

# 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

$\omega_n(a)$ :  $n$ th cavity mode frequency

## Casimir force per unit area

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

$A$ : the area of the boundary plates

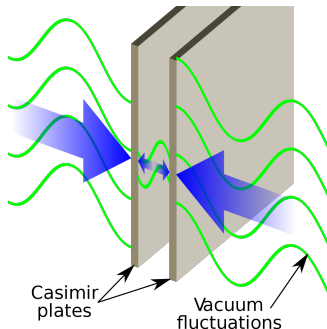
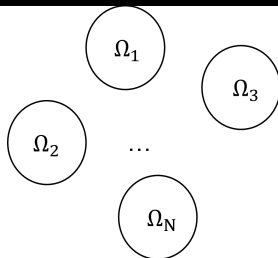


Image: Emok, "Casimir forces on parallel plates ", Wikipedia,  
[https://en.wikipedia.org/wiki/Casimir\\_effect/media/File:Casimir\\_plates.svg](https://en.wikipedia.org/wiki/Casimir_effect/media/File:Casimir_plates.svg)

- 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)

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



- $k$  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

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

## Birman-Krein Formula

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When  $f(x) = x$ :

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

## Casimir energy formula<sup>a</sup> — Scattering matrix method

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

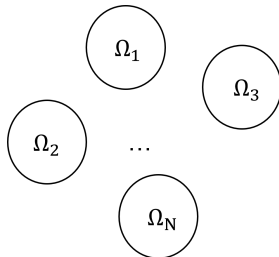
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<sup>a</sup>Hanisch F, Strohmaier A, Waters A. A relative trace formula for obstacle scattering[J]. arXiv preprint arXiv:2002.07291, 2020.

- $\Omega$ : 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  $k > 0$ ,

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

## Relation between the single-layer operator and KSSF

For  $k > 0$ ,

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

This relation can help to derive:

## Casimir energy formula<sup>a b</sup> — Single-layer operator method

$$\mathcal{E}_{\text{slp}} = -\frac{\hbar c}{2\pi} \int_0^\infty \Xi(ik) dk$$

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

<sup>b</sup>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 formula — Single-layer operator method

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

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



**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:**

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

where

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

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

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

with

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

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

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

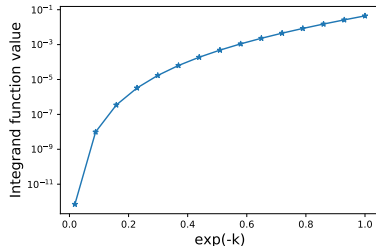
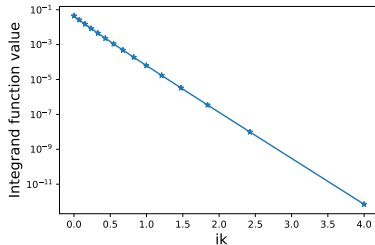
where

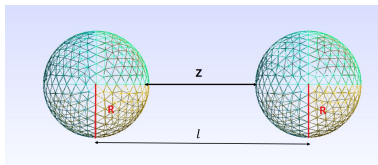
$$V_{ij}^{(m,n)}(k) = \langle V_{ij}(k) \phi_m^{(i)}, \phi_n^{(j)} \rangle = \int_{\Gamma} \overline{\phi_n^{(j)}}(\mathbf{x}) \int_{\Gamma} g_k(\mathbf{x}, \mathbf{y}) \phi_m^{(i)}(\mathbf{y}) dS_{\mathbf{y}} dS_{\mathbf{x}}$$

and  $\phi^{(i)} = [\phi_1^{(i)} \quad \phi_2^{(i)} \quad \cdots \quad \phi_N^{(i)}] \subset P_h^1(\Gamma)$  is the set of basis functions defined on the  $i$ th object.

**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  $y$  with  $k = -\log(y)$ , we can apply the normal trapezoidal rule to compute the integral.

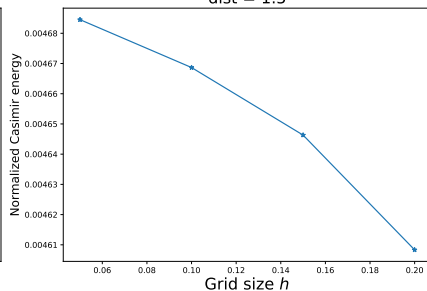
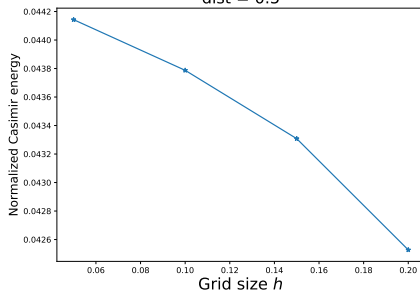


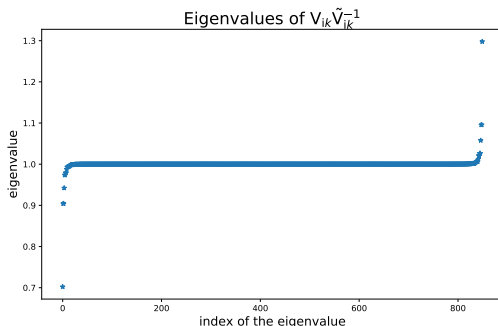


## Normalized Casimir energy in the scalar case

dist = 0.5

dist = 1.5



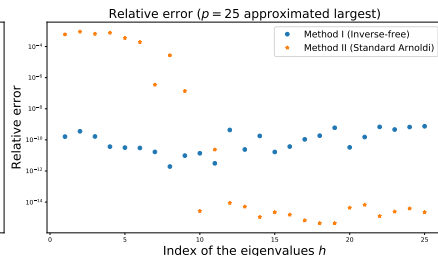
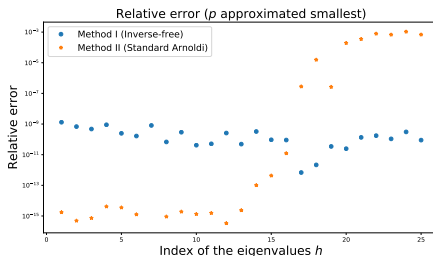
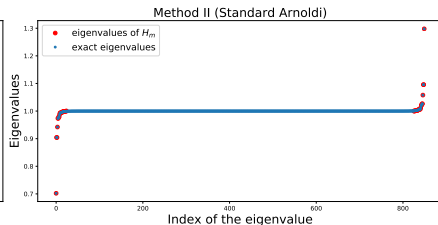
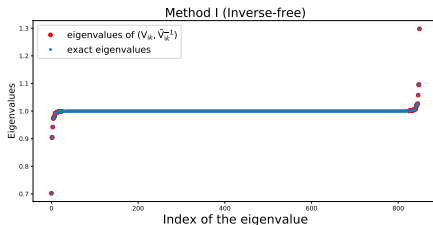


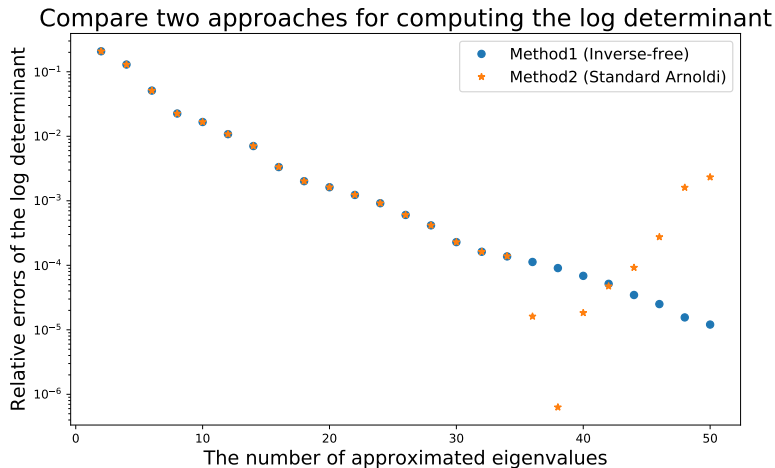
The eigenvalues of the matrix  $V_{ik}\tilde{V}_{ik}^{-1}$  when  $ik = 0.8i$ .

$\tilde{V}_{ik}$  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.

- **Method I:** Inverse-free Krylov subspace method for computing  $p$  smallest (largest) eigenvalues of  $V_{ik} \tilde{\mathbf{x}} = \lambda \tilde{V}_{ik} \tilde{\mathbf{x}}$  ( $V_{ik} \tilde{V}_{ik}^{-1} \tilde{\mathbf{x}} = \lambda \tilde{\mathbf{x}}$ ).
  - Construct a basis  $\hat{Z}_i$  of the  $i$ th Krylov subspace  $K_m(V_{ik} - \theta_i \tilde{V}_{ik}, x_i)$  with dimension  $m$ , for  $i = 1, 2, \dots, p$
  - Orthonormalize  $[\hat{Z}_1 \dots \hat{Z}_p]$  to obtain  $Z$  and project  $V_{ik}$  and  $\tilde{V}_{ik}$  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  $\tilde{V}_{ik}$
  - Apply the standard Arnoldi iterations on  $V_{ik} \tilde{V}_{ik}^{-1}$  to compute projected Hessenberg matrix

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







- Casimir energy can be computed via evaluating the log determinant of the single-layer boundary operators
- Efficiently computing the Casimir energy by avoiding directly 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.

- $\Omega$ : a domain assembling from individual objects  $\Omega_i$
- $M_k$ : 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

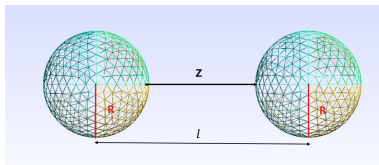
$$\Xi(k) = \log \det \left( M_k \tilde{M}_k^{-1} \right)$$

## Casimir energy formula<sup>a</sup> — electric-field operator method

$$\mathcal{E}_{\text{elec}} = -\frac{\hbar c}{2\pi} \int_0^\infty \Xi(ik) dk$$

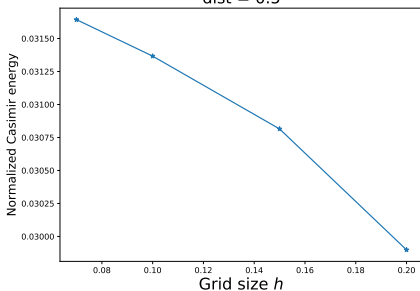
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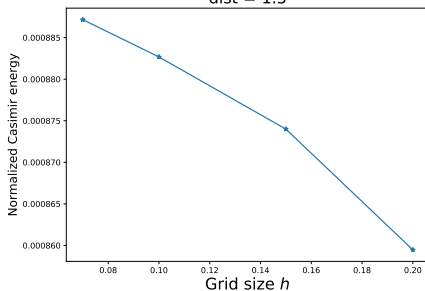


## Normalized Casimir energy in the vector case

dist = 0.5



dist = 1.5



- Xiaoshu Sun, Timo Betcke, Alexander Strohmaier. *Numerical aspects of Casimir energy computation in acoustic scattering* (2021) [**In preparation**]
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