The origin of van-der-Waals forces

Fundamental concepts and their consequences

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UNIVERSITY OF BERGEN

Acknowledgements

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- Lennard-Jones Potential

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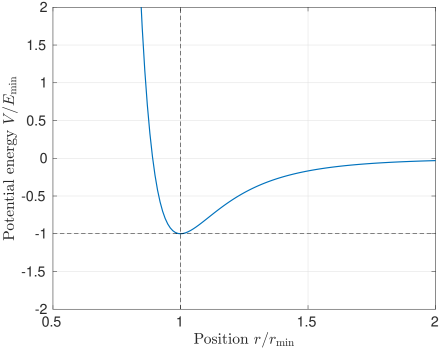

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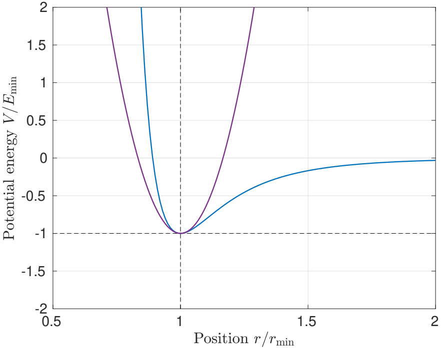

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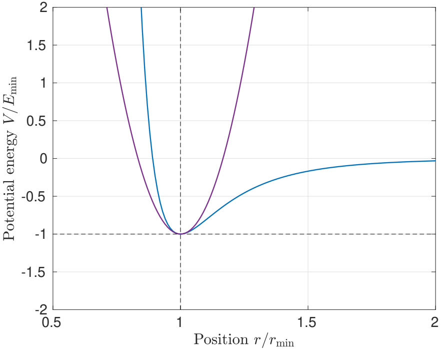

- Origin:
  - Repulsive C_{12}: Pauli blocking

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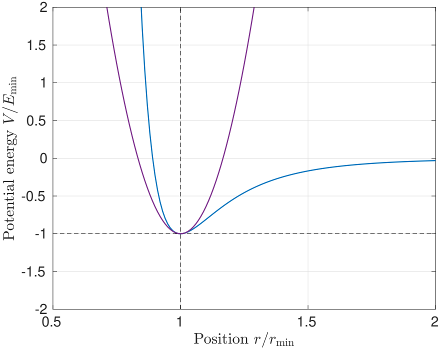

- Origin:
  - Repulsive C_{12}: Pauli blocking
  - Attractive C_6: van-der-Waals Coefficient, tabled somewhere

Unsatisfying situation

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- How does the vdW coefficient depend on the materials?
- Force discovered in 1873 by Johannes Diderik van der Waals, and still, there are tabled values.
- Nowadays, several DFT simulations still use tabled values, e.g. Grimme, Tkatchenko–Scheffler

Difficult situation

	Gravity	Electromagnetism	Weak interaction	Strong interaction
Acting on	mass	charges	quarks and leptons	quarks
Range	∞	∞	$< 10^{-17}\,\mathrm{m}$	$\approx 10^{-15}\,\mathrm{m}$
Rel. strength	1	10^{36}	10^{25}	10^{38}
Long-range	$1/r$	$1/r$	e^{-mr}/r	r

Table: Overview of the fundamental interactions: gravity, electromagnetism, weak and strong interactions concerning the corresponding property of the interaction objects (acting on), their range, their relative strength (rel. strength) compared to gravity, and their long-range behaviour.

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Where is the van-der-Waals force?

Relevance of vdW forces for daily life

[1] HBG Casimir, Proc. Kon. Ned. Akad. Wet. **51**, 793 (1948).

Relevance of vdW forces for daily life

https://www.nwzonline.de/wirtschaft/weser-ems/nordenham-drei-zimmer-fuer-nur-einen-euro_a_1,0,606668192.html

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Relevance of vdW forces for daily life

https://www.gutefrage.net/frage/wandinnenfarbe-noch-gut-oder-nicht

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- Common question: Can I still use it?

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https://de.wikipedia.org/wiki/Hendrik_Casimir

- Common question: Can I still use it?
- Scientific question: Why is that?
- H.B.G. Casimir: That's something to do with the vacuum fluctuations

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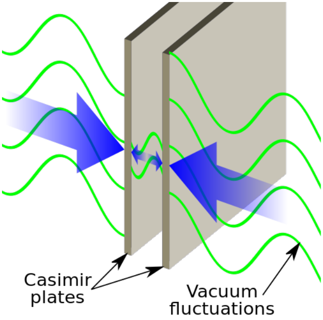

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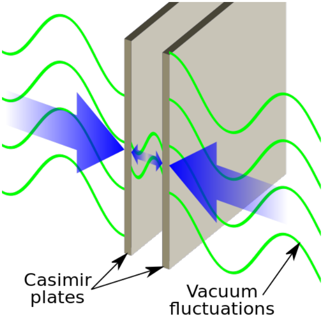

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- Difference of zero-point energy inside and outside[1]

[1] HBG Casimir, Proc. Kon. Ned. Akad. Wet. **51**, 793 (1948).

Table of contents

Table of Contents

References

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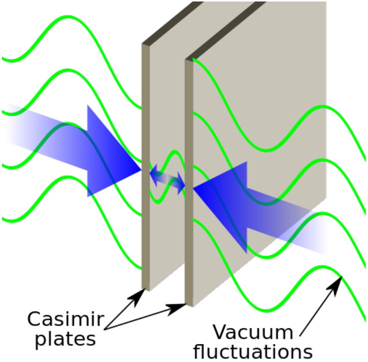
- Script: http://www.dr-fiedler.eu/pages/teaching.php

Requirements for the theory



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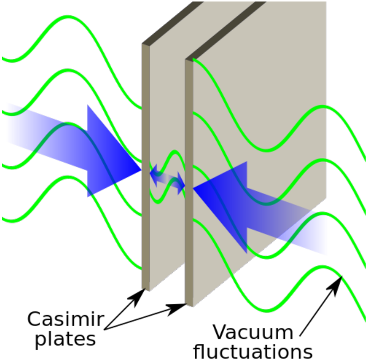

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- Effect of the ground-state fluctuations or zero-point energy of the em field

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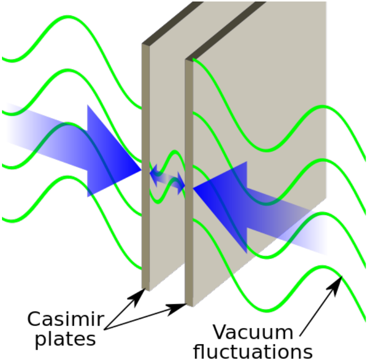

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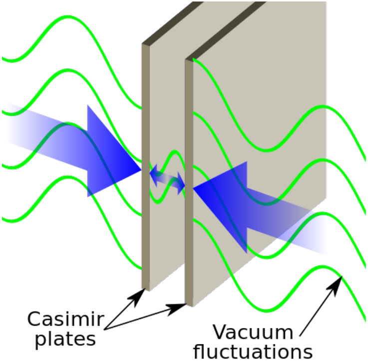

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$\rightarrow$ Quantum mechanics

- Effect involves neutral, dielectric or polarisable objects

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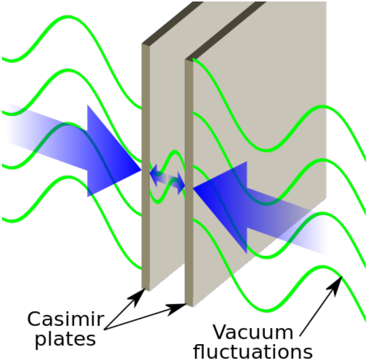

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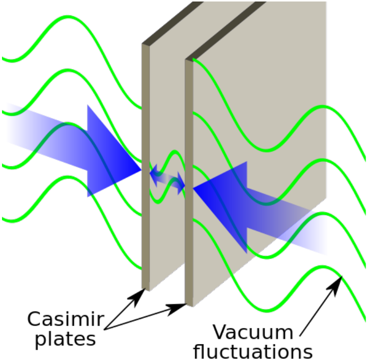

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$\rightarrow$ Macroscopic Maxwell Equations

$\rightarrow$ Solution via Green functions to be applicable to arbitrary geometries

Table of Contents

em field in presence of mac. dielectrics

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- mac. Maxwell equations: absence of external sources and currents

$$
\begin{aligned}
\nabla \cdot \boldsymbol{B}(\boldsymbol{r}, t) &= 0\,, \\
\nabla \times \boldsymbol{E}(\boldsymbol{r}, t) &= -\dot{\boldsymbol{B}}(\boldsymbol{r}, t)\,, \\
\nabla \cdot \boldsymbol{D}(\boldsymbol{r}, t) &= 0\,, \\
\nabla \times \boldsymbol{H}(\boldsymbol{r}, t) &= \dot{\boldsymbol{D}}(\boldsymbol{r}, t)\,.
\end{aligned}
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- displacement field $\boldsymbol{D}(\boldsymbol{r})$, magnetic field $\boldsymbol{H}(\boldsymbol{r})$

$$\boldsymbol{D}(\boldsymbol{r}) = \varepsilon_0 \boldsymbol{E}(\boldsymbol{r}) + \boldsymbol{P}(\boldsymbol{r})\,, \qquad \boldsymbol{H}(\boldsymbol{r}) = \frac{1}{\mu_0}\boldsymbol{B}(\boldsymbol{r}) - \boldsymbol{M}(\boldsymbol{r})\,,$$

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- polarisation $\boldsymbol{P}(\boldsymbol{r})$ and magnetisation $\boldsymbol{M}(\boldsymbol{r})$

Noise currents and density

- medium responds linearly and locally to the externally applied fields
  $\rightarrow$ linear response function

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$$

- noise polarisation and noise magnetisation $\boldsymbol{P}_N(\boldsymbol{r},t)$, $\boldsymbol{M}_N(\boldsymbol{r},t)$ consequence of the fluctuation–dissipation theorem

- $\boldsymbol{P}_N(\boldsymbol{r}, t)$, $\boldsymbol{M}_N(\boldsymbol{r}, t) \Longleftrightarrow$ noise current and noise density

$$\varrho_N(\boldsymbol{r},\omega) = -\nabla\cdot\boldsymbol{P}_N(\boldsymbol{r},\omega)\,, \quad \boldsymbol{j}_N(\boldsymbol{r},\omega) = -i\omega\boldsymbol{P}_N(\boldsymbol{r},\omega)+\nabla\times\boldsymbol{M}_N(\boldsymbol{r},\omega)$$

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- sources for Maxwell equations (temporal Fourier space)

$$\begin{aligned}
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\varepsilon_0\nabla\cdot[\varepsilon(\boldsymbol{r},\omega)\boldsymbol{E}(\boldsymbol{r},\omega)] &= \varrho_N(\boldsymbol{r},\omega)\,,\\
\nabla\times[\kappa(\boldsymbol{r},\omega)\boldsymbol{B}(\boldsymbol{r},\omega)] + i\frac{\omega}{c^2}\varepsilon(\boldsymbol{r},\omega)\boldsymbol{E}(\boldsymbol{r},\omega) &= \mu_0\boldsymbol{j}_N(\boldsymbol{r},\omega)\,,
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\end{aligned}$$

- Maxwell equations $\rightarrow$ vector HELMHOLTZ equation for the electric field

$$\nabla\times[\kappa(\boldsymbol{r},\omega)\nabla\times\boldsymbol{E}(\boldsymbol{r},\omega)] - \frac{\omega^2}{c^2}\varepsilon(\boldsymbol{r},\omega)\boldsymbol{E}(\boldsymbol{r},\omega) = i\omega\mu_0\boldsymbol{j}_N(\boldsymbol{r},\omega)$$

Fundamental solution of the Helmholtz equation

$$\nabla \times \nabla \times \boldsymbol{E}(\boldsymbol{r},\omega) - \frac{\omega^2}{c^2}\varepsilon(\boldsymbol{r},\omega)\boldsymbol{E}(\boldsymbol{r},\omega) = i\omega\mu_0\boldsymbol{j}_N(\boldsymbol{r},\omega)$$

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- dyadic GREEN function $\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)$

$$\nabla \times \nabla \times \mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega) - \frac{\omega^2}{c^2}\varepsilon(\boldsymbol{r},\omega)\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega) = \boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')\,,$$

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- electric field:

$$\boldsymbol{E}(\boldsymbol{r},\omega) = i\omega\mu_0 \int \mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\boldsymbol{j}_N(\mathbf{r}',\omega)\mathrm{d}^3r'\,.$$

dyadic Green function

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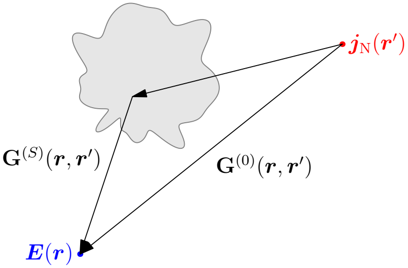
- Separation of Green tensor



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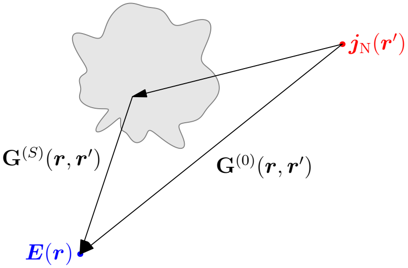
- free propagation (vacuum, bulk) $\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}')$



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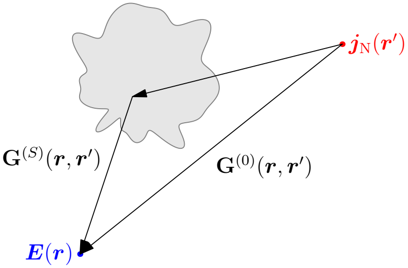

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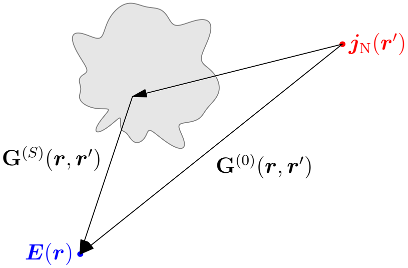

Quantisation of the em field

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- Hamiltonian of em field

$$H = \frac{1}{2}\int \mathrm{d}^3 r \left[\varepsilon_0 \boldsymbol{E}^2(\boldsymbol{r},t) + \frac{1}{\mu_0}\boldsymbol{B}^2(\boldsymbol{r},t)\right]$$

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- with second Maxwell equation

$$\nabla \times \boldsymbol{E}(\boldsymbol{r},\omega) = i\omega \boldsymbol{B}(\boldsymbol{r},\omega)$$

$\rightarrow$

$$H = \frac{1}{2}\int \mathrm{d}^3 r \left[\varepsilon_0 \boldsymbol{E}^2(\boldsymbol{r},t) - \frac{1}{\omega^2\mu_0}\left[\nabla \times \boldsymbol{E}(\boldsymbol{r},t)\right]^2\right]$$

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- e field induced by noise currents

$$\boldsymbol{E}(\boldsymbol{r},\omega) = i\omega\mu_0 \int \mathbf{G}(\boldsymbol{r},\mathbf{r}',\omega)\cdot \boldsymbol{j}_N(\mathbf{r}',\omega)\mathrm{d}^3 r'$$

Quantisation of the em field

- currents induced by external e field

$$\boldsymbol{j}(\boldsymbol{r},\omega) = \int \mathbf{Q}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\boldsymbol{E}(\boldsymbol{r}',\omega)\mathrm{d}^3r' + \boldsymbol{j}_N(\boldsymbol{r},\omega)$$

with complex conductivity tensor **Q**

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- 2^{nd} quantisation: canonical variable noise currents $\boldsymbol{j}_N(\boldsymbol{r},\omega)\to\hat{\boldsymbol{j}}_N(\boldsymbol{r},\omega)$
- fluctuation–dissipation theorem:

$$\left[\hat{\boldsymbol{j}}_N(\boldsymbol{r},\omega),\hat{\boldsymbol{j}}_N^\dagger(\boldsymbol{r}',\omega')\right]=\frac{\hbar\omega}{\pi}\delta(\omega-\omega')\boldsymbol{\sigma}(\boldsymbol{r},\boldsymbol{r}',\omega)$$

Quantisation of the em field

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$$\boldsymbol{j}(\boldsymbol{r},\omega) = \int \mathbf{Q}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\boldsymbol{E}(\boldsymbol{r}',\omega)\mathrm{d}^3r' + \boldsymbol{j}_N(\boldsymbol{r},\omega)$$

  with complex conductivity tensor $\mathbf{Q}$
- its real part $\boldsymbol{\sigma}(\boldsymbol{r},\boldsymbol{r}',\omega) = \mathrm{Re}\,\mathbf{Q}(\boldsymbol{r},\boldsymbol{r}',\omega)$
- 2^{nd} quantisation: canonical variable noise currents $\boldsymbol{j}_N(\boldsymbol{r},\omega) \to \hat{\boldsymbol{j}}_N(\boldsymbol{r},\omega)$
- fluctuation–dissipation theorem:

$$\left[\hat{\boldsymbol{j}}_N(\boldsymbol{r},\omega),\hat{\boldsymbol{j}}_N^\dagger(\boldsymbol{r}',\omega')\right] = \frac{\hbar\omega}{\pi}\delta(\omega-\omega')\boldsymbol{\sigma}(\boldsymbol{r},\boldsymbol{r}',\omega)$$

- $\hat{H} = \pi\int\mathrm{d}\omega\int\mathrm{d}^3r\mathrm{d}^3r'\,\hat{\boldsymbol{j}}_N^\dagger(\boldsymbol{r},\omega)\cdot\boldsymbol{\sigma}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\hat{\boldsymbol{j}}_N(\boldsymbol{r}',\omega)$

field–medium operators

- bosonic creation operator

$$\hat{\boldsymbol{f}}(\boldsymbol{r},\omega) = \sqrt{\frac{\hbar\omega}{\pi}} \int \mathrm{d}^3 r' \mathbf{K}(\boldsymbol{r},\boldsymbol{r}',\omega) \cdot \hat{\boldsymbol{j}}_N(\boldsymbol{r}',\omega)$$

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- Hamiltonian

$$\hat{H} = \int \mathrm{d}\omega \int \mathrm{d}^3 r\, \hbar\omega\, \hat{\boldsymbol{f}}^\dagger(\boldsymbol{r},\omega) \cdot \hat{\boldsymbol{f}}(\boldsymbol{r},\omega)$$

What is $\mathbf{K}(\boldsymbol{r}, \boldsymbol{r}', \omega)$?

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- quantised e-field

$$\hat{\boldsymbol{E}}(\boldsymbol{r},\omega) = i\mu_0\omega\sqrt{\frac{\hbar\omega}{\pi}}\int \mathrm{d}^3 s \int \mathrm{d}^3 r' \mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\mathbf{K}(\boldsymbol{r}',\boldsymbol{s},\omega)\cdot\hat{\boldsymbol{f}}(\boldsymbol{s},\omega)$$

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Useful relations

Useful relations

- Excitations
  - Annihilation: $\hat{\boldsymbol{f}}(\boldsymbol{r},\omega)\,|\{0\}\rangle = \boldsymbol{0}$
  - Creation: $\hat{\boldsymbol{f}}^\dagger(\boldsymbol{r},\omega)\,|\{0\}\rangle = |\boldsymbol{1}(\boldsymbol{r},\omega)\rangle$
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  - Describe excitations of field **and** media. Often called polaritons
- local mode density:
$$\left\langle \hat{\boldsymbol{E}}(\boldsymbol{r},\omega)\otimes\hat{\boldsymbol{E}}^{\dagger}(\boldsymbol{r}',\omega')\right\rangle = \frac{\hbar}{\pi\varepsilon_0}\frac{\omega^2}{c^2}\mathrm{Im}\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\delta(\omega-\omega')$$

Table of Contents

Quantum-mechanics of a free particle

$$\hat{H} = \hat{T}_c + \hat{T}_e + \hat{V}_{ee} + \hat{V}_{cc} + \hat{V}_{ec}\,, \tag{1}$$

- Kinetic energy of core $\hat{T}_c$
- Kinetic energy of electrons $\hat{T}_e$
- Interaction potential between the electrons $\hat{V}_{ee}$
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Typically solved via DFT

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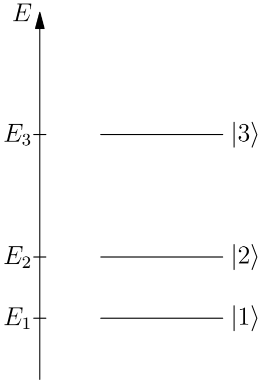
Typically solved via DFT
Too complicated for QED

Particles in the QED framework

- Solving the Hamiltonian yields energy spectrum



Particles in the QED framework

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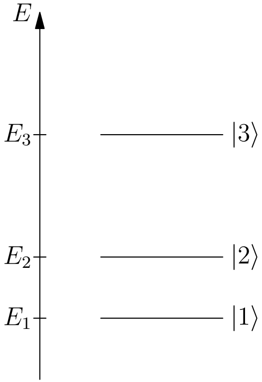

Particles in the QED framework

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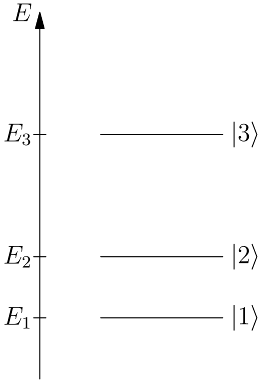
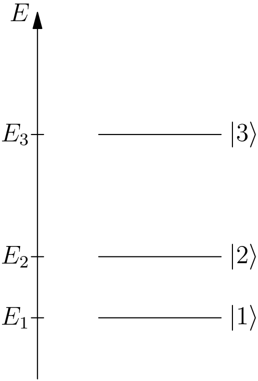


Particles in the QED framework

- Solving the Hamiltonian yields energy spectrum
- Energies $E_1 < E_2 < E_3 < \dots$
- States $|1\rangle, |2\rangle, |3\rangle, \dots$
- Expand Hamiltonian in energy states

$$\hat{H} = \sum_n E_n |n\rangle \langle n| \tag{2}$$

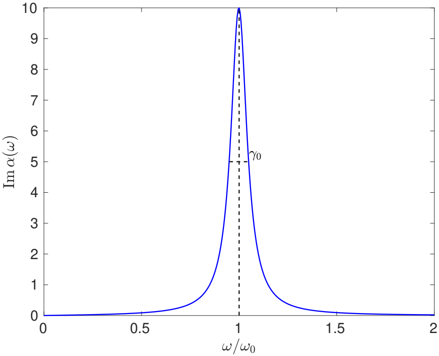


Particle's spectrum

Particle's spectrum

- Characterised by polarisability

$$\alpha_0(\omega) = \sum_j \frac{c_{0j}}{\omega_{0j}^2 - \omega^2 - i\gamma_{j0}\omega}$$



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$$\alpha_0(\omega) = \sum_j \frac{c_{0j}}{\omega_{0j}^2 - \omega^2 - i\gamma_{j0}\omega}$$

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- Linewidth γ_{0j}
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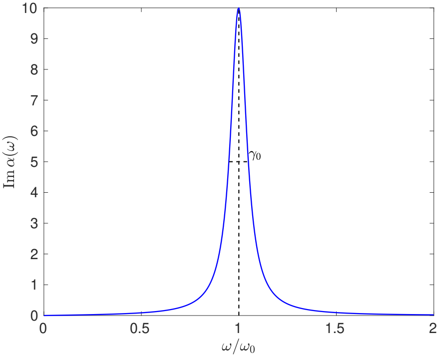

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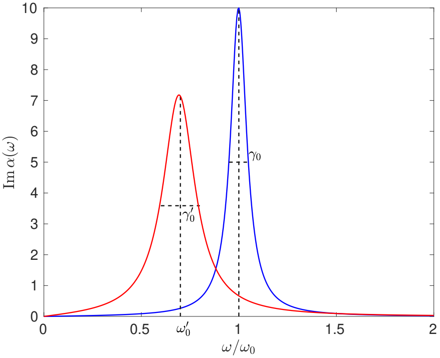

- Near surface: $\omega_0' = \omega_0 + \Delta\omega_0(\boldsymbol{r})$, $\gamma_0' = \gamma_0 + \Delta\gamma_0(\boldsymbol{r})$

Table of Contents

Dipole coupling

$$\hat{H}_{\mathrm{int}} = -\hat{\boldsymbol{d}} \cdot \hat{\boldsymbol{E}}$$

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$$\hat{\boldsymbol{d}} = e\hat{\boldsymbol{r}}$$

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Dipole coupling

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- Dipole operator

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  acting on the particle
- Field operator

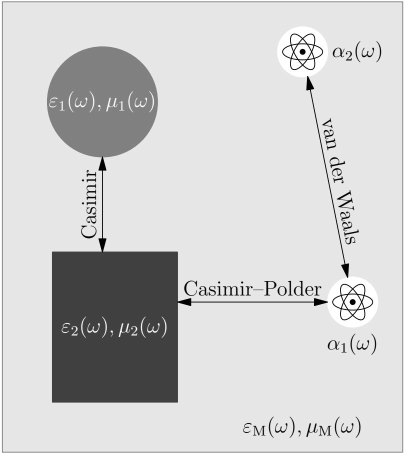
$$\hat{\boldsymbol{E}}(\boldsymbol{r},\omega) = i\sqrt{\frac{\hbar}{\pi\varepsilon_0}}\frac{\omega^2}{c^2}\int \mathrm{d}^3r'\sqrt{\mathrm{Im}\chi(\boldsymbol{r}',\omega)}\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\hat{\boldsymbol{f}}(\boldsymbol{r}',\omega)$$

  acting on the field (including media)

Dispersion Forces

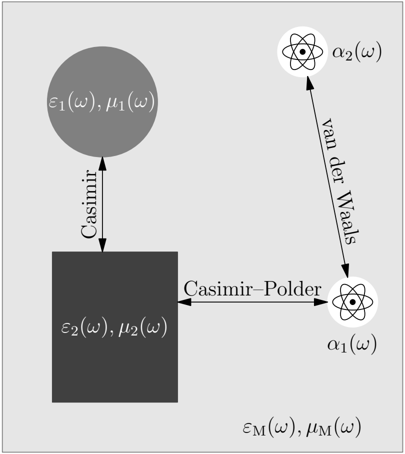
Dispersion Forces

- Casimir force: Interaction between two macroscopic dielectric bodies $\varepsilon_{1,2}$



Dispersion Forces

- Casimir force: Interaction between two macroscopic dielectric bodies $\varepsilon_{1,2}$
- Casimir–Polder force: Interaction between a polarisable particle α and a dielectric body ε



Dispersion Forces

- Casimir force: Interaction between two macroscopic dielectric bodies $\varepsilon_{1,2}$
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- Van der Waals force: Interaction between two polarisable particles $\alpha_{1,2}$

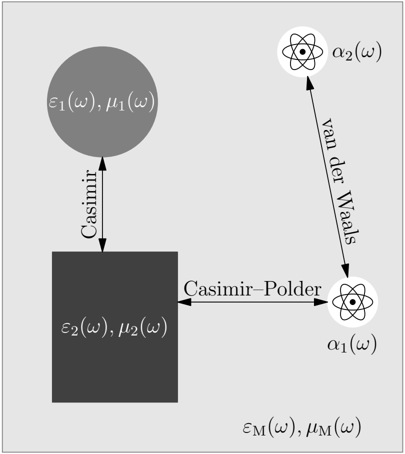


Table of Contents

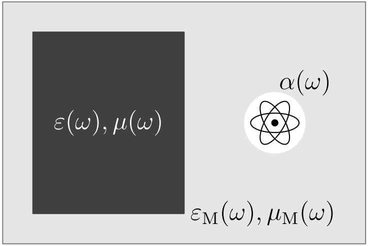
Origin of Dispersion forces

Dispersion interaction	origin
Casimir force	$\left\langle \hat{\varrho}\hat{\boldsymbol{E}} + \hat{\boldsymbol{j}} \times \hat{\boldsymbol{B}} \right\rangle$
Casimir–Polder force	$\left\langle \hat{\boldsymbol{d}} \cdot \hat{\boldsymbol{E}} \right\rangle_2$
van der Waals force	$\left\langle \hat{\boldsymbol{d}}_1 \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_1) + \hat{\boldsymbol{d}}_2 \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_2) \right\rangle_4$

Table of Contents

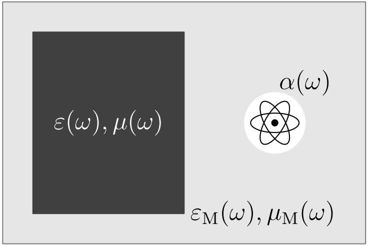
Casimir–Polder potential

- Situation: particle in front of a dielectric body $[\varepsilon(\omega), \mu(\omega)]$



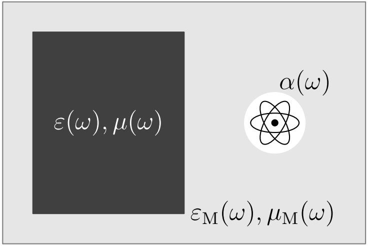
Casimir–Polder potential

- Situation: particle in front of a dielectric body $[\varepsilon(\omega), \mu(\omega)]$
- Particle in ground state: $|0\rangle$



Casimir–Polder potential

- Situation: particle in front of a dielectric body [$\varepsilon(\omega), \mu(\omega)$]
- Particle in ground state: $|0\rangle$
- Field in ground state: $|\{0\}\rangle$



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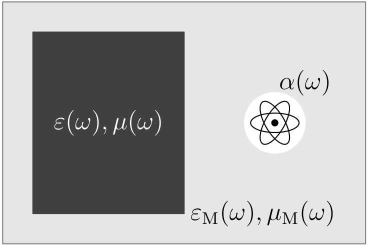

- Hamiltonian $\hat{H} = \hat{H}_F + \hat{H}_A + \hat{H}_{AF}$

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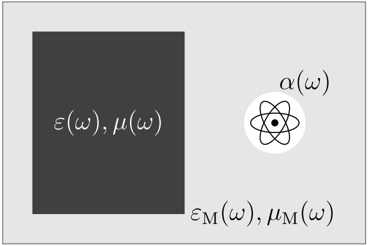
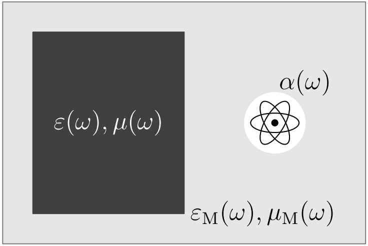


- Hamiltonian $\hat{H} = \hat{H}_F + \hat{H}_A + \hat{H}_{AF}$
- without interaction

Casimir–Polder potential



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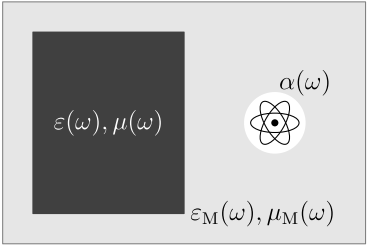
Casimir–Polder potential



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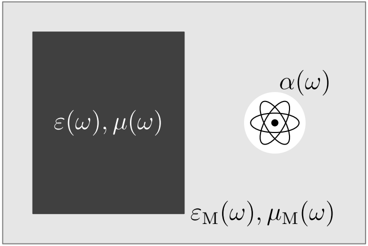

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- without interaction
  - Hamiltonian $\hat{H}_0 = \hat{H}_F + \hat{H}_A$
  - State $|0, \{0\}\rangle$

$\rightarrow$ Perturbation theory

Casimir–Polder potential

- e field: $\hat{\boldsymbol{E}}(\boldsymbol{r},\omega) = i\sqrt{\frac{\hbar}{\pi\varepsilon_0}}\frac{\omega^2}{c^2}\int \mathrm{d}^3r'\sqrt{\mathrm{Im}\chi(\boldsymbol{r}',\omega)}\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\hat{\boldsymbol{f}}(\boldsymbol{r}',\omega)$

Casimir–Polder potential

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- state: $|0,\{0\}\rangle$; interaction: $\hat{H}_{AF} = -\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}$

Casimir–Polder potential

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- state: $|0,\{0\}\rangle$; interaction: $\hat{H}_{AF} = -\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}$
- Perturbation:

$$
\begin{aligned}
\Delta E = &- \langle 0,\{0\}|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|0,\{0\}\rangle \\
&- \sum_k \int \mathrm{d}^3r\mathrm{d}\omega \frac{\langle 0,\{0\}|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|k,\mathbf{1}(\boldsymbol{r},\omega)\rangle\langle k,\mathbf{1}(\boldsymbol{r},\omega)|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|0,\{0\}\rangle}{\hbar\left(\omega_k-\omega\right)} \\
&+ \cdots
\end{aligned}
$$

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- Perturbation:

$$\begin{aligned}\Delta E =& -\langle 0,\{0\}|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|0,\{0\}\rangle \\ & -\sum_k\int \mathrm{d}^3r\mathrm{d}\omega\frac{\langle 0,\{0\}|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|k,\mathbf{1}(\boldsymbol{r},\omega)\rangle\langle k,\mathbf{1}(\boldsymbol{r},\omega)|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}\,|0,\{0\}\rangle}{\hbar\,(\omega_k-\omega)} \\ & +\cdots\end{aligned}$$

- Intermediate states $|k,\mathbf{1}(\boldsymbol{r},\omega)\rangle$: one field excitation, particle excited to state k

Casimir–Polder potential

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& +\cdots
\end{aligned}
$$

- Intermediate states $|k,\mathbf{1}(\boldsymbol{r},\omega)\rangle$: one field excitation, particle excited to state k
- First order vanishes

Casimir–Polder potential

- Matrix element

$$\langle k, \mathbf{1}(\boldsymbol{r},\omega)|\,\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}(\boldsymbol{r}_A)\,|0,\{0\}\rangle = \boldsymbol{d}_{k0}\cdot\mathbf{G}^{*,T}(\boldsymbol{r}_A,\boldsymbol{r},\omega)$$

Casimir–Polder potential

- Matrix element

$$\langle k, \mathbf{1}(\boldsymbol{r},\omega)|\, \hat{\boldsymbol{d}} \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_A)\, |0, \{0\}\rangle = \boldsymbol{d}_{k0} \cdot \mathbf{G}^{*,T}(\boldsymbol{r}_A, \boldsymbol{r}, \omega)$$

- Energy shift:

$$\Delta E = -\sum_k \int \mathrm{d}^3 r \int \frac{\mathrm{d}\omega}{\hbar(\omega_k - \omega)} \left(\boldsymbol{d}_{0k} \cdot \mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}, \omega) \cdot \mathbf{G}^{*,T}(\boldsymbol{r}, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0} \right)$$

Casimir–Polder potential

- Matrix element

$$\langle k, \mathbf{1}(\boldsymbol{r}, \omega)| \,\hat{\boldsymbol{d}} \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_A) \,|0, \{0\}\rangle = \boldsymbol{d}_{k0} \cdot \mathbf{G}^{*,T}(\boldsymbol{r}_A, \boldsymbol{r}, \omega)$$

- Energy shift:

$$\Delta E = -\sum_k \int \mathrm{d}^3 r \int \frac{\mathrm{d}\omega}{\hbar(\omega_k - \omega)} \left(\boldsymbol{d}_{0k} \cdot \mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}, \omega) \cdot \mathbf{G}^{*,T}(\boldsymbol{r}, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0}\right)$$

- Integral relation:

$$\int \mathrm{d}^3 s \, \mathbf{G}(\boldsymbol{r}, \boldsymbol{s}, \omega) \cdot \mathbf{G}^{*,T}(\boldsymbol{s}, \boldsymbol{r}', \omega) = \frac{\hbar\mu_0}{\pi} \omega^2 \mathrm{Im}\, \mathbf{G}(\boldsymbol{r}, \boldsymbol{r}', \omega)$$

Casimir–Polder potential

- Energy shift:

$$\Delta E = -\sum_k \int \frac{\mathrm{d}\omega\, \mu_0 \omega^2}{\pi(\omega_k - \omega)} \boldsymbol{d}_{0k} \cdot \operatorname{Im} \mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0}$$

Casimir–Polder potential

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$$\Delta E = -\sum_k \int \frac{\mathrm{d}\omega\,\mu_0\omega^2}{\pi(\omega_k - \omega)} \boldsymbol{d}_{0k} \cdot \mathrm{Im}\,\mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0}$$

- Recalling: local mode density (slide 20):
$\left\langle \hat{\boldsymbol{E}}(\boldsymbol{r},\omega) \otimes \hat{\boldsymbol{E}}^\dagger(\boldsymbol{r}',\omega') \right\rangle = \frac{\hbar}{\pi\varepsilon_0}\frac{\omega^2}{c^2}\mathrm{Im}\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\delta(\omega-\omega')$
interpretation: CP force proportional to the local mode density of the vacuum field

Casimir–Polder potential

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  interpretation: CP force proportional to the local mode density of the vacuum field
- Separation of the Green function (slide 15)

$$\Delta E = -\sum_k \int \frac{\mathrm{d}\omega\,\mu_0\omega^2}{\pi(\omega_k-\omega)} \times \left(\boldsymbol{d}_{0k}\cdot \mathrm{Im}\left[\mathbf{G}^{(0)}(\boldsymbol{r}_A,\boldsymbol{r}_A,\omega)+\mathbf{G}^{(S)}(\boldsymbol{r}_A,\boldsymbol{r}_A,\omega)\right]\cdot \boldsymbol{d}_{k0}\right)$$

Lamb shift

- free-space Green tensor in coincidence limit is dependent on $\boldsymbol{r}$

$$\mathrm{Im}\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r},\omega)=\frac{\omega}{6\pi c}\mathbf{1}$$

Lamb shift

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- Lamb shift:

$$\Delta E_{Lamb} = -\sum_k \int \frac{\mathrm{d}\omega\,\mu_0\omega^2}{\pi(\omega_k-\omega)} \left(\boldsymbol{d}_{0k}\cdot \mathrm{Im}\,\mathbf{G}^{(0)}(\boldsymbol{r}_A,\boldsymbol{r}_A,\omega)\cdot \boldsymbol{d}_{k0}\right)$$

Lamb shift

- free-space Green tensor in coincidence limit is dependent on $\boldsymbol{r}$

$$\mathrm{Im}\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r},\omega) = \frac{\omega}{6\pi c}\mathbf{1}$$

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$$\Delta E_{Lamb} = -\sum_k \int \frac{\mathrm{d}\omega\,\mu_0\omega^2}{\pi(\omega_k-\omega)}\left(\boldsymbol{d}_{0k}\cdot\mathrm{Im}\,\mathbf{G}^{(0)}(\boldsymbol{r}_A,\boldsymbol{r}_A,\omega)\cdot\boldsymbol{d}_{k0}\right)$$

- limiting integral range to $\hbar\omega_k \ll m_e c^2$ (non-relativistic)

$$\Delta E_{Lamb} = \frac{\mu_0}{6\pi^2 c}\sum_k \omega_k^3\,|\boldsymbol{d}_{0k}|^2 \ln\left(\frac{m_e c^2}{\hbar\omega_k}\right)$$

Casimir–Polder potential

- Energy shift due to the scattering Green function

$$\Delta E = -\sum_k \int \frac{\mathrm{d}\omega \, \mu_0 \omega^2}{\pi(\omega_k - \omega)} \left(\boldsymbol{d}_{0k} \cdot \operatorname{Im} \mathbf{G}^{(S)}(\boldsymbol{r}_A, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0} \right)$$

Casimir–Polder potential

- Energy shift due to the scattering Green function

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- spatial dependent potential $\rightarrow$ Casimir–Polder potential $U_{CP}(\boldsymbol{r}_A)$

Casimir–Polder potential

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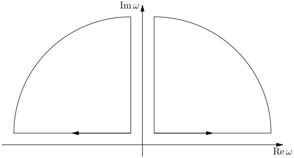
- spatial dependent potential $\to$ Casimir–Polder potential $U_{CP}(\boldsymbol{r}_A)$
- using $\mathrm{Im}\mathbf{G} = (\mathbf{G}-\mathbf{G}^*)/2i$ and
  Schwarz reflection principle $\mathbf{G}^*(\omega) = \mathbf{G}(-\omega^*)$

$$U_{CP}(\boldsymbol{r}_A) = \frac{\mu_0}{2i\pi}\sum_k \left[\int_0^\infty \frac{\mathrm{d}\omega}{\omega_k+\omega} - \int_0^{-\infty} \frac{\mathrm{d}\omega}{\omega_k-\omega}\right] \times\omega_k\omega\boldsymbol{d}_{0k}\cdot\mathbf{G}^{(S)}(\boldsymbol{r}_A,\boldsymbol{r}_A,\omega)\cdot\boldsymbol{d}_{k0}$$

Casimir–Polder potential

$$U_{CP}(\boldsymbol{r}_A) = \frac{\mu_0}{2i\pi} \sum_k \left[\int_0^{\infty} \frac{\mathrm{d}\omega}{\omega_k + \omega} - \int_0^{-\infty} \frac{\mathrm{d}\omega}{\omega_k - \omega} \right]$$
$$\times \omega_k \omega \boldsymbol{d}_{0k} \cdot \mathbf{G}^{(S)}(\boldsymbol{r}_A, \boldsymbol{r}_A, \omega) \cdot \boldsymbol{d}_{k0}$$

- Contour-integral techniques
- Green function analytic in the upper half plane
- Contour along infinite quarter-circles vanishes



$$U_{CP}(\boldsymbol{r}_A) = \frac{\mu_0}{\pi} \sum_k \int_0^{\infty} \mathrm{d}\xi \frac{\omega_k \xi^2}{\omega_k^2 + \xi^2} \mathbf{d}_{0k} \cdot \mathbf{G}^{(S)}(\boldsymbol{r}_A, \boldsymbol{r}_A, i\xi) \cdot \mathbf{d}_{k0}$$

- $\boldsymbol{a} \cdot \mathbf{A} \cdot \boldsymbol{b} = a_i A_{ij} b_j = b_j a_i A_{ij} = \mathrm{tr}[\boldsymbol{b} \otimes \boldsymbol{a} \cdot \mathbf{A}]$

- $\boldsymbol{a} \cdot \mathbf{A} \cdot \boldsymbol{b} = a_i A_{ij} b_j = b_j a_i A_{ij} = \mathrm{tr}[\boldsymbol{b} \otimes \boldsymbol{a} \cdot \mathbf{A}]$
- dispersion formula for ground-state polarisability

$$\boldsymbol{\alpha}(\omega) = \lim_{\epsilon \to 0+} \frac{1}{\hbar} \sum_k \left(\frac{\boldsymbol{d}_{k0} \otimes \boldsymbol{d}_{0k}}{\omega + \omega_k + i\epsilon} - \frac{\boldsymbol{d}_{0k} \otimes \boldsymbol{d}_{k0}}{\omega - \omega_k + i\epsilon} \right)$$

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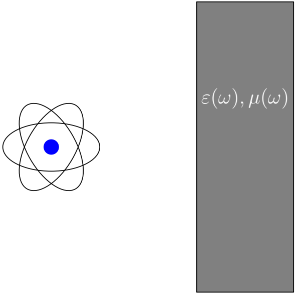
- Casimir–Polder potential

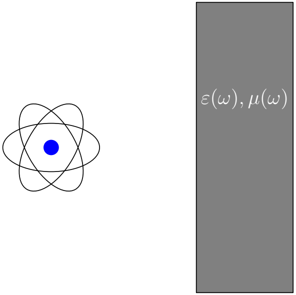
$$U_{CP}(\boldsymbol{r}_A) = \frac{\hbar\mu_0}{2\pi} \int_0^\infty \mathrm{d}\xi\, \xi^2\, \mathrm{tr}\left[\boldsymbol{\alpha}(i\xi) \cdot \mathbf{G}^{(S)}(\boldsymbol{r}_A, \boldsymbol{r}_A, i\xi) \right]$$

Example: an atom in front of an infinite half-space



Example: an atom in front of an infinite half-space

- Green tensor for a half space [S.Y. Buhmann; Dispersion forces I]

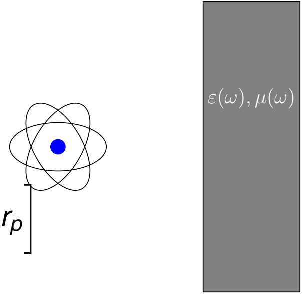


Example: an atom in front of an infinite half-space

- Green tensor for a half space [S.Y. Buhmann; Dispersion forces I]
- Casimir–Polder potential

$$U_{CP}(z_A) = \frac{\hbar\mu_0}{8\pi^2}\int_0^\infty \mathrm{d}\xi\,\xi^2\alpha(i\xi)$$

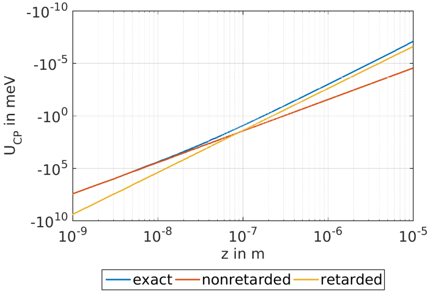
$$\times \int_{\xi/c}^\infty \mathrm{d}k_z \mathrm{e}^{-2k_z z_A}\left[r_s - \left(2\frac{k_z^2c^2}{\xi^2}-1\right)r_p\right]$$



$$r_s = \frac{k_{1z}-k_{2z}}{k_{1z}+k_{2z}}\,,\quad r_p = \frac{\varepsilon_2(\omega)k1z - \varepsilon_1(\omega)k_{2z}}{\varepsilon_2(\omega)k_{1z}+\varepsilon_1(\omega)k_{2z}}$$

Asymptotic behaviour

$$U_{CP}(z_A) = \frac{\hbar\mu_0}{8\pi^2}\int\limits_0^\infty \mathrm{d}\xi\,\xi^2\alpha(i\xi)\int\limits_{\xi/c}^\infty \mathrm{d}k_z \mathrm{e}^{-2k_z z_A}\left[r_s - \left(2\frac{k_z^2c^2}{\xi^2} - 1\right)r_p\right]$$



Asymptotic behaviour

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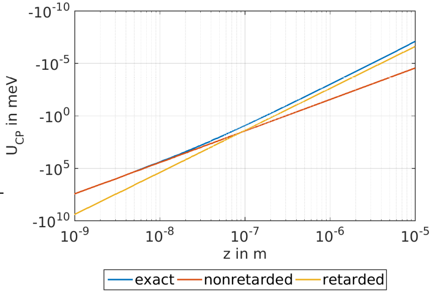
- long distances: $z_A \gg c/\omega_{min}$: main part of the integrant $\xi \to 0 \to$ static fields (yellow)

$$U_{CP}(z_A) = -\frac{23\hbar c\alpha(0)(\varepsilon(0) - 1}{640\pi^2\varepsilon_0\, z_A^4}$$



Asymptotic behaviour

$$U_{CP}(z_A) = \frac{\hbar\mu_0}{8\pi^2}\int_0^\infty \mathrm{d}\xi\,\xi^2\alpha(i\xi)\int_{\xi/c}^\infty \mathrm{d}k_z \mathrm{e}^{-2k_z z_A}\left[r_s - \left(2\frac{k_z^2c^2}{\xi^2}-1\right)r_p\right]$$

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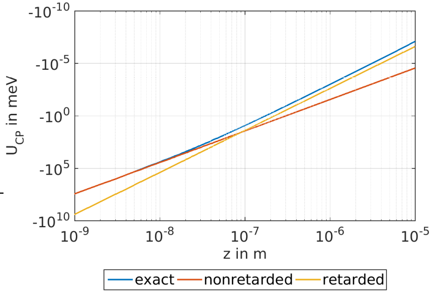

Asymptotic behaviour

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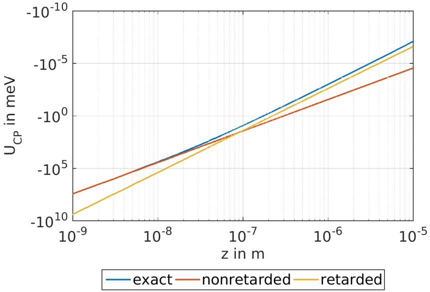

Asymptotic behaviour

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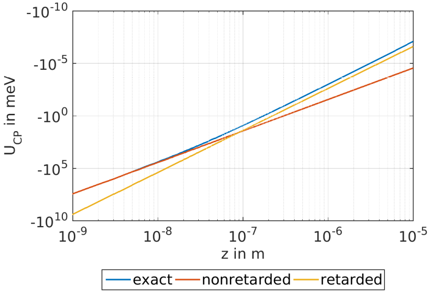
  $\mathrm{e}^{-2k_z z_A} \approx 1 - 2k_z z_A$

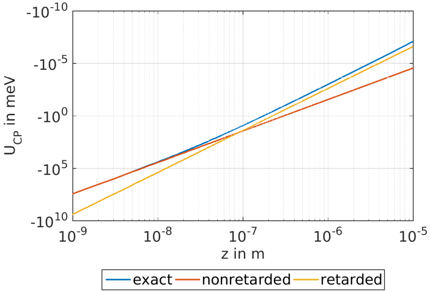


Asymptotic behaviour

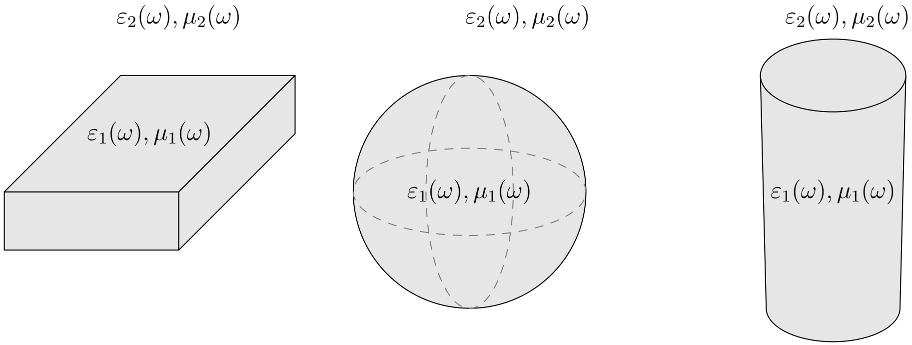
$$U_{CP}(z_A) = \frac{\hbar\mu_0}{8\pi^2} \int\limits_0^\infty \mathrm{d}\xi\, \xi^2 \alpha(i\xi) \int\limits_{\xi/c}^\infty \mathrm{d}k_z \mathrm{e}^{-2k_z z_A} \left[r_s - \left(2\frac{k_z^2 c^2}{\xi^2} - 1 \right) r_p \right]$$

- short distances: $z_A \ll c/\omega_{max}$
  $\mathrm{e}^{-2k_z z_A} \approx 1 - 2k_z z_A$
- $U_{CP}(z_A) = -\frac{C_3}{z_A^3}$ (red)

$$C_3 = \frac{\hbar}{16\pi^2\varepsilon_0} \int\limits_0^\infty \alpha(i\xi) \frac{\varepsilon(i\xi) - 1}{\varepsilon(i\xi) + 1} \mathrm{d}\xi$$



Other known geometries



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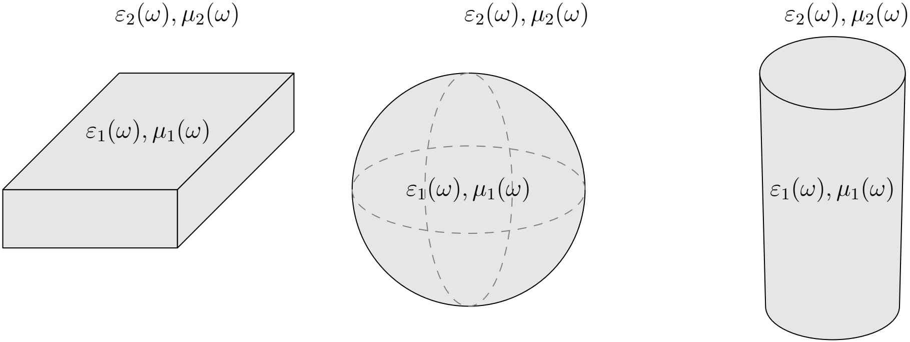
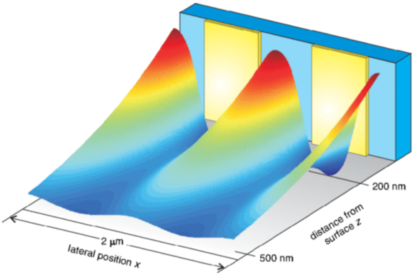


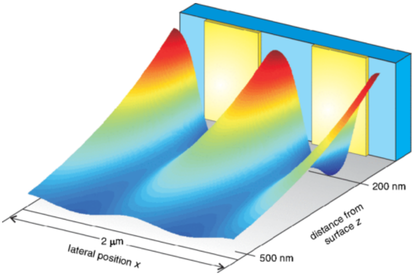
Approximation of the scattering Green tensor



H. Bender, JF *et al.*, PRX **4**, 011029 (2014).

- Sapphire periodically covered with gold stripes

Approximation of the scattering Green tensor



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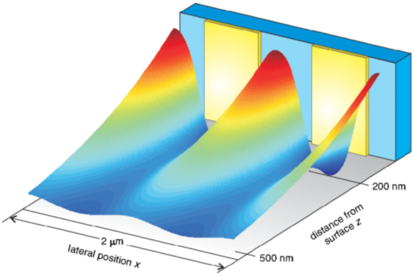

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- Green tensor by Rayleigh expansion
- Series expansion in wave vector ***k***

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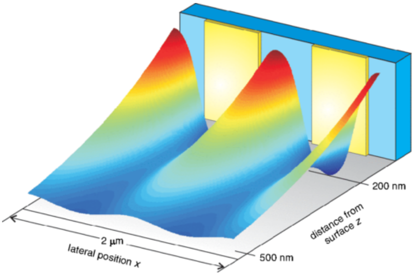
Approximation of the scattering Green tensor



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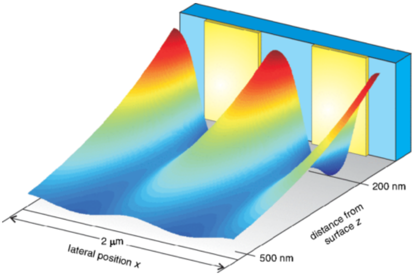
- Large distances: periodic structure not resolvable, $\Longleftrightarrow$ Green tensor for plate

Approximation of the scattering Green tensor



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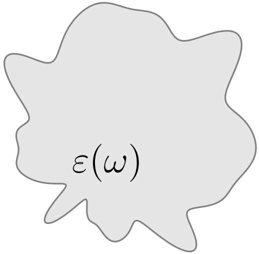
- Series expansion in wave vector $\boldsymbol{k}$
- Large distances: periodic structure not resolvable, $\Longleftrightarrow$ Green tensor for plate
- Disadvantage: Only applicable to periodic structures

Table of Contents

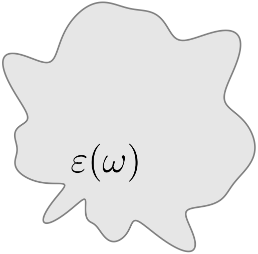
Born series expansion



- Non-periodic scatterer?

$\mathbf{r}\,\bullet$

Born series expansion



- Non-periodic scatterer?
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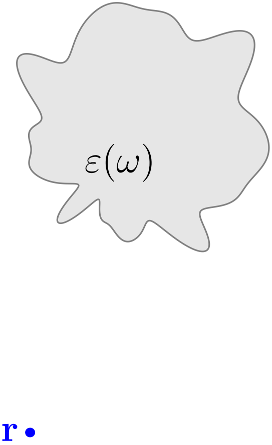
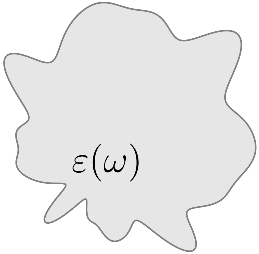
$\mathbf{r}\,\bullet$

Born series expansion



- Non-periodic scatterer?
- Green tensor by Born series expansion
- Series expansion number of interactions inside the scatterer

Born series expansion



- Non-periodic scatterer?
- Green tensor by Born series expansion
- Series expansion number of interactions inside the scatterer
- Disadvantage: Convergence is not guaranteed in general

$\mathbf{r}$ •

Born series expansion

Green tensor = Fundamental solution of the Helmholtz equation

$$\left[\nabla\times\nabla\times-\frac{\omega^2}{c^2}\varepsilon(\boldsymbol{r},\omega)\right]\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)=\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$

Born series expansion

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Reference Green tensor satisfies another Helmholtz equation (bulk, vacuum, layered media, ...)

$$\left[\nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon_0(\boldsymbol{r},\omega)\right]\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}',\omega) = \boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$

Born series expansion

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Difference of both

$$\left[\nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon_0(\boldsymbol{r})\right]\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}') = \frac{\omega^2}{c^2}\delta\varepsilon\left[\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') + \mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}')\right]$$

Born series expansion

$$\left[\nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon_0(\boldsymbol{r})\right] \mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{\omega^2}{c^2}\delta\varepsilon \left[\mathbf{G}^{(0)}(\boldsymbol{r}, \boldsymbol{r}') + \mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}')\right]$$

with $\delta\varepsilon = \varepsilon(\boldsymbol{r}, \omega) - \varepsilon_0(\boldsymbol{r}, \omega)$

Born series expansion

$$\left[\nabla \times \nabla \times -\frac{\omega^2}{c^2}\varepsilon_0(\boldsymbol{r})\right] \mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}') = \frac{\omega^2}{c^2}\delta\varepsilon\left[\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}') + \mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}')\right]$$

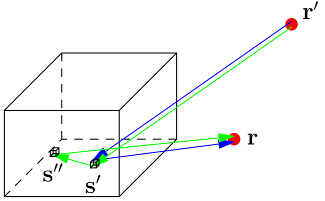
with $\delta\varepsilon = \varepsilon(\boldsymbol{r},\omega) - \varepsilon_0(\boldsymbol{r},\omega)$

Formal solution

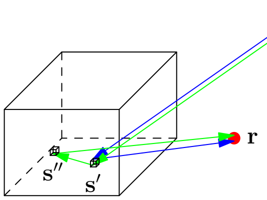
$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega) = \int \mathrm{d}^3 s\, \mathbf{G}^{(0)}(\boldsymbol{r},\mathbf{s},\omega)\cdot\frac{\omega^2}{c^2}\delta\varepsilon\left[\mathbf{G}^{(0)}(\mathbf{s},\boldsymbol{r}',\omega) + \mathbf{G}^{(S)}(\mathbf{s},\boldsymbol{r}',\omega)\right]$$

Born series expansion

- Iterative solution



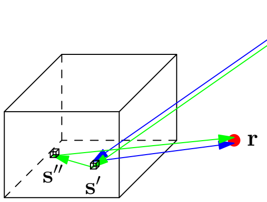
Born series expansion



- Iterative solution
- First order

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{\omega^2}{c^2} \times \int \mathrm{d}^3 s' \mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)\cdot\delta\varepsilon(\boldsymbol{s}',\omega) \cdot \mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{r}',\omega)$$

Born series expansion

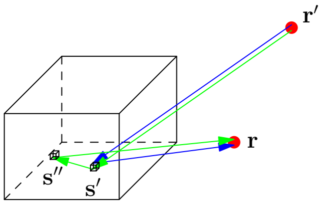


- Iterative solution
- First order

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega)=\frac{\omega^2}{c^2}$$
$$\times\int \mathrm{d}^3 s'\,\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)\cdot\delta\varepsilon(\boldsymbol{s}',\omega)$$
$$\cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{r}',\omega)$$

- Hamaker approach, one interaction between particle and volume element (blue path)

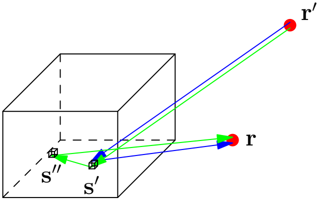
Born series expansion



- Second order

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}') = \left(\frac{\omega^2}{c^2}\right)^2 \times \int \mathrm{d}^3s'\mathrm{d}^3s''\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}')\cdot\delta\varepsilon(\boldsymbol{s}') \cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{s}'')\cdot\delta\varepsilon(\boldsymbol{s}'')\cdot\mathbf{G}^{(0)}(\boldsymbol{s}'',\boldsymbol{r}')$$

Born series expansion

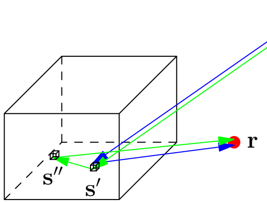


- Second order

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}') = \left(\frac{\omega^2}{c^2}\right)^2 \times \int \mathrm{d}^3 s' \mathrm{d}^3 s'' \mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}') \cdot \delta\varepsilon(\boldsymbol{s}') \cdot \mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{s}'') \cdot \delta\varepsilon(\boldsymbol{s}'') \cdot \mathbf{G}^{(0)}(\boldsymbol{s}'',\boldsymbol{r}')$$

- Leads to Axilrod-Teller potential, two body interactions (green path)

Born series expansion



- Second order

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}') = \left(\frac{\omega^2}{c^2}\right)^2 \times \int \mathrm{d}^3 s' \mathrm{d}^3 s'' \mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}')\cdot\delta\varepsilon(\boldsymbol{s}') \cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{s}'')\cdot\delta\varepsilon(\boldsymbol{s}'')\cdot\mathbf{G}^{(0)}(\boldsymbol{s}'',\boldsymbol{r}')$$

- Leads to Axilrod-Teller potential, two body interactions (green path)
- Analogue for higher orders

Local-field correction of the Born series

- Recalling Born series expansion

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega)=\frac{\omega^2}{c^2}\int \mathrm{d}^3s'\,\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)\cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{r}',\omega)$$
$$+\left(\frac{\omega^2}{c^2}\right)^2\int \mathrm{d}^3s'\,\mathrm{d}^3s''\,\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)$$
$$\cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{s}'',\omega)\cdot\delta\varepsilon(\boldsymbol{s}'',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}'',\boldsymbol{r}',\omega)+\ldots$$

Local-field correction of the Born series

- Recalling Born series expansion

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega)=\frac{\omega^2}{c^2}\int \mathrm{d}^3s'\,\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)\cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{r}',\omega)$$
$$+\left(\frac{\omega^2}{c^2}\right)^2\int \mathrm{d}^3s'\,\mathrm{d}^3s''\,\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{s}',\omega)$$
$$\cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}',\boldsymbol{s}'',\omega)\cdot\delta\varepsilon(\boldsymbol{s}'',\omega)\cdot\mathbf{G}^{(0)}(\boldsymbol{s}'',\boldsymbol{r}',\omega)+\dots$$

- Singularity extraction (for isotropic media)

$$\mathbf{G}^{(0)}(\boldsymbol{r},\boldsymbol{r}',\omega)=\lambda\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')+\mathbf{R}(\boldsymbol{r},\boldsymbol{r}',\omega)$$

with $\lambda=-c^2/(3\omega^2)$ for vacuum

Local-field correction of the Born series

- Inserting in Born series expansion

$$
\begin{aligned}
\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega) = {} & \frac{\omega^2}{c^2}\int \mathrm{d}^3 s' \left[\lambda\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{s}') + \mathbf{R}(\boldsymbol{r},\boldsymbol{s}',\omega)\right]\cdot\delta\varepsilon(\boldsymbol{s}',\omega) \\
& \cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}'-\boldsymbol{r}') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{r}',\omega)\right] \\
& + \left(\frac{\omega^2}{c^2}\right)^2 \int \mathbf{d}^3 s' \mathbf{d}^3 s'' \left[\lambda\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{s}') + \mathbf{R}(\boldsymbol{r},\boldsymbol{s}',\omega)\right] \\
& \cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}'-\boldsymbol{s}'') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{s}'',\omega)\right]\cdot\delta\varepsilon(\boldsymbol{s}'',\omega) \\
& \cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}''-\boldsymbol{r}') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{r}',\omega)\right] + \dots
\end{aligned}
$$

Local-field correction of the Born series

- Inserting in Born series expansion

$$\begin{aligned}\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{\omega^2}{c^2}\int \mathrm{d}^3 s' \left[\lambda\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{s}') + \mathbf{R}(\boldsymbol{r},\boldsymbol{s}',\omega)\right] \cdot \delta\varepsilon(\boldsymbol{s}',\omega)\\ \cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}'-\boldsymbol{r}') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{r}',\omega)\right]\\ + \left(\frac{\omega^2}{c^2}\right)^2 \int \mathbf{d}^3 s' \mathbf{d}^3 s'' \left[\lambda\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{s}') + \mathbf{R}(\boldsymbol{r},\boldsymbol{s}',\omega)\right]\\ \cdot\delta\varepsilon(\boldsymbol{s}',\omega)\cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}'-\boldsymbol{s}'') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{s}'',\omega)\right]\cdot\delta\varepsilon(\boldsymbol{s}'',\omega)\\ \cdot\left[\lambda\boldsymbol{\delta}(\boldsymbol{s}''-\boldsymbol{r}') + \mathbf{R}(\boldsymbol{s}',\boldsymbol{r}',\omega)\right] + \ldots\end{aligned}$$

- Performing integration over $\boldsymbol{\delta}$

Local-field correction of the Born series

- Result for first order, (assuming $\boldsymbol{r}, \boldsymbol{r}' \notin V$)

$$\mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}', \omega) = \frac{\omega^2}{c^2}\delta\varepsilon(\omega) \int \mathrm{d}^3 s \sum_{i=0}^{\infty} \left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]^i \mathbf{R}(\boldsymbol{r}, \boldsymbol{s}, \omega) \cdot \mathbf{R}(\boldsymbol{s}, \boldsymbol{r}', \omega)$$

Local-field correction of the Born series

- Result for first order, (assuming $\boldsymbol{r}, \boldsymbol{r}' \notin V$)

$$\mathbf{G}^{(S)}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{\omega^2}{c^2}\delta\varepsilon(\omega)\int \mathrm{d}^3 s \sum_{i=0}^{\infty}\left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]^i \mathbf{R}(\boldsymbol{r},\boldsymbol{s},\omega)\cdot\mathbf{R}(\boldsymbol{s},\boldsymbol{r}',\omega)$$

- geometric series

$$\sum_{i=0}^{\infty}\left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]^i = \left(1-\left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]\right)^{-1}$$

Local-field correction of the Born series

- Result for first order, (assuming $\boldsymbol{r}, \boldsymbol{r}' \notin V$)

$$\mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}', \omega) = \frac{\omega^2}{c^2}\delta\varepsilon(\omega) \int \mathrm{d}^3 s \sum_{i=0}^{\infty} \left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]^i \mathbf{R}(\boldsymbol{r}, \boldsymbol{s}, \omega) \cdot \mathbf{R}(\boldsymbol{s}, \boldsymbol{r}', \omega)$$

- geometric series

$$\sum_{i=0}^{\infty} \left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]^i = \left(1 - \left[\frac{\omega^2}{c^2}\lambda\delta\varepsilon\right]\right)^{-1}$$

- In free-space

$$\mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}', \omega) = \frac{\omega^2}{c^2} \frac{\chi(\omega)}{1 + \chi(\omega)/3} \int \mathrm{d}^3 s \mathbf{R}(\boldsymbol{r}, \boldsymbol{s}, \omega) \cdot \mathbf{R}(\boldsymbol{s}, \boldsymbol{r}', \omega)$$

Local-field correction of the Born series

- Factor equivalent to Mie reflection coefficient for a sphere

$$\frac{\chi(\omega)}{1+\chi(\omega)/3} = 3\frac{\varepsilon-1}{\varepsilon+2}$$

Local-field correction of the Born series

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- equivalent to Clausius-Mossotti relation

$$3\frac{\varepsilon-1}{\varepsilon+2} = \frac{\alpha}{\varepsilon_0}$$

Local-field correction of the Born series

- Factor equivalent to Mie reflection coefficient for a sphere

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- equivalent to Clausius-Mossotti relation

$$3\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{\alpha}{\varepsilon_0}$$

- Green function for scattering at a point particle at $\boldsymbol{r}_B$ $[\delta(\boldsymbol{r}_B - \boldsymbol{s})]$

$$\mathbf{G}^{(S)}(\boldsymbol{r}, \boldsymbol{r}', \omega) = \frac{\omega^2}{\varepsilon_0 c^2}\alpha_B(\omega)\mathbf{R}(\boldsymbol{r}, \boldsymbol{r}_B, \omega) \cdot \mathbf{R}(\boldsymbol{r}_B, \boldsymbol{r}', \omega)$$

Table of Contents

Van-der-Waals potential

- Inserting in Casimir–Polder potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathbf{d}\xi\,\xi^4\,\mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi)\cdot\mathbf{R}(\boldsymbol{r}_A,\boldsymbol{r}_B,i\xi)\cdot\boldsymbol{\alpha}_B(i\xi)\cdot\mathbf{R}(\boldsymbol{r}_B,\boldsymbol{r}_A,i\xi)\right]$$

Van-der-Waals potential

- Inserting in Casimir–Polder potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}\xi\, \xi^4\, \mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi)\cdot\mathbf{R}(\boldsymbol{r}_A, \boldsymbol{r}_B, i\xi)\cdot\boldsymbol{\alpha}_B(i\xi)\cdot\mathbf{R}(\boldsymbol{r}_B, \boldsymbol{r}_A, i\xi)\right]$$

- equivalent to fourth order perturbation theory of the interaction Hamiltonian $\hat{H}_{int} = -\hat{\boldsymbol{d}}_A \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_A) - \hat{\boldsymbol{d}}_B \cdot \hat{\boldsymbol{E}}(\boldsymbol{r}_B)$

van–der–Waals potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}\xi\,\xi^4\,\mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_A,\boldsymbol{r}_B,i\xi)\cdot\boldsymbol{\alpha}_B(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_B,\boldsymbol{r}_A,i\xi)\right]$$

van–der–Waals potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) =$$

$$-\frac{\hbar\mu_0^2}{2\pi}\int\limits_0^\infty \mathbf{d}\xi\, \xi^4\, \mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_A,\boldsymbol{r}_B,i\xi)\cdot\boldsymbol{\alpha}_B(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_B,\boldsymbol{r}_A,i\xi)\right]$$

scattering Green tensor for bulk material (non-retarded)

$$\mathbf{G}(\boldsymbol{r},\boldsymbol{r}'\omega) = -\frac{1}{\pi k^2\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\left(\mathbf{I}-3\mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'}\otimes\mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'}\right)$$

van–der–Waals potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) =$$

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$$\mathbf{G}(\boldsymbol{r},\boldsymbol{r}'\omega) = -\frac{1}{\pi k^2\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\left(\mathbf{I}-3\mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'}\otimes\mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'}\right)$$

- vacuum: $k=\omega/c \to U(\boldsymbol{r}_A,\boldsymbol{r}_B) = -\frac{3\hbar}{16\pi^3\varepsilon_0^2|\boldsymbol{r}_A-\boldsymbol{r}_B|^6}\int_0^\infty \mathrm{d}\xi\,\alpha_A(i\xi)\alpha_B(i\xi)$

van–der–Waals potential

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) =$$

$$-\frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}\xi\, \xi^4 \operatorname{tr}\left[\boldsymbol{\alpha}_A(i\xi) \cdot \mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}_B, i\xi) \cdot \boldsymbol{\alpha}_B(i\xi) \cdot \mathbf{G}(\boldsymbol{r}_B, \boldsymbol{r}_A, i\xi)\right]$$

scattering Green tensor for bulk material (non-retarded)

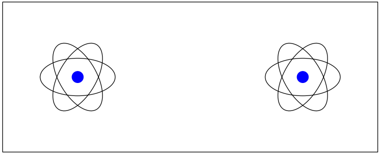
$$\mathbf{G}(\boldsymbol{r}, \boldsymbol{r}'\omega) = -\frac{1}{\pi k^2 \left|\boldsymbol{r} - \boldsymbol{r}'\right|^3} \left(\mathbf{I} - 3\mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'} \otimes \mathbf{e}_{\boldsymbol{r}-\boldsymbol{r}'}\right)$$

- vacuum: $k = \omega/c \to U(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{3\hbar}{16\pi^3\varepsilon_0^2|\boldsymbol{r}_A - \boldsymbol{r}_B|^6} \int_0^\infty \mathrm{d}\xi\, \alpha_A(i\xi)\alpha_B(i\xi)$
- bulk: $k = \omega\sqrt{\varepsilon(\omega)}/c \to U(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{3\hbar}{16\pi^3\varepsilon_0^2|\boldsymbol{r}_A - \boldsymbol{r}_B|^6} \int_0^\infty \mathrm{d}\xi\, \frac{\alpha_A(i\xi)\alpha_B(i\xi)}{\varepsilon^2(i\xi)}$

Interpretation

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}\xi\, \xi^4\, \mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi) \cdot \mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}_B, i\xi) \cdot \boldsymbol{\alpha}_B(i\xi) \cdot \mathbf{G}(\boldsymbol{r}_B, \boldsymbol{r}_A, i\xi)\right]$$

- Two neutral particles



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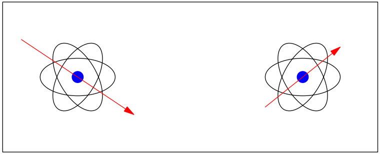
- Two neutral particles
- Quantum vacuum spontaneously excites the particles



Interpretation

$$U_{vdW}(\boldsymbol{r}_A, \boldsymbol{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int\limits_0^\infty \mathrm{d}\xi\,\xi^4\,\mathrm{tr}\left[\boldsymbol{\alpha}_A(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_A, \boldsymbol{r}_B, i\xi)\cdot\boldsymbol{\alpha}_B(i\xi)\cdot\mathbf{G}(\boldsymbol{r}_B, \boldsymbol{r}_A, i\xi)\right]$$

- Two neutral particles
- Quantum vacuum spontaneously excites the particles
- Leading to attractive dipole force