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

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Casimir energy

Sum of zero-point energy:

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

a: the distance between two plates

$\omega_n(a)$: nth cavity mode frequency

Casimir force per unit area

$$F(a) = -\frac{1}{A}\frac{\partial\mathcal{E}}{\partial a} = -\frac{\hbar c\pi^2}{240a^4}$$

A: the area of the boundary plates

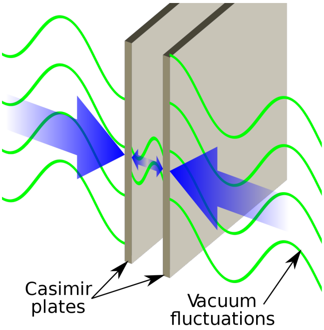
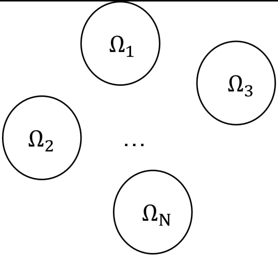


Image: Emok, "Casimir forces on parallel plates ", Wikipedia, *https://en.wikipedia.org/wiki/Casimir_effect/media/File:Casimir_plates.svg*

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)



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 ith object
- $T_{i,k}$ is the T-matrix associated with the ith 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 $f(x) = x$:

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

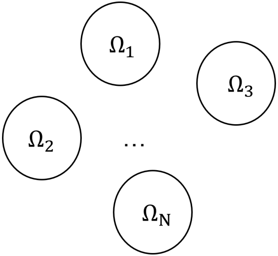
Casimir energy formula[a] — Scattering matrix method

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

[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

- Ω: a domain assembling from individual objects Ω_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] [b] — 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.

[b] Reid M T H, Rodriguez A W, White J, et al. Efficient computation of Casimir interactions between arbitrary 3D objects[J]. Physical review letters, 2009, 103(4): 040401.

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 $\log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right)$ by using the Galerkin discretization form of operators

Single-layer boundary operator:

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

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:

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

with

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

Matrix representation of Galerkin discretised single-layer boundary operator:

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

where

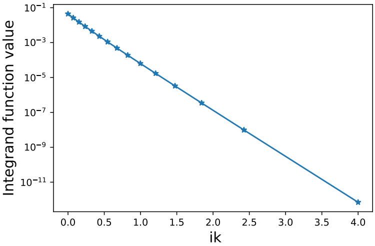
$$\mathrm{V}_{ij}^{(m,n)}(k) = \langle V_{ij}(k)\phi_m^{(i)}, \phi_n^{(j)} \rangle = \int_\Gamma \overline{\phi_n^{(j)}}(\boldsymbol{x}) \int_\Gamma g_k(\boldsymbol{x}, \boldsymbol{y})\phi_m^{(i)}(\boldsymbol{y}) dS_{\boldsymbol{y}} dS_{\boldsymbol{x}}$$

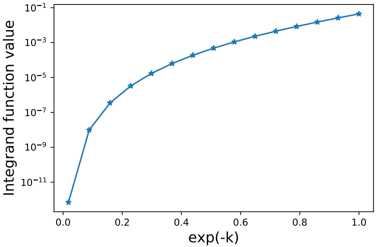
and $\phi^{(i)} = \begin{bmatrix} \phi_1^{(i)} & \phi_2^{(i)} & \ldots & \phi_N^{(i)} \end{bmatrix} \subset P_h^1(\Gamma)$ is the set of basis functions defined on the ith object.

Compute the Casimir energy

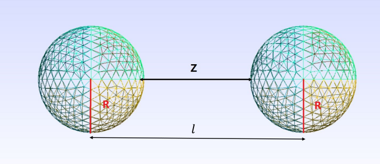
Task 2: Evaluate the integral $\int_0^\infty \log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right) dk$ via the trapezoidal rule

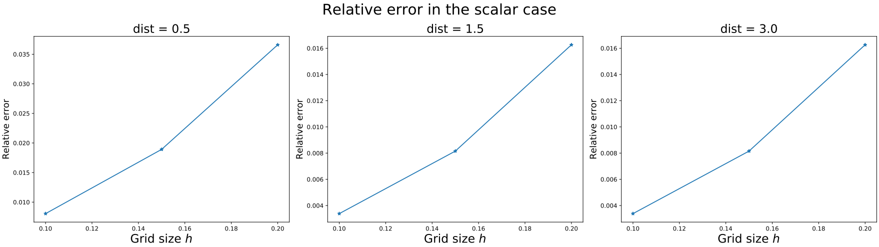
- (Left) The integrand value $\log\det\left(V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}\right)$ exponentially decay with the increasing k.
- (Right) By changing the variable from k to y with $k = -\log(y)$, we can apply the normal trapezoidal rule to compute the integral.



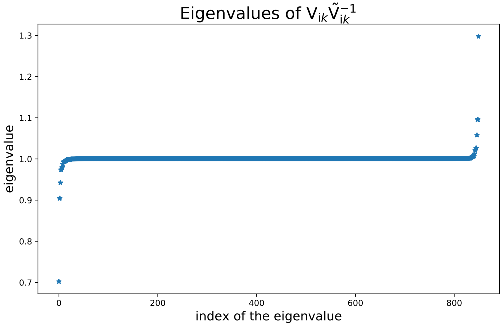


Numerical experiments: *h*-convergence





Speed up Casimir computations



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

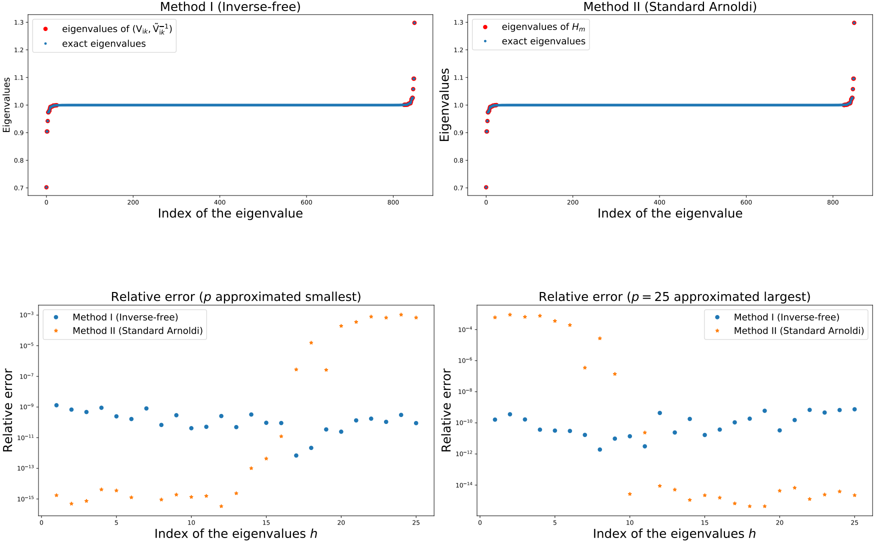
$\tilde{V}_{ik}$ is a compact perturbation of V_{ik} $\implies$ most of the eigenvalues of $V_{ik}\tilde{V}_{ik}^{-1}$ are around 1, which contribute nothing on the log determinant.

Speed up Casimir computations

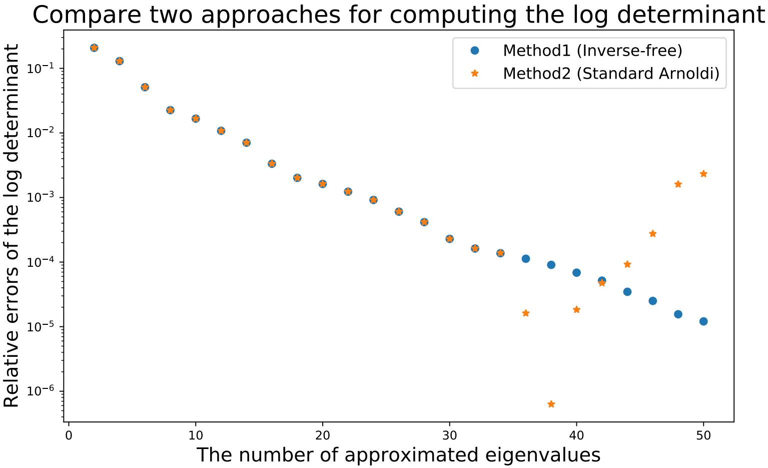
- **Method I:** Inverse-free Krylov subspace method for computing p smallest (largest) eigenvalues of $\mathrm{V}_{\mathrm{i}k}\tilde{\boldsymbol{x}} = \lambda\tilde{\mathrm{V}}_{\mathrm{i}k}\tilde{\boldsymbol{x}}$ ($\mathrm{V}_{\mathrm{i}k}\tilde{\mathrm{V}}_{\mathrm{i}k}^{-1}\tilde{\boldsymbol{x}} = \lambda\tilde{\boldsymbol{x}}$).
  - Construct a basis $\hat{Z}_i$ of the ith Krylov subspace $K_m(\mathrm{V}_{\mathrm{i}k} - \theta_i\tilde{\mathrm{V}}_{\mathrm{i}k}, x_i)$ with dimension m, for $i = 1, 2, \ldots, p$
  - Orthonormalize $\left[\hat{Z}_1 \cdots \hat{Z}_p\right]$ to obtain Z and project $\mathrm{V}_{\mathrm{i}k}$ and $\tilde{\mathrm{V}}_{\mathrm{i}k}$ on Z
  - Compute the p smallest (or largest) eigenvalues for this pair of projected matrices
- **Method II:** LU decomposition for inverting the matrix.
  - Use LU decomposition to compute the inverse of each diagonal block matrix in $\tilde{\mathrm{V}}_{\mathrm{i}k}$
  - Apply the standard Arnoldi iterations on $V_{\mathrm{i}k}\tilde{V}_{\mathrm{i}k}^{-1}$ to compute projected Hessenberg matrix

Compare two methods

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



Compare two 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 directyly computing the 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.

Bonus: Casimir energy in the Maxwell case

- Ω: a domain assembling from individual objects Ω_i
- M_k: the Maxwell electric-field boundary operator defined on the boundary $\partial\Omega = \bigcup_{i=1}^{N} \partial\Omega_i$
- $\tilde{M}_k$: the “diagonal part” of M_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

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

Casimir energy formula[a] — electric-field operator method

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

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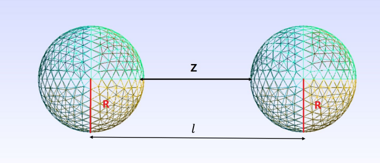
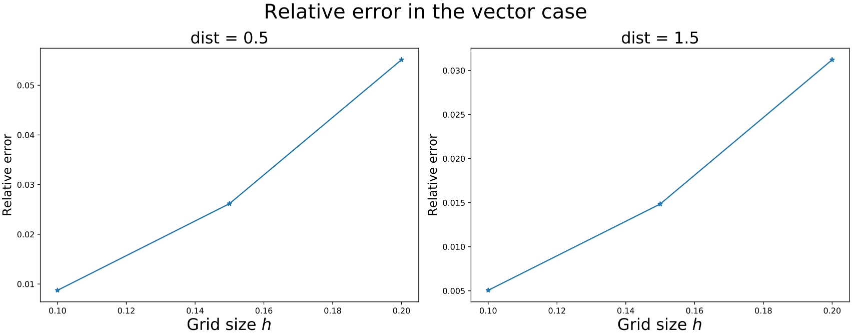
Numerical experiments: *h*-convergence





Papers

- Xiaoshu Sun, Timo Betcke, Alexander Strohmaier. *Numerical aspects of Casimir energy computation in acoustic scattering* (2021) [**In preparation**]
- Casimir H B G, Polder D. *The influence of retardation on the London-van der Waals forces[J]*. Physical Review, 1948, 73(4): 360. [**First Casimir paper**]
- Reid M T H, Rodriguez A W, White J, et al. Efficient computation of Casimir interactions between arbitrary 3D objects[J]. Physical review letters, 2009, 103(4): 040401. [**Casimir energy derived from the path-integral expression**]
- 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]**