Casimir and Casimir-Polder forces with dissipation from first principles

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Abstract:
We consider Casimir-Polder and Casimir forces with finite dissipation by coupling heat baths to the dipoles introducing, this way, dissipation from 'first principles'. We derive a representation of the free energy as an integral over real frequencies, which can be viewed as an generalization of the 'remarkable formula' introduced by Ford et. al. 1985. For instance, we obtain a nonperturbative representation for the atom-atom and atom-wall interactions. We investigate several limiting cases. From the limit $T \to 0$ we show that the third law of thermodynamics cannot be violated within the given approach, where the dissipation parameter cannot depend on temperature 'by construction'.

ArXiv 1707.06214, 1710.00300

Motivation

The Casimir-Polder force describes the basic electromagnetic interaction between molecules or between a molecule and a wall, and the Lifshitz formula describes the interaction between macroscopic bodies. Their theoretical foundation is commonly based on stochastic electrodynamics and/or vacuum fluctuations and it incorporates material properties in terms of permittivity or polarizability. This way, it is possible to account for the real structure of the interacting objects and to make predictions for high precision measurements, which constitute a highly actual and important topic.

The free energy F is described by the Lifshitz formula

$$F = T \sum_l \int \frac{d\boldsymbol{k}_{||}}{(2\pi)^2} \sum_{\text{TE,TM}} \ln\left(1 - r^2 e^{-2a\eta}\right) \equiv F_0 + \Delta_T F$$

reflection coefficients: $r_{\text{TE}} = \dfrac{\eta - \varkappa}{\eta + \varkappa}, \quad r_{\text{TM}} = \dfrac{\varepsilon(i\xi_l)\eta - \varkappa}{\varepsilon(i\xi_l)\eta + \varkappa}$

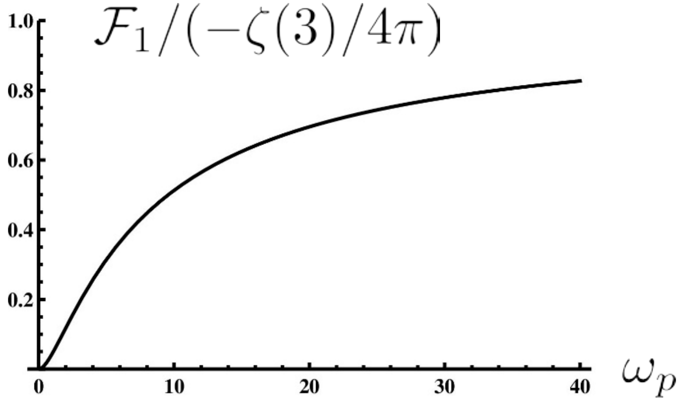
$$-\xi_l = k_{||}^2 - \eta^2$$
$$-\varepsilon(i\xi_l)\xi_l = k_{||}^2 - \varkappa^2$$

permittivity: $\varepsilon(i\xi_l) = 1 + \frac{\omega_p^2}{\xi_l^2 + \xi_l \gamma}$, γ is the dissipation parameter

physically, for metals it appears from scattering of the conduction electrons off thermally excited phonons (there are more mechanisms)

Problems

- $\lim_{\gamma \to 0} \Delta_T F = \Delta_T F(\gamma = 0) + \mathcal{F}_1 T$
- $\Delta_T F \underset{T\to 0}{=} \mathcal{F}_1 T + O(T^2)$ (provided $\gamma(T) \sim T^\alpha$ $(\alpha > 1)$)



Q: How does γ come into the Lifshitz formula?

Simplest answer: inserted 'by hand', using the Drude permittivity $\varepsilon_\mathrm{D} = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$

better answer: use FDT

advanced answer: add heat baths to the matter dipoles

heat bath allows to derive the LF with dissipation from 'first principles' since the initial system under consideration has a Hamiltonian (with no imaginary parts), resp. it has unitarity

Model: oscillators (dipoles) for the matter, electromagnetic field and heat bathes attached to the oscillators simplest model: in $(1+1)$ dimensions, consider oscillators (dipoles) for the matter, electromagnetic field and heat bathes attached to the oscillators

$$\mathcal{L} = \int dx \, \frac{1}{2} \left(\dot{\phi}(t,x)^2 - \phi'(t,x)^2 \right) + \sum_{i=1}^{2} \frac{m}{2} \left(\dot{\xi}_i(t)^2 - \Omega^2 \xi_i(t)^2 \right) \\ - e \sum_{i=1}^{2} \xi_i(t) \phi(t, a_i) + \sum_{i=1}^{2} \int_0^\infty d\omega \, \frac{\mu}{2} \left(\dot{q}_{i\omega}(t)^2 - \omega^2 \left(q_{i\omega}(t) - \xi_i(t) \right)^2 \right)$$

now 'integrate out' the bath variables, for this use cration and anihilation operators,

$$\hat{q}_{i\omega} = \frac{l_0}{\sqrt{2}} \left(\hat{b}_{i\omega} + \hat{b}^\dagger_{i\omega} \right), \quad \hat{p}_{i\omega} = \frac{\hbar}{i\sqrt{2} l_0} \left(\hat{b}_{i\omega} - \hat{b}^\dagger_{i\omega} \right), \qquad l_0 = \sqrt{\frac{\hbar}{\mu\omega}}$$

which obey the Heisenberg equations of motion,

$$\dot{\hat{b}}_{i\omega}(t) = \frac{i}{\hbar} [\hat{H}, \hat{b}_{i\omega}(t)] = -i\omega \hat{b}_{i\omega}(t) + i \frac{\omega}{\sqrt{2} l_0} \hat{\xi}(t), \qquad \dot{\hat{b}}^\dagger_{i\omega}(t) = \frac{i}{\hbar} [\hat{H}, \hat{b}^\dagger_{i\omega}(t)] = i\omega \hat{b}^\dagger_{i\omega}(t) - i \frac{\omega}{\sqrt{2} l_0} \hat{\xi}(t),$$

their retarded solutions are

$$\hat{b}_{i\omega}(t) = e^{-i\omega t}\hat{b}_{i\omega}(0) - \frac{i\omega}{\sqrt{2}l_0}\int_{-\infty}^{t} dt'\, e^{-i\omega(t-t')}\hat{\xi}(t'), \quad \hat{b}^{\dagger}_{i\omega}(t) \quad = e^{i\omega t}\hat{b}^{\dagger}_{i\omega}(0) + \frac{i\omega}{\sqrt{2}l_0}\int_{-\infty}^{t} dt'\, e^{i\omega(t-t')}\hat{\xi}(t'),$$

insert these into the eom for the oscillators,

$$m\left(-\omega^2 + \Omega^2\right)\tilde{\xi}_{i\omega} = -e\tilde{\phi}_{i\omega}(a_i) + \int_0^{\infty} d\omega\, \mu\omega^2 \left(\frac{l_0}{\sqrt{2}}\left(\hat{b}_{i\omega} + \hat{b}^{\dagger}_{i\omega}\right) - \tilde{\xi}_{i\omega}\right),$$

we get new equations,

$$m\Big(\underbrace{-\omega^2 + i\gamma\omega + \Omega^2}_{\equiv N(\omega)}\Big)\tilde{\xi}_{i\omega} = -e\tilde{\phi}_{i\omega}(a_i) + \tilde{F}_{i\omega}$$

with the Langevin force

$$\tilde{F}_{i\omega} = 2\pi\sqrt{\frac{\gamma m}{\pi}\hbar\omega}\left(\Theta(-\omega)\hat{b}_{-\omega} + \Theta(\omega)\hat{b}^{\dagger}_{\omega}\right)$$

and the damping term where γ came in from $\mu = \frac{2\gamma m}{\pi\omega^2}$.

In addition we have the equation for the field $\left(-\omega^2 - \partial_x^2\right)\tilde{\phi}_{\omega}(x) = -e\sum_{i=1}^{2}\tilde{\xi}_{i\omega}\delta(x - a_i),$

Now we solve these equation. First, we solve for the oscillators

$$\tilde{\xi}_{i\omega} = -\frac{e}{mN(\omega)}\tilde{\phi}_\omega(a_i) + \frac{\tilde{F}_{i\omega}}{mN(\omega)},$$

Now we insert this solution into the equation for the field,

$$\left(-\omega^2 - \partial_x^2 - \frac{e^2}{mN(\omega)}\sum_{i=1}^{2}\delta(x-a_i)\right)\tilde{\phi}_\omega(x) = -\frac{e}{mN(\omega)}\sum_{i=1}^{2}\delta(x-a_i)\tilde{F}_{i\omega}.$$

This equation can be solved also easily. It is important to mention, that we take the inhomogeneous solutions only. This is because the homogeneous one are proportional to $\exp(-\frac{\gamma}{2}t)$ and disappear after time, when the equilibrium is reached.

This way, we express the field $\tilde{\phi}_\omega(x)$ and the oscillators, $\tilde{\xi}_{i\omega}$, in terms of the bath operators $b_{i\omega}$, $b^\dagger_{i\omega}$
Next, we insert these solutions into the Hamiltonian, $H = H_{\text{field}} + H_{\text{osc}} + H_{\text{int}}$, with

$$H_{\text{field}} = \int dx\,\frac{1}{2}\left(\dot{\phi}(t,x)^2 + \phi'(t,x)^2\right),\; H_{\text{osc}} = \sum_{i=1}^{2}\frac{m}{2}\left(\dot{\xi}_i(t)^2 + \Omega^2\xi_i(t)^2\right),\; H_{\text{int}} = e\sum_{i=1}^{2}\xi_i(t)\phi(t,a_i).$$

The Hamiltonian appears expressed in terms of the bath operators (via the Langevin forces).

Now we calculate the averages, $E = \langle H \rangle$ for the internal energy using

$$\langle \hat{b}_\omega \hat{b}^\dagger_{\omega'} + \hat{b}^\dagger_\omega \hat{b}_{\omega'} \rangle = \delta(\omega - \omega') \mathcal{N}_T(\omega), \qquad \langle \ldots \rangle = \frac{1}{Z} \mathrm{Tr} \ldots e^{-\beta H}$$

the result reads (after some calculation)

$$E = \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega \mathcal{N}_T(\omega) \partial_\omega \delta(\omega), \quad F = \int_0^\infty \frac{d\omega}{\pi} \left(\frac{\hbar\omega}{2} + T \ln \left(1 - e^{-\beta\hbar\omega}\right) \right) \partial_\omega \delta(\omega)$$

(for the free energy we used the relation $E = \frac{\partial}{\partial\beta}(\beta F)$) where $\delta(\omega) = \frac{1}{2i} \mathrm{Tr} \ln \frac{\hat{\Phi}(\omega)}{\hat{\Phi}(-\omega)}$ with

$$\left(\hat{\Phi}(\omega)\right)_{rs} = (-\omega^2 + i\gamma\omega + \Omega^2)\delta_{rs} - \frac{e^2}{m} G_0(a_r, a_s)$$

Here, $G_0(x, x')$ is the free Green's function of the field $\phi(t, x)$.

remarks

- This way, we have a representation of the free energy in terms of an integral over real frequencies. However, these are in no way related to the eigenfrequencies (modes) of the system (field+oscillators).
- This formula can be viewed as a generalization of the 'remarkable formula', derived in [1] for a single oscillator (and used later in several places)
- $\delta(\omega)$ can be rewritten in terms of the imaginary part of a Green's function
- the above techniques allows to derive FDT's for various Green's functions, e.g., for $\phi(t, x)$ or for $\xi_i(t)$
- the above techniques allows to average over different ensembles, not necessarily Gibbs ensembles
- the heat bath is a microscopic model for the thermodynamic notion of a reservoir
- time reversal is broken by taking the retarded solutions for the bath operators
- it was shown in [2] that the 'independent oscillator model' (this is what we use here) allows to model any admissible damping (including with memory)

[1] G. W. Ford, J. T. Lewis, and R. F. O'Connell. Quantum Oscillator in a Blackbody Radiation Field. *Phys. Rev. Lett.*, 55:2273–2276, 1985.

[2] G. W. Ford, J. T. Lewis, and R. F. O'Connell. Quantum Langevin Equation. *Phys. Rev. A*, 37:4419–4428, 1988.

Electromagnetic field and dipoles [1710.00300]

do the same as before for the more realistic system

$$(-\omega^2 - \Delta + \boldsymbol{\nabla} \circ \boldsymbol{\nabla})\tilde{\boldsymbol{E}}_\omega(\mathbf{x}) = 4\pi e \omega^2 \sum_i \tilde{\boldsymbol{\xi}}_{\omega,i} \delta^{(3)}(\mathbf{x} - \mathbf{a}_i),$$

$$m\underbrace{(-\omega^2 - i\gamma\omega + \Omega^2)}_{= N(\omega)}\tilde{\boldsymbol{\xi}}_{\omega,i} = e\tilde{\boldsymbol{E}}_\omega(\mathbf{a}_i) + \tilde{\boldsymbol{F}}_{\omega,i},$$

this is after Fourier transform, point dipoles $\mathbf{p}_i = e\boldsymbol{\xi}_i$ ($\boldsymbol{\xi}_i$ - displacement of the i-th charge), dipole approximation is taken and the bath variables are already integrated out, providing dissipation and Langevin forces
from the Langevin forces we need only the averages

$$\langle \tilde{\boldsymbol{F}}_{\omega,i} \tilde{\boldsymbol{F}}_{\omega',j} \rangle = \frac{\gamma m \omega}{\pi} \delta(\omega + \omega') \delta_{ij} \coth \frac{\beta\omega}{2}.$$

'It remains' to solve these equations, i.e., to get expressions for the electric field $\tilde{\boldsymbol{E}}_\omega(\mathbf{x})$ and for the displacements $\tilde{\boldsymbol{\xi}}_{\omega,i}$, in terms of the Langevin forces $\tilde{\boldsymbol{F}}_{\omega,i}$

If we solve the second equation,

$$\tilde{\xi}_{\omega,i} = \frac{1}{mN(\omega)} \left(e\tilde{\boldsymbol{E}}_\omega(\mathbf{a}_i) + \tilde{\boldsymbol{F}}_{\omega,i} \right)$$

and insert into the first one, we get

$$\left(-\omega^2 - \Delta + \boldsymbol{\nabla} \circ \boldsymbol{\nabla} - 4\pi\alpha(\omega)\omega^2 \sum_i \delta^{(3)}(\mathbf{x} - \mathbf{a}_i) \right) \tilde{\boldsymbol{E}}_\omega(\mathbf{x}) = \frac{4\pi\alpha(\omega)\omega^2}{e} \sum_i \delta^{(3)}(\mathbf{x} - \mathbf{a}_i)\tilde{\boldsymbol{F}}_{\omega,i}$$

This is an effective equation for the electric field. It is like a Schrödinger equation with delta function potentials. The delta functions in this equation are three dimensional and therefor the equation is ill defined. All known methods to handle this situation were recently discussed in [1]. In terms of electrodynamics, one needs to exclude from the solution of this equation the action of the electric field created from a dipole acting on the dipole itself, i.e., its self-field.

[1] M. Bordag and J.M. Munoz-Castaneda. Dirac Lattices, Zero-Range Potentials and Self Adjoint Extension. *Phys. Rev. D*, 91:065027, 2015.

now we insert the solution into the Hamiltonian

$$H = H_{\rm ED} + H_{\rm dipole} \text{ with } H_{\rm ED} = \frac{1}{8\pi}\int d^3\mathbf{x}\left(\boldsymbol{E}(t,\mathbf{x})^2 + \mathbf{B}(t,\mathbf{x})^2\right), H_{\rm dipole} = \sum_i \frac{m}{2}\left(\dot{\boldsymbol{\xi}}_i(t)^2 + \Omega^2\boldsymbol{\xi}_i(t)^2\right);$$

and calculate the internal energy, $E = \langle H\rangle$ and, from here, the free energy. After calculation, we get

$$F = \int_0^\infty \frac{d\omega}{\pi}\left(\frac{\omega}{2} + T\ln\left(1 - e^{-\beta\omega}\right)\right)\partial_\omega\delta(\omega).$$

with

$$\delta(\omega) = \frac{1}{2i}\operatorname{tr}\ln\frac{\hat{\boldsymbol{T}}(\omega)}{\hat{\boldsymbol{T}}(-\omega)}.$$

and $\hat{\boldsymbol{T}}(\omega)$ is the scattering T-operator of the effective equation of the electric field. Its inverse reads

$$T^{-1}_{ij}(\omega) = \frac{1}{4\pi\alpha(\omega)\omega^2}\left(\delta_{ij} - 4\pi\alpha(\omega)\omega^2\boldsymbol{G}^{(0)}_{\omega,ij}\right), \quad \alpha(\omega) = \frac{e^2}{mN(\omega)}$$

where

$$\boldsymbol{G}^{(0)}_{\omega,ij} = \begin{cases} 0, & i = j, \\ \boldsymbol{G}^{(0)}_{\omega}(\mathbf{a}_i - \mathbf{a}_j), & i \neq j, \end{cases}$$

Configurations considered

- atom-atom $\qquad \boldsymbol{\xi}_i(t), \quad$ i=1,2

- atom-wall $\qquad$ i=0 and i=1,2,... $\qquad \mathbf{a}_i \to \quad \mathbf{x}, \quad \sum_{i=1}^{\infty} \to \rho \int d\mathbf{x}\, \Theta(-z),$

$$\delta_{ij} \to \qquad \rho\delta^{(3)}(\mathbf{x}-\mathbf{x}'),$$

- wall-wall $\qquad$ i=-1,-2,... and i=1,2,...

for atom-atom, literally the above formulas

for atom-wall we have $\quad \ln L(\omega) = \ln(1 - 4\pi\alpha(\omega)\omega^2 \Delta G_{\text{wall}})$ with
$\Delta G_{\text{wall}} = \int \frac{d\mathbf{k}_{||}}{(2\pi)^2} \left(r_{\text{TE}} + \frac{-q^2+k_{||}^2}{\omega^2} r_{\text{TM}} \right) \frac{e^{2iqa}}{-2iq}.$
for wall-wall we get

$$F = \int_0^{\infty} \frac{d\omega}{\pi} \int \frac{d\mathbf{k}_{||}}{(2\pi)^2} \left(\frac{\hbar\omega}{2} + T \ln\left(1 - e^{-\beta\omega}\right) \right) \partial_\omega \operatorname{Tr} \ln \frac{\boldsymbol{L}(\omega)}{\boldsymbol{L}(\omega)^*}, \qquad \boldsymbol{L}(\omega) = 1 - r^2 e^{2iaq}$$

$(\omega^2 = k_{||}^2 + q^2)$

special cases

1. $\gamma \to 0$ restore results with pure T except for wall-wall, where $\lim_{\gamma\to 0} \Delta_T F = \Delta_T F(\gamma = 0) + \mathcal{F}_1 T$ is restored

2. $T \to 0$ in each case $F \sim T^2$ found

3. transition to Matsubara representation delivers the known formulas, except for A-A and A-W configurations in case the oscillators have vanishing intrinsic frequency Ω. In such cases, the $l = 0$ – contribution becomes modified
   modification also in case of criticality

Comments

- reobtained known results, except for non-perturbative treatment of atom-wall case
- modification of $l = 0$ – contribution in some special cases
- no problem with thermodynamics possible. Within the given approach, the dissipation parameter γ cannot depend on temperature, different approach needed

Thank you for attention