The Casimir energy and radiative heat transfer between nanostructured surfaces

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The computation of the Casimir force¹ at thermal equilibrium T is well understood between parallel plates (*Fabry-Pérot cavity*).



[1] H. Casimir, Proc. K. Ned. Akad. Wet. 51, 793 (1948).

But when $T_1 \neq T_2$, we deal with the Casimir force out-of-thermal equilibrium and the radiative heat flux². These are well understood between parallel plates, but real technological applications rarely display such simple geometries.







We will consider *nanostructured surfaces*, where the calculation of these observables is considerably less trivial due to the diffraction of the modes.



Calculations of these observables so far relied on approximation methods. We use an *exact* method based on scattering theory.

Derjaguin's Proximity Approximation (PA) considers the total force as a sum of the local plane-plane contributions.

The *Effective Media Approximation* (EMA) considers rough surfaces as planes with mixed permittivities between the media at interface.



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Casimir plane-plane theory at T=0

The quantum theory predicts a non-zero vacuum energy per mode :

$$E(\omega,T) = \hbar\omega \left(\frac{1}{2} + \overline{n}(\omega,T)\right) = \frac{1}{2}\hbar\omega \coth\frac{\hbar\omega}{2k_BT} \qquad \text{for} \qquad \overline{n}(\omega,T) = \frac{1}{e^{\hbar\omega/k_BT} - 1}$$

This leads to the Casimir force as a pressure from vacuum, written as a sum over all field modes characterized by frequency ξ (= -i ω), **k**, and polarization p :

$$F = \frac{A\hbar c}{8\pi^3} \sum_p \int_{k_x \in \mathbb{R}} dk_x \int_{k_y \in \mathbb{R}} dk_y \int_0^\infty d\xi \kappa \frac{r_{\mathbf{k},1}^p(i\xi)e^{-\kappa L}r_{\mathbf{k},2}^p(i\xi)e^{-\kappa L}}{1 - r_{\mathbf{k},1}^p(i\xi)e^{-\kappa L}r_{\mathbf{k},2}^p(i\xi)e^{-\kappa L}}$$

Ζ,

E₀

$$\kappa = \sqrt{rac{\xi^2}{c^2} + \mathbf{k}^2} = ik_z$$
 $rac{\omega^2}{c^2} = k_x^2 + k_y^2 + k_z^2 = \mathbf{k}^2 + k_z^2$

 $\text{Perfect mirrors}: \ r^{\text{TE}} = -r^{\text{TM}} = -1 \quad \Longrightarrow \quad F = \frac{A\hbar c\pi^2}{240L^4}$

Casimir theory at T=0

Evanescent waves are present by necessity in the vicinity of an interface. They contribute to the Casimir effect and especially to the heat flux.

Refracted wave

Evanescent wave



Interface



Interface Evanescent zone

Ordinary propagative waves belong to the range $(\omega > c|\mathbf{k}|)$ and evanescent waves to $(\omega < c|\mathbf{k}|)$.

We consider two gratings made of rectangular periodic corrugations, separated by a vacuum slit. We determine each grating's S-matrix through the *Rigorous Coupled-Wave Analysis* (RCWA)^{3,4}.



The reflection is no longer specular as in the plane-plane case. We need the S-matrix associated with each grating : then we can compute *both* the Casimir energy and the heat flux.

[3] M. G. Moharam, E. B. Grann, D. A. Pommet, and T. K. Gaylord, J. Opt. Soc. Am. A 12, 1068 (1995). [4] P. Lalanne and G. M. Morris, J. Opt. Soc. Am. A 13, 779 (1996).

We need to find the longitudinal components outside the corrugated region (z > a) and within the transmitted region (z < 0). We consider p incident modes and n diffracted modes, with p, n \in [2N +1], as basis of our S-matrix.



Then for I_p , R_{np} , and T_{np} being the incidence, reflection, and transmission matrices of dimension 2N+1, we can generalize the Rayleigh expansion for an incident monochromatic wave for the field outside the corrugations (z > a):

$$E_{y}(x,z) = I_{p}^{(e)}e^{i(\alpha_{p}x-\beta_{p}^{(1)}z)} + \sum_{\substack{n=-\infty\\n=-\infty}}^{+\infty} R_{np}^{(e)}e^{i(\alpha_{n}x+\beta_{n}^{(1)}z)}$$
$$H_{y}(x,z) = I_{p}^{(h)}e^{i(\alpha_{p}x-\beta_{p}^{(1)}z)} + \sum_{\substack{n=-\infty\\n=-\infty}}^{+\infty} R_{np}^{(h)}e^{i(\alpha_{n}x+\beta_{n}^{(1)}z)}$$

and within the transmitted region (z < 0):

$$E_{y}(x,z) = \sum_{n=-\infty}^{+\infty} T_{np}^{(e)} e^{i(\alpha_{n}x - \beta_{n}^{(2)}z)} \quad H_{y}(x,z) = \sum_{n=-\infty}^{+\infty} T_{np}^{(h)} e^{i(\alpha_{n}x - \beta_{n}^{(2)}z)}$$

For :
$$\alpha_{p} = k_{x} + \frac{2\pi p}{d} \quad \text{and} \quad \alpha_{n} = k_{x} + \frac{2\pi n}{d}$$

 $\beta_p^{(1)2} = \omega^2 - k_y^2 - \alpha_p^2$ and $\beta_n^{(1)2} = \omega^2 - k_y^2 - \alpha_n^2$

 $\beta_n^{(2)2} = \omega^2 \epsilon \mu - k_z^2 - \alpha_n^2$

We rewrite the Maxwell equations inside the corrugated region 0 < z < a through a set of first-order differential equations :

$$\partial_z \mathbf{F} = \mathbf{M} \mathbf{F} \quad \text{for } \mathbf{F}^\top = (E_y, E_x, H_y, H_x)$$

for M a constant square matrix of dimension 8N + 4. The solution of the fields is then of the form :

$$\mathbf{F}(z) = e^{\mathbf{M}z}\mathbf{F}(0)$$

From now on, our strategy will be to write the fields inside the grating in this form, and match them by continuity relations for each E_y , H_y , E_x , H_x , with our previous equations at boundary z = a for z > a, and at boundary z = 0 for z < 0.

The Casimir force between gratings eventually becomes⁵:

$$F = rac{A\hbar c}{8\pi^3} \int_{k_x = -\pi/d}^{+\pi/d} dk_x \int_{k_y \in \mathbb{R}} dk_y \int_0^\infty d\xi \operatorname{Tr}\left[\mathbf{Z}_1 \mathbf{Z}_2
ight]$$

$$\mathbf{Z}_{1} = \left[I - \mathbf{R}_{1}(i\xi)\mathbf{K}(i\xi)\mathbf{R}_{2}(i\xi)\mathbf{K}(i\xi)\right]^{-1}$$

$$\mathbf{Z}_{2} = \mathbf{R}_{1}(i\xi)\operatorname{diag}(\kappa)\mathbf{K}(i\xi)\mathbf{R}_{2}(i\xi)\mathbf{K}(i\xi) + \mathbf{R}_{1}(i\xi)\mathbf{K}(i\xi)\mathbf{R}_{2}(i\xi)\operatorname{diag}(\kappa)\mathbf{K}(i\xi)$$

$$K(i\xi) = \operatorname{diag}\left[\exp\left(-L\sqrt{\xi^{2} + k_{y}^{2} + [k_{x} + (2n\pi/d)]^{2}}\right)\right] \quad \text{and} \quad n = -N, \dots, +N$$

$$\mathbf{R}_{1}(i\xi) = \left(\begin{array}{cc}r_{01}^{\mathrm{TE}} & 0\\ 0 & r_{01}^{\mathrm{TM}}\end{array}\right) \longrightarrow \mathbf{R}_{1}(i\xi) = \left(\begin{array}{cc}r_{01}^{\mathrm{TE}/\mathrm{TE}} & r_{01}^{\mathrm{TE}/\mathrm{TM}}\\ r_{01}^{\mathrm{TM}/\mathrm{TE}} & r_{01}^{\mathrm{TM}/\mathrm{TM}}\end{array}\right)$$
Specular (no coupling)
$$\mathbf{R}_{1}(i\xi) = \left(\begin{array}{cc}r_{01}^{\mathrm{TE}/\mathrm{TE}} & r_{01}^{\mathrm{TM}/\mathrm{TM}}\\ r_{01}^{\mathrm{TM}/\mathrm{TE}} & r_{01}^{\mathrm{TM}/\mathrm{TM}}\end{array}\right)$$

[5] A. Lambrecht and V. Marachevsky, Phys. Rev. Lett. 101, 160403 (2008).

Casimir force VS distance F(L) at T=0 d=200nm, a=100nm, p=50%

• Casimir force (∞r^2) much larger for metals than for dielectrics.



Casimir force VS groove depth F(a) at T=0 L=200nm, d=200nm, p=50%

• At a = 0 nm, we recover the plane-plane values of separation distances L = 200 nm.





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Casimir between arbitrary gratings at T=0

Arbitrary profiles can be modeled as stacks of K horizontal rectangular slices :



Number of slices K

A similar differential equation can be solved within each slice (i) to relate the fields at boundary z = ia/K and z = (i+1)a/K, so that the field at z = a is related to the field at z = 0 via the relation :

$$\mathbf{F}(a) = \left[\prod_{i=K}^{1} \exp^{\mathbf{M}^{(i)} \frac{a}{K}}\right] \mathbf{F}(0)$$

Casimir between arbitrary gratings at T=0

Eventually we can define all kinds of arbitrary periodic profiles :



Casimir between arbitrary gratings at T=0 L=100nm, d=400nm, a=50nm, d₁(z)>200nm, Si

Casimir energy as a function of lateral shift $E(\delta)$ for four different (but *proportionally equivalent*) arbitrary periodic profiles :



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For T≠0, we must take into account the thermal contribution to the vacuum energy density $E(\omega,T)$. This will appear as a coth factor in the integrand of the Casimir force expression, with its poles appearing as *Matsubara frequencies* (avoided by η) :

$$\left(F = \frac{A}{4\pi^2} k_B T \sum_{m=0}^{\prime} \int_{k_x = -\pi/d}^{+\pi/d} dk_x \int_{k_y \in \mathbb{R}} dk_y \operatorname{Tr} \left[\mathbf{Z}_1 \mathbf{Z}_2\right]\right)$$

Matsubara frequencies :

$$\omega_m = i\xi_m = im rac{2\pi k_B T}{\hbar} o 0$$

The zero temperature limit is recovered when :

$$\omega_T = \frac{2\pi k_B T}{\hbar} \to 0 \qquad \qquad \lambda_T = \frac{\hbar c}{k_B T} = \frac{2\pi c}{\omega_T}$$

So for distances beyond the value of $\lambda_T/2$, the thermal contributions to the zero temperature Casimir force become important.

Casimir energy VS distance L for T≠0 Gratings have d=200nm, a=100nm, p=50%.

- Regardless of the chosen material, the value of the Casimir energy at long separation distances increases with temperature.
- This is especially true for larger distances due to the thermal wavelength contribution.



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Casimir between gratings for $T_1 \neq T_2$

First let us define the wave vector $\mathbf{k} = (k_{\perp}, k_{z})$ such that :

$$k_z = \sqrt{\omega^2/c^2 - k_\perp^2} \qquad ext{for} \qquad -rac{\pi}{2} < rg k_z \leqslant +rac{\pi}{2}$$

We define the following projectors on the propagative and evanescent sectors^{6,7}:

$$egin{aligned} \Sigma_n^{ ext{pw}} &= k_z^n \Pi^{ ext{pw}} & ext{for} & \Pi_{
ho
ho'}^{ ext{pw}} &= \delta_{
ho
ho'} rac{1+s_lpha}{2} \ \end{aligned}$$
 $\Sigma_n^{ ext{ew}} &= k_z^n \Pi^{ ext{ew}} & ext{for} & \Pi_{
ho
ho'}^{ ext{ew}} &= \delta_{
ho
ho'} rac{1-s_lpha}{2} \end{aligned}$

with $s_{\alpha} \equiv \operatorname{sgn}(\omega^2/c^2 - k_{\perp}^2)$

[6] G. Bimonte, Phys. Rev. A 80, 042102 (2009).
[7] R. Messina and M. Antezza, Phys. Rev. A 84, 042102 (2011).

Casimir between gratings for $T_1 \neq T_2$

Eventually we obtain the normalized scattering expression of the Casimir force out-of-thermal equilibrium⁸ for real frequencies :

$$F_z^{(\text{neq})}(T_1, T_2) = \frac{1}{2} F_z^{(\text{eq})}(T_1) + \frac{1}{2} F_z^{(\text{eq})}(T_2) + \frac{1}{2} \Delta F_z^{(\text{neq})}(T_1, T_2)$$

$$F_{z}^{(\text{eq})}(T) = \frac{1}{8\pi^{3}} 2\text{Re} \int_{\omega>0} \frac{E(\omega,T)}{\omega} \int_{k_{x}=-\pi/d}^{+\pi/d} \int_{k_{y}\in\mathbb{R}} \text{Tr} \left[k_{z} \left(\mathbf{U}^{12}\mathbf{S}^{1}\mathbf{S}^{2} + \mathbf{U}^{21}\mathbf{S}^{2}\mathbf{S}^{1}\right)\right] dk_{y} dk_{x} d\omega$$

$$\Delta F_{z}^{(\text{neq})}(T_{1}, T_{2}) = \frac{1}{8\pi^{3}} \int_{\omega > 0} \frac{E(\omega, T_{1}) - E(\omega, T_{2})}{\omega} \int_{k_{x} = -\pi/d}^{+\pi/d} \int_{k_{y} \in \mathbb{R}} \text{Tr} \left[\mathbf{J}^{12} - \mathbf{J}^{21} \right] dk_{y} dk_{x} d\omega$$

 $\begin{aligned} \mathsf{For}: \qquad E(\omega,T) &= \hbar\omega \left(\frac{1}{2} + \overline{n}(\omega,T)\right) \qquad \text{for} \qquad \overline{n}(\omega,T) = \frac{1}{e^{\hbar\omega/k_BT} - 1} \\ \mathbf{J}^{12} &= \mathbf{U}^{12} \left(\mathbf{\Sigma}_{-1}^{\mathrm{pw}} - \mathbf{S}^{1} \mathbf{\Sigma}_{-1}^{\mathrm{pw}} \mathbf{S}^{1\dagger} + \mathbf{S}^{1} \mathbf{\Sigma}_{-1}^{\mathrm{ew}} - \mathbf{\Sigma}_{-1}^{\mathrm{ew}} \mathbf{S}^{1\dagger}\right) \qquad \mathbf{U}^{12} &= \left[1 - S^{1} S^{2}\right]^{-1} \\ &\times \mathbf{U}^{12\dagger} \left(\mathbf{\Sigma}_{2}^{\mathrm{pw}} + \mathbf{S}^{2\dagger} \mathbf{\Sigma}_{2}^{\mathrm{pw}} \mathbf{S}^{2} + \mathbf{S}^{2\dagger} \mathbf{\Sigma}_{2}^{\mathrm{ew}} + \mathbf{\Sigma}_{2}^{\mathrm{ew}} \mathbf{S}^{2}\right) \end{aligned}$

[8] M. Antezza, L. Pitaevskii, and S. Stringari, Phys. Rev. Lett. 95, 113202 (2005).

Casimir $F^{tot}(a)$ between gratings for $T_1 \neq T_2$

L=100nm, d=500nm, p=50%, T1=250K, T2=350K, SiO2/SiC

 We can expect the total Casimir force to converge with larger a's beyond a groove depth of a > 500 nm.



Casimir F^{neq}(L) between planes for $T_1 \neq T_2$ $\langle T \rangle$ =350K, SiO₂/SiC

- Existence of a separation distance L_s where all profiles have the same $F^{neq}=0$.
- For L>L_s the contribution Fneq is negative and the total force may be potentially repulsive.

$\Delta F^{neq}/F^{eq}$ between planes for $T_1 \neq T_2$ L=3000nm, SiO₂/SiC

- Eventually we find the larger ratio F^{neq}/F^{eq} at greater separation distances.
- Possibility of experimental measurements, and further study towards the repulsive regime⁷.

$\langle \mathbf{T} angle$	ΔT	$\mathbf{T_1}$	T_2	$\left {\Delta {{f F}^{\left({ m{neq}} ight)} / {f F}^{\left({ m{eq}} ight)} } ight $
350	200	450	250	22.12%
350	150	425	275	$\mathbf{18.11\%}$
350	100	400	300	$\mathbf{10.78\%}$
350	50	375	325	$\mathbf{5.98\%}$
350	200	450	250	22.12%
250	200	350	150	$\mathbf{16.89\%}$
150	200	250	50	$\mathbf{11.50\%}$

[7] R. Messina and M. Antezza, Phys. Rev. A 84, 042102 (2011)

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Heat flux in the scattering theory

We can use our former scattering formalism for the Casimir force out of thermal equilibrium and use the cavity statistical quantum average to derive the radiative heat transfer coefficient between two gratings⁶ at temperatures T_1 and T_2 :

$$h = \frac{1}{8\pi^3 |T_1 - T_2|} \int_{\omega > 0} \left(E(\omega, T_1) - E(\omega, T_2) \right) \int_{k_x = -\pi/d}^{+\pi/d} \int_{k_y \in \mathbb{R}} \operatorname{Tr} \left[\mathbf{H}^{12} \right] dk_y dk_x d\omega$$

with:

$$egin{aligned} \mathbf{H}^{12} &= \left[\mathbf{U}^{12} \left(\mathbf{\Sigma}_{-1}^{\mathrm{pw}} - \mathbf{S}^1 \mathbf{\Sigma}_{-1}^{\mathrm{pw}} \mathbf{S}^{1\dagger} + \mathbf{S}^1 \mathbf{\Sigma}_{-1}^{\mathrm{ew}} - \mathbf{\Sigma}_{-1}^{\mathrm{ew}} \mathbf{S}^{1\dagger}
ight) \ & imes \mathbf{U}^{12\dagger} \left(\mathbf{\Sigma}_{1}^{\mathrm{pw}} - \mathbf{S}^{2\dagger} \mathbf{\Sigma}_{1}^{\mathrm{pw}} \mathbf{S}^2 + \mathbf{S}^{2\dagger} \mathbf{\Sigma}_{1}^{\mathrm{ew}} - \mathbf{\Sigma}_{1}^{\mathrm{ew}} \mathbf{S}^2
ight)
ight] \end{aligned}$$

[6] G. Bimonte, Phys. Rev. A 80, 042102 (2009).

Heat flux between various plates $T_1=290K, T_2=310K$

 In contrast to the Casimir force, stronger flux (∝1-r²) for dielectrics than metals.

Heat flux between SiO₂ plates

We see three domains of respective power laws with contributions from specific physical effects : A- the extreme near-field below 200nm (dipole-dipole interaction), B- the near-field from 200nm to 10 μ m (surface phonon-polaritons), and C- the domain of Stefan–Boltzmann's law beyond 10 μ m (classical radiative heat transfer).

Flux as a function of distance h(L) for gratings d=1500nm, p=20%, a=500nm, T1=290K, T2=310K, SiO₂

- Large variation between $\delta/d=0\%$ et $\delta/d=50\%$ and in near-field, but convergence beyond 0.5µm.
- Usefulness of an exact method instead of an approximation.

Heat flux between gratings

The flux modulation factor between $\delta/d=0\%$ and $\delta/d=50\%$ at L=25nm on the first plot is 36.

Hence the idea of application of a *thermal modulator*⁹ based on the simple lateral shift of two gratings in extreme near-field.

[9] J. Lussange, R. Guérout, F. Rosa, J.-J. Greffet, A. Lambrecht, and S. Reynaud, Phys. Rev. B 86, 085432 (2012)

Flux as a function of lateral shift $h(\delta)$ for gratings L=100nm, d=a=500nm, p=30%, T1=290K, T2=310K, SiO₂

• Smooth transition with lateral shift, with application of progressive modulation.

Flux as a function of period h(d) for gratings L=100nm, p=20%, a=500nm, T1=290K, T2=310K, SiO₂

- Great difference between $\delta/d=0\%$ et $\delta/d=50\%$ for larger periods.
- The Proximity Approximation is inaccurate for smaller periods.

Flux as a function of groove depth h(a) for gratings

- L=100nm, d=500nm, p=20%, T1=290K, T2=310K, SiO2
 - Fast convergence beyond an inflexion point a > 100nm.
 - The flux decreases with larger groove depths, in contrast to gold.

Flux as a function of groove depth h(a) for gratings L=1µm, p=50%, T1=290K, T2=310K, Au

• Increase of the flux with groove depth due to digging of wave-guides enhancing the surface-plasmon polariton coupling¹⁰.

• Additional modes in the thermal frequency window contributing to the heat transfer.

[10] R. Guérout, J. Lussange, F. Rosa, J.-P. Hugonin, D. Dalvit, J.-J. Greffet, A. Lambrecht, and S. Reynaud, Phys. Rev. B **85**, 180301(R) (2012)

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Conclusion

By deriving the S-matrix of a given profile through the RCWA, we have performed the first *exact* numerical calculations based on scattering theory of both the Casimir force and the radiative heat transfer between nanostructured surfaces. Most notably, our calculations present new insights on :

- 1. The Casimir force between *arbitrary gratings*, with direct engineering applications.
- 2. The Casimir force between gratings *out-of-thermal equilibrium*, with a presentation of the first results for experimentalists.
- 3. The *heat flux between gratings*, with large modulations in the case of a lateral shift of the profiles.

Conclusion

Finally, this theoretical work has direct potential applications :

- Potential modulation of the Casimir force and hence of reducing the problem of stiction in NEMS and MEMS through a temperature control of gratings.
- Many electromechanical systems must be grounded, often through the use of gold coatings. Importance of non-trivial heat flux issues in the case of gold gratings.
- The heat flux between gratings, with the potential design of a thermal modulator of factor 36.

Thank you for your attention