Bohr-van Leeuwen theorem and the thermal Casimir effect for conductors

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Overview

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2. Asymptotic results from microscopic theory
3. The Bohr-van Leeuwen theorem
4. The fluctuating e.m. field outside macroscopic bodies
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The thermal Casimir force

The Casimir pressure for two homogeneous and isotropic parallel plates is (Lifshitz 1955):

$$P(d,T) = -\frac{k_B T}{\pi} \sum_{n=0}^{\infty} \left(1 - \frac{1}{2}\delta_{n0}\right) \int_0^{\infty} dk_\perp \, k_\perp \, q_n \sum_{\alpha=s,p} \left(\frac{e^{2q_n d}}{r_1^{(\alpha)}(i\xi_n, k_\perp)\, r_2^{(\alpha)}(i\xi_n, k_\perp)} - 1 \right)^{-1}$$

Matsubara frequencies $\xi_n = 2\pi n k_B T/\hbar \quad n = 0, 1, 2, \ldots$

The non-zero Matsubara terms are commonly evaluated using optical tabulated data, and pose no problems

Problems arise from the **n=0** zero Matsubara modes. This requiires extrapolating optical data to **zero frequency.**

The TM zero mode is no problem for good conductors $r_i^{(p)}(0, k_\perp) = 1$

There is no agreement on the value of the n=0 contribution for transverse electric (s) polarization for good (normal) conductors.

$r_i^{(s)}(0, k_\perp) = 0$ (**Drude prescription**)

Suggested alternatives for the **TE** zero mode:

$$r_i^{(s)}(0, k_\perp) = \frac{\sqrt{\Omega_P^2/c^2 + k_\perp^2} - k_\perp}{\sqrt{\Omega_P^2/c^2 + k_\perp^2} + k_\perp}$$ (**plasma prescription**)

The most striking difference between these prescriptions is seen at large distances and/or T $\frac{k_B T a}{\hbar c} \gg 1$

In this limit the entire force results from the n=0 Matsubara terms:

$$P_{\text{Drude}} = \frac{1}{2} P_{\text{plasma}} = P_{\text{ideal}} = \frac{k_B T}{4\pi a^3} \zeta(3)$$

Results from microscopic theory

(Buenzli, Martin PRE **77**, 011114 (2008))

The conductors are modelled as a system of quantum mobile charges confined within two slabs by a confining potential
The Hamiltonian in the **Coulomb gauge** is

$$H_{\Lambda,L,d} = \sum_{i=1}^{N} \frac{1}{2m_{\gamma_i}} \left(P_i - \frac{e_{\gamma_i}}{c} A(r_i) \right)^2 + \sum_{i<j} e_{\gamma_i} e_{\gamma_j} v(r_i - r_j) + \sum_{i=1}^{N} V^{\text{walls}}(r_i, \gamma_i) + H_{0,\Lambda}^{\text{rad}}$$

$$v(r_i - r_j) = \frac{1}{|r_i - r_j|}.$$

$V^{\text{walls}}(r_i, \gamma_i)$ is the confining potential

$H_{0,\Lambda}^{\text{rad}}$ Free Hamiltonian of e.m. field

Particles spins are neglected

The mobile charges are considered in **thermal equilibrium** with the photon field at positive temperature T

Fluctuations of all degrees of freedom, matter and field, are treated according to the principles of **QED and statistical physics** without recourse to approximations

The assumption is made that the plates are conducting,:
λ_{screen} **« plates thickness, plates separation**

Result: in the asymptotic limit of large separations the Casimir pressure f(d) approaches the value predicted by the **Drude** model:

$$f(d) \sim -\frac{\zeta(3) k_B T}{8\pi d^3}, \quad d \to \infty$$

Remark: the Casimir effect is an equilibrium phenomenon

Question: can we use statistical physics to derive model-independent constraints on the permitted behavior of the reflection coefficients?

Example: Onsager's relations on reflection coefficients implied by microscopic reversibility

$$\begin{aligned} r_{ss}(\omega,\vec{k}_\perp;\mathbf{B}_{\rm ext}) &= r_{ss}(\omega,-\vec{k}_\perp;-\mathbf{B}_{\rm ext})\,, \\ r_{pp}(\omega,\vec{k}_\perp;\mathbf{B}_{\rm ext}) &= r_{pp}(\omega,-\vec{k}_\perp;-\mathbf{B}_{\rm ext})\,, \\ r_{sp}(\omega,\vec{k}_\perp;\mathbf{B}_{\rm ext}) &= -r_{ps}(\omega,-\vec{k}_\perp;-\mathbf{B}_{\rm ext})\,. \end{aligned}$$

Example: chiral materials

Born-Drude model $\mathbf{D}=\epsilon\,\mathbf{E}-f\,\nabla\times\mathbf{E}\,,\quad \mathbf{B}=\mathbf{H}\,.$ does not pass Onsager criterion

Fedorov model $\mathbf{D}=\epsilon\,(\mathbf{E}+\beta\,\nabla\times\mathbf{E})\,,\quad \mathbf{B}=\mu\,(\mathbf{H}+\beta\,\nabla\times\mathbf{H})$ OK

Question: can we use statistical physics to obtain information also on the zero frequency limit of reflection coefficients?

The Bohr-van Leeuwen th.

Van-Leeuwen (1921)

Consider the microscopic Hamiltonian for a system of charged particles. In the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$

$$H = \sum_{i=1}^{N} \frac{1}{2m_{\gamma_i}} \left(P_i - \frac{e_{\gamma_i}}{c} A(r_i) \right)^2 + \sum_{i<j} e_{\gamma_i} e_{\gamma_j} v(r_i - r_j) + \sum_{i=1}^{N} V^{\text{walls}}(r_i, \gamma_i) + H_{0,\Lambda}^{\text{rad}}$$

$v(\mathbf{r}_i - \mathbf{r}_j)$ Coulomb potential

$H_{0,\Lambda}^{\text{rad}}$ Free Hamiltonian of e.m. field

The CLASSICAL partition function for the e.m. field is

$$Z[\mathbf{J}(\mathbf{x}), \mathbf{\Psi}(\mathbf{x})] = \int d\mu_{rad} \int \prod_{i=1}^{N} d\mathbf{r}_i d\mathbf{P}_i \, e^{-\beta H + \int d^3\mathbf{x} (\mathbf{J}(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) + \mathbf{\Psi}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x}))}$$

By the canonical change of variable

$$\mathbf{P}_i \to \mathbf{P}_i' = \mathbf{P}_i - \frac{e_{\gamma_i}}{c} \mathbf{A}(\mathbf{r}_i)$$

one finds that the partition function **factorizes**: $Z[\mathbf{J}(\mathbf{x}), \mathbf{\Psi}(\mathbf{x})] = \mathcal{K} \times Z_{0,\Lambda}^{\text{rad}}[\mathbf{J}(\mathbf{x}), \mathbf{\Psi}(\mathbf{x})]$

$$Z_{0,\Lambda}^{\text{rad}}[\mathbf{J}(\mathbf{x}), \mathbf{\Psi}(\mathbf{x})] = \int d\mu_{rad} \, e^{-\beta H_{0,\Lambda}^{\text{rad}} + \int d^3\mathbf{x} (\mathbf{J}(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) + \mathbf{\Psi}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x}))}$$

partition functiton of the e.m. field
In free space

$$\mathcal{K} = \int \prod_{i=1}^{N} d\mathbf{r}_i d\mathbf{P}_i \, \exp\left[-\beta \left(\sum_{i=1}^{N} \frac{\mathbf{P}_i^2}{2m_{\gamma_i}} + \sum_{i<j} e_{\gamma_i} e_{\gamma_j} v(\mathbf{r}_i - \mathbf{r}_j) \right) \right]$$

partition function of the charges

Conclusion: **CLASSICALLY, at thermal equilibrium the e.m. fields decouples from matter**

The theorem explains why normal metals do not show strong diamagnetism.

Fluctuations of the e.m. field outside macroscopic bodies

$$H_{\rm ext} = \int d^3\mathbf{r}\left[U(\mathbf{r},t)\rho^{(\rm ext)}(\mathbf{r},t) - \frac{1}{c}\mathbf{A}_\perp(\mathbf{r},t)\cdot\mathbf{j}_\perp^{(\rm ext)}(\mathbf{r},t)\right],$$

$$\nabla\cdot\mathbf{j}_\perp^{(\rm ext)} = 0.$$

$$U(\mathbf{r},t) = \int_{-\infty}^{t} dt'\int d^3\mathbf{r}'\, G(\mathbf{r},\mathbf{r}',t-t')\rho^{(\rm ext)}(\mathbf{r}',t')$$

$$\mathbf{A}_\perp(\mathbf{r},t) = \frac{1}{c}\int_{-\infty}^{t} dt'\int d^3\mathbf{r}'\,\mathbf{G}_\perp(\mathbf{r},\mathbf{r}',t-t')\cdot\mathbf{j}_\perp^{(\rm ext)}(\mathbf{r}',t'),$$

MACROSCOPIC Maxwell Eqs. for the Green functions

$$\nabla\cdot[\epsilon(\mathbf{r},\omega)\nabla\tilde{G}] = -4\pi\delta(\mathbf{r}-\mathbf{r}')$$

$$[\Delta + \epsilon(\mathbf{r},\omega)\omega^2/c^2]\tilde{\mathbf{G}}_\perp(\mathbf{r},\mathbf{r}',\omega) = -4\pi\delta_\perp(\mathbf{r}-\mathbf{r}')$$

From the fluctuation dissipation th. one obtains

$$\langle\{U(\mathbf{r},t)U(\mathbf{r}',0)\}\rangle = -\frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}E_\beta(\omega)\,\mathrm{Im}[\tilde{G}(\mathbf{r},\mathbf{r}',\omega)]\cos(\omega t),$$

$$E_\beta(\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)$$

$$\langle\{A_{\perp i}(\mathbf{r},t)A_{\perp j}(\mathbf{r}',0)\}\rangle = \frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}E_\beta(\omega)\,\mathrm{Im}[\tilde{G}_{\perp ij}(\mathbf{r},\mathbf{r}',\omega)]\cos(\omega t)$$

Outside material bodies it is convenient to write

$$G(\mathbf{r},\mathbf{r}',t-t') = G^{(0)}(\mathbf{r}-\mathbf{r}',t-t') + F^{(\rm mat)}(\mathbf{r},\mathbf{r}',t-t'),$$

$$\mathbf{G}_\perp(\mathbf{r},\mathbf{r}',t-t') = \mathbf{G}_\perp^{(0)}(\mathbf{r}-\mathbf{r}',t-t') + \mathbf{F}_\perp^{(\rm mat)}(\mathbf{r},\mathbf{r}',t-t').$$

$$\delta\langle\{E_{\parallel i}(\mathbf{r},0)\,E_{\parallel j}(\mathbf{r}',0)\}\rangle = -\frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}\,E_\beta(\omega)\,\mathrm{Im}\left(\frac{\partial^2 \tilde{F}^{(\mathrm{mat})}}{\partial x_i \partial x'_j}\right)$$

$$\delta\langle\{E_{\perp i}(\mathbf{r},0)\,E_{\perp j}(\mathbf{r}',0)\}\rangle = \frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}\,E_\beta(\omega)\,k_0^2\,\mathrm{Im}\,[\tilde{F}^{(\mathrm{mat})}_{\perp ij}(\mathbf{r},\mathbf{r}',\omega)]$$

$$k_0 = \omega/c$$

$$\delta\langle\{B_i(\mathbf{r},0)\,B_j(\mathbf{r}',0)\}\rangle = \frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega}\,E_\beta(\omega)\,\mathrm{Im}\,[(\vec{\nabla}_{\mathbf{r}} \times \tilde{\mathbf{F}}^{(\mathrm{mat})}_\perp \times \overleftarrow{\nabla}_{\mathbf{r}'})_{ij}]$$

In the classical limit: $E_\beta(\omega) \to k_B T$

After a Wick rotation to imaginary frequencies

$$\lim_{\hbar\to 0}\,\delta\langle\{E_{\perp i}(\mathbf{r},0)E_{\perp j}(\mathbf{r}',0)\}\rangle = k_B T\,\mathcal{E}^{(\mathrm{cl})}_{\perp ij}(\mathbf{r},\mathbf{r}')$$

$$\lim_{\hbar\to 0}\,\delta\langle\{B_{\perp i}(\mathbf{r},0)B_{\perp j}(\mathbf{r}',0)\}\rangle = k_B T\,\mathcal{B}^{(\mathrm{cl})}_{\perp ij}(\mathbf{r},\mathbf{r}'),$$

$$\mathcal{E}^{(\mathrm{cl})}_{\perp ij}(\mathbf{r},\mathbf{r}') = \lim_{\omega\to 0}\left(\frac{\omega^2}{c^2}\,\tilde{F}^{(\mathrm{mat})}_{\perp ij}(\mathbf{r},\mathbf{r}',\omega)\right)$$

$$\mathcal{B}^{(\mathrm{cl})}_{\perp ij}(\mathbf{r},\mathbf{r}') = \lim_{\omega\to 0}(\vec{\nabla}_{\mathbf{r}} \times \tilde{\mathbf{F}}^{(\mathrm{mat})}_\perp \times \overleftarrow{\nabla}_{\mathbf{r}'})_{ij}.$$

The Bohr-van Leeuwen th. is sarisfied iff: $\boxed{\mathcal{E}^{(\mathrm{cl})}_{\perp ij} = \mathcal{B}^{(\mathrm{cl})}_{\perp ij} = 0}$

(G. Bimonte, PRA **79**, 042107 (2009))

Important conclusion: only the zero-frequency limit matters for establishing if the theorem is satisfied

NOTA BENE: **this conclusion holds for any number of bodies of any shape**

Simple case: the field outside one-slab

Outside a slab occupying the z<0 halfspace, we find: $\bar{\mathbf{k}}^{(\pm)} = \mathbf{k}_\perp \pm i k_\perp \hat{\mathbf{z}}$ $\quad \mathbf{e}_\perp = \hat{\mathbf{z}} \times \hat{\mathbf{k}}_\perp$

$$\mathcal{E}^{(\mathrm{cl})}_{\perp ij} = \lim_{\omega\to 0} \int \frac{d^2\mathbf{k}_\perp}{2\pi\, k_\perp} \left\{ k_0^2\, r^{(s)}(\omega, k_\perp)\, e_{\perp i} e_{\perp j} + [r^{(p)}(\omega, k_\perp) - \bar{r}(\omega)]\, \bar{k}^{(+)}_i \bar{k}^{(-)}_j \right\} e^{i\bar{\mathbf{k}}^{(+)}\cdot\mathbf{r} - i\bar{\mathbf{k}}^{(-)}\mathbf{r}'}$$

$$\mathcal{B}^{(\mathrm{cl})}_{\perp ij} = \lim_{\omega\to 0} \int \frac{d^2\mathbf{k}_\perp}{2\pi\, k_\perp} \left\{ r^{(s)}(\omega, k_\perp)\, \bar{k}^{(+)}_i \bar{k}^{(-)}_j + k_0^2\, r^{(p)}(\omega, k_\perp)\, e_{\perp i} e_{\perp j} \right\} e^{i\bar{\mathbf{k}}^{(+)}\cdot\mathbf{r} - i\bar{\mathbf{k}}^{(-)}\mathbf{r}'}$$

$$r^{(s)}(\omega, k_\perp) = \frac{k_z - s}{k_z + s} \qquad r^{(p)}(\omega, k_\perp) = \frac{\epsilon(\omega)\, k_z - s}{\epsilon(\omega)\, k_z + s} \qquad \bar{r}(\omega) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}\,.$$

Whether the Bohr-van Leeuwen is satisfied or not depends exclusively on the reflection coeffcients for zero frequency

$$\epsilon(\omega) = \epsilon_0 + O(\omega) \quad (\mathrm{insulator}) \qquad \mathcal{E}^{(\mathrm{cl})}_{\perp ij} = \mathcal{B}^{(\mathrm{cl})}_{\perp ij} = 0$$

$$\epsilon(\omega) = \frac{4\pi i \sigma_0}{\omega} + O(1); \quad (\mathrm{Drude-like\ models}) \qquad \mathcal{E}^{(\mathrm{cl})}_{\perp ij} = \mathcal{B}^{(\mathrm{cl})}_{\perp ij} = 0$$

$$\epsilon(\omega) = -\frac{\Omega_P^2}{\omega^2} + O(\omega^{-1}) \quad (\mathrm{plasma-like\ models}) \qquad \mathcal{E}^{(\mathrm{cl})}_{\perp ij} = 0\,, \quad \mathcal{B}^{(\mathrm{cl})}_{\perp ij} \neq 0$$

Conclusion: **insulators and Drude-like models of conductors satisfy the theorem, plasma-like mdels of conductors do not**.

The Casimir case

Evaluation of the longitudinal and transverse contributions to the Casimir force results in:

$$\langle T^{(\mathrm{mat})}_{\|zz}\rangle = \frac{1}{\pi^2}\mathrm{Im}\int_0^\infty \frac{d\omega}{\omega}E_\beta(\omega)\int dk_\perp\, k_\perp^2\,\left[\left(1-\frac{e^{2k_\perp d}}{\bar r_1 \bar r_2}\right)^{-1}\right]$$

$$\langle T^{(\mathrm{mat})}_{\perp zz}\rangle = -\frac{1}{\pi^2}\mathrm{Im}\int_0^\infty \frac{d\omega}{\omega}E_\beta(\omega)\int_0^\infty dk_\perp\, k_\perp \left\{ q\sum_{\alpha=s,p}\left(\frac{e^{-2ik_z d}}{r_1^{(\alpha)} r_2^{(\alpha)}}-1\right)^{-1} - k_\perp\left(\frac{e^{2k_\perp d}}{\bar r_1 \bar r_2}-1\right)^{-1}\right\}$$

By taking the classical limit of $\langle T^{(\mathrm{mat})}_{\perp zz}\rangle$ we find

$$\lim_{\hbar\to 0}\langle T^{(\mathrm{mat})}_{\perp zz}\rangle = -\frac{k_B T}{2\pi}\int_0^\infty dk_\perp\, k_\perp^2\left(\frac{e^{2k_\perp d}}{(r^{(s)}(0,k_\perp))^2}-1\right)^{-1}$$

The Bohr-van Leeuwen requires that this quantity vanishes, and this is only possible if $r^{(s)}(0,k_\perp)=0$

Conclusions

1. The Casimir effect is an equilibrium phenomenon and therefore it should obey the principles of statistical physics for equilibrium systems
2. The Bohr-van Leeuwen th. of classical statistical physics implies that, in the classical limit, the reflection coefficient for transverse electric fields must vanish for zero frequency
3. For normal metals, plasma-like prescriptions for the n=0 Matsubara mode violate the Bohr-van Leewuen th., while Drude-like prescriptions satisfy it
4. The Bohr-van Leeuwen theorem does not apply in the case of magnetic materials and superconductors, where quantum effects are determinant

The fluctuation-dissipation th.

Callen,Welton (1951)
Kubo (1966)

Consider a Hamiltonian system at thermal equilibrium perturbed by small external forces

$$H_{\text{ext}} = -\int d^3\mathbf{r} \sum_j Q_j(\mathbf{r},t) f_j(\mathbf{r},t), \qquad \delta\langle Q_i(\mathbf{r},t)\rangle = \sum_j \int d^3\mathbf{r} \int_{-\infty}^{t} dt' \phi_{ij}(\mathbf{r},\mathbf{r}',t-t') f_j(\mathbf{r}',t').$$

Admittance $\tilde{\phi}_{ij}(\mathbf{r},\mathbf{r}',\omega) = \int_0^\infty dt \phi_{ij}(\mathbf{r},\mathbf{r}',t) e^{i\omega t}.$

The admittance is analytic for Im(w)>0

$$\tilde{\phi}_{ij}(\mathbf{r},\mathbf{r}',-w^*) = \tilde{\phi}^*_{ij}(\mathbf{r},\mathbf{r}',w).$$

To first order in perturbation theory $\phi_{ij}(\mathbf{r},\mathbf{r}',t-t') = \Delta_{ij}(\mathbf{r},\mathbf{r}',t-t')\theta(t-t').$ $\quad \Delta_{ij}(\mathbf{r},\mathbf{r}',t-t') = \frac{i}{\hbar}\langle [Q_i(\mathbf{r},t), Q_j(\mathbf{r}',t')]\rangle,$

At equilibrium: $\int_{-\infty}^{\infty} dt \Delta_{ij}(\mathbf{r},\mathbf{r}',t) e^{i\omega t} = \frac{i\omega}{E_\beta(\omega)} \int_{-\infty}^{\infty} dt \langle\{Q_i(\mathbf{r},t) Q_j(\mathbf{r}',0)\}\rangle e^{i\omega t},$ $\quad E_\beta(\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_B T}\right)$

If $\Delta_{ij}(\mathbf{r},\mathbf{r}',t)$ is odd in time $\int_{-\infty}^{\infty} dt \Delta_{ij}(\mathbf{r},\mathbf{r}',t) e^{i\omega t} = 2i \int_0^\infty dt \Delta_{ij}(\mathbf{r},\mathbf{r}',t)\sin(\omega t) = 2i\,\text{Im}[\tilde{\phi}_{ij}(\mathbf{r},\mathbf{r}',\omega)].$

$$\langle\{Q_i(\mathbf{r},t) Q_j(\mathbf{r}',0)\}\rangle = \frac{2}{\pi}\int_0^\infty \frac{d\omega}{\omega} E_\beta(\omega)\,\text{Im}[\tilde{\phi}_{ij}(\mathbf{r},\mathbf{r}',\omega)]\cos(\omega t).$$

In the classical limit $\lim_{\hbar\to 0}\langle\{Q_i(\mathbf{r},0) Q_j(\mathbf{r}',0)\}\rangle = k_B T \tilde{\phi}_{ij}(\mathbf{r},\mathbf{r}',0).$

In the classical limit, the equilibrium values of the correlators depend exlusively on the zero-frequency limit of the admittance