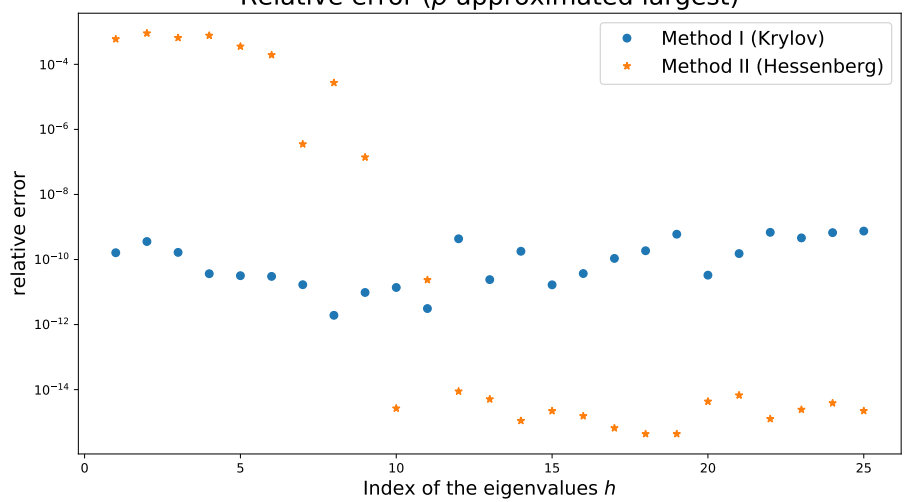
# Compare two inverse-free methods

Compare the exact eigenvalues of $V_{ik}\tilde{V}_{ik}^{-1}$ with approximated ones ($m = 50$)

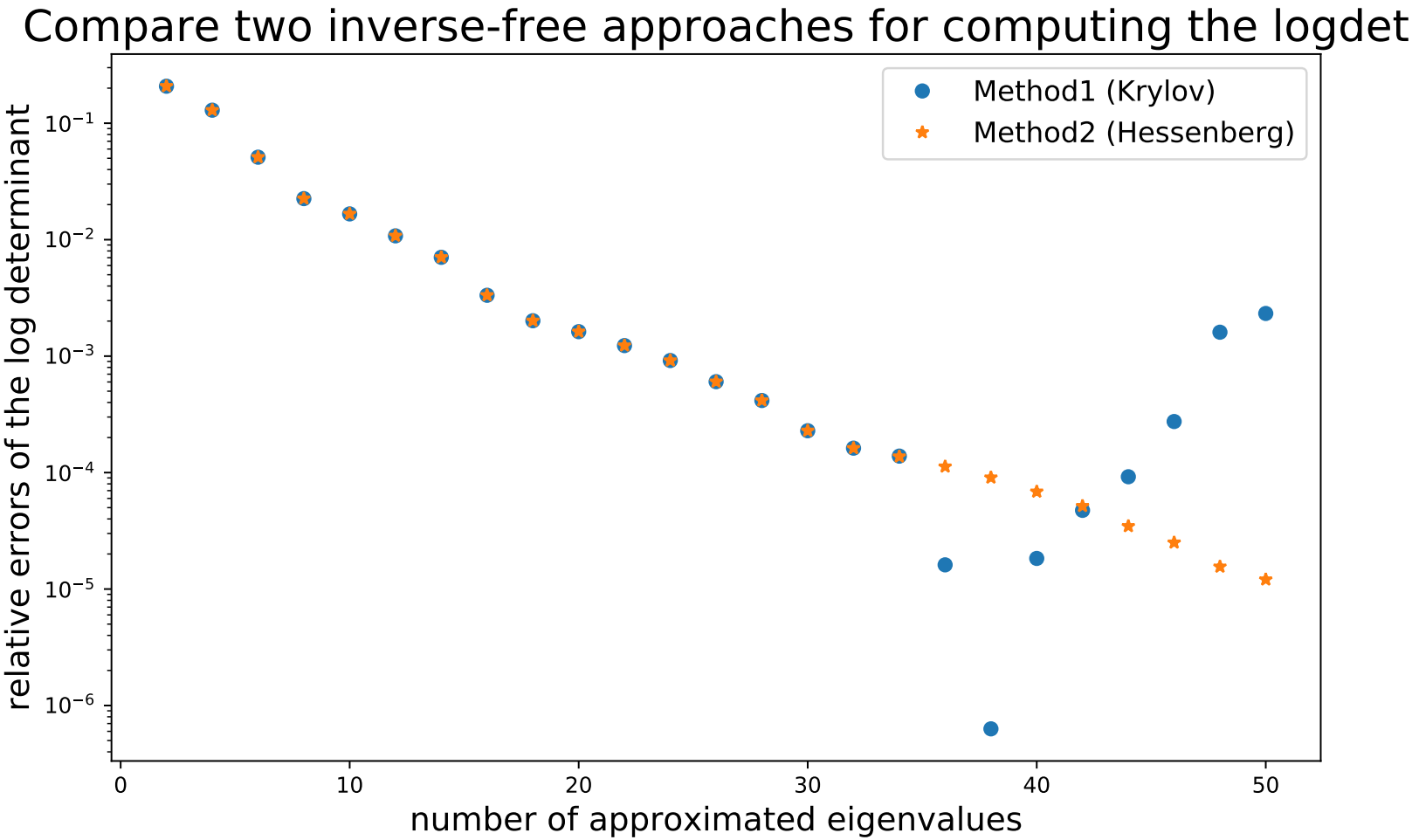


# Compare two inverse-free methods



# Summary

- Casimir energy can be computed via evaluating the log determinant of the single-layer boundary operators
- Efficiently computing the Casimir enengy by avoiding computing any inverse matrix and only approximating multiple extreme eigenvalues.
- Next step is to focus on the maxwell case, which needs us to change the operator to the electric field boundary operator.

# Papers


- Hanisch F, Strohmaier A, Waters A. *A relative trace formula for obstacle scattering*. arXiv preprint arXiv:2002.07291, 2020. **[KSSF and Casimir energy]**
- Quillen P, Ye Q. *A block inverse-free preconditioned Krylov subspace method for symmetric generalized eigenvalue problems*. Journal of computational and applied mathematics, 2010, 233(5): 1298-1313. **[Inverse-free Krylov subspace method for generalized eigenvalue problem]**
- Saad Y. *Numerical methods for large eigenvalue problems: revised edition*. Society for Industrial and Applied Mathematics, 2011. **[Arnoldi iteration]**