Van der Waals interaction between an atom with spherical plasma shell

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We consider the van der Waals energy of an atom near the infinitely thin sphere with finite conductivity which model the fullerene. We put the sphere into spherical cavity inside the infinite dielectric media, then calculate the energy of vacuum fluctuations in framework of the zeta-function approach. The energy for a single atom is obtained from this expression by consideration of the rare media. In the limit of the infinite radius of the sphere the Casimir-Polder expression for an atom and plate is recovered. For finite radius of sphere the energy of an atom monotonously falls down as d^{-3} close to the sphere and d^{-7} far from the sphere. For hydrogen atom on the surface of the fullerene C_{60} we obtain that the energy is $3.8eV$. We obtain also that the polarizability of fullerene is merely cube of its radius.

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I. INTRODUCTION

The general theory of the van der Waals force was developed by Lifshits in Ref. [1, 2] in framework of the statistical physics. In the case of interaction between particle and plate it is commonly referred to as the Casimir-Polder force [3]. For small distance the potential of interaction is proportional to inverse third degree of distance from the plate. For great distance the retardation of the interaction had taken into account and the potential falls down as fourth degree of distance. The last advantages in Casimir effect have been discussed in great depth in books and reviews [4–6].

The van der Waals force is very important for interaction the graphene (graphite layers) with bodies [7–14] and microparticles [15–18]. An understanding of the mechanisms of molecule-nanostructure interaction is of importance for the problem of hydrogen storage in carbon nanostructures [19]. The microscopic mechanisms underlying the absorption phenomenon remain unclear (see, for example review [20]).

In the present paper we use model of the fullerene in terms of the two dimensional free electron gas [21]. This model was applied and developed for the molecule C_{60} in Refs. [22, 23], for flat plasma sheet in Ref. [24] and for spherical plasma surface in Ref. [25]. In the framework of this model the conductive surface is considered as infinitely thin shell with the specific wave number $\Omega = 4\pi ne^2/mc^2$, where n is surface density of electrons in the surface and m is its mass. Due to the fact that the surface is infinitely thin, the information about the properties of the surface is encoded in the boundary conditions on the conductive surface which are different for TE and TM modes. As it was shown in Ref. [25] the energy of the vacuum electromagnetic fluctuations for surface shaped as sphere has a maximum for radius of sphere approximately equals to the specific wavelength of the model $\lambda_\Omega = 2\pi/\Omega$. It means that the Casimir force tries to expand sphere with radius larger then λ_Ω and try to shrink the sphere with radius larger then λ_Ω. In the limit $\Omega \to \infty$ the Boyer result [26] is recovered.

In the present paper the same model of fullerene is adopted – the conductive singular sphere with radius R in vacuum. To obtain the van der Waals energy for an atom near to this sphere we use the following approach (see Refs. [1, 2, 13, 18]). We put the sphere inside the spherical cavity with radius $L = R + d > R$ which is inside the dielectric media with coefficients μ, ε. Then we find the zero-point energy of this system by using the zeta-function regularization approach, and take the limit of the rared media with $\varepsilon = 1 + 4\pi N\alpha + O(N^2)$, where $N \to 0$ is the volume density of the atoms and α is the polarizability of the unit atom. The energy per unit atom with distance d from the sphere may be found by simple formula

$$E_a(s) = -\lim_{N\to 0} \frac{\partial_d E(s)}{4\pi N(R+d)^2},$$

where $E(s)$ is the zeta-regularized energy with regularization parameter s.

The paper is organized as follows. In Sec. II we derive the boundary conditions for conductive sphere and the boundary of the cavity. Section III is devoted to the solution the boundary conditions and obtaining the conditions for energy spectrum. In Sec. IV the expression for the van der Waals energy is found which is analyzed in the limit of infinite radius of the sphere and close and far from that sphere. Section V contains the numerical calculations for hydrogen atom with fullerene C_{60}. In the last section we discuss results obtained.

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II. MAXWELL'S EQUATIONS AND MATCHING CONDITIONS

Let us consider a conductive infinitely thin sphere with radius R in vacuum spherical cavity with radius $L = R + d$ inside the dielectric media with parameters μ, ε (see fig. 1). We have two spheres and we should

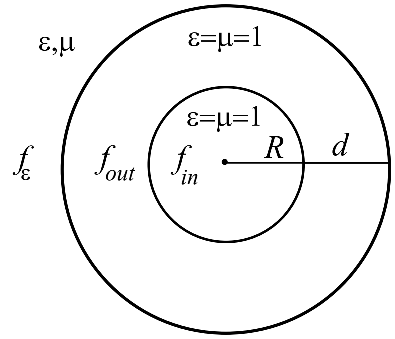

FIG. 1: The infinitely thin conductive sphere with radius R is located inside the vacuum spherical cavity with radius $L = R + d$ into dielectric media with $\varepsilon, \mu \neq 1$.

consider the boundary conditions on two spherical boundaries.

I. First of all we consider spherical boundary with radius $L = R + d$. Inside the sphere we have vacuum, $\varepsilon = \mu = 1$ and outside – the dielectric media with $\varepsilon, \mu \neq 1$. For spherical symmetric case the electromagnetic field has two independent polarizations usually called as TE and TM modes. The Maxwell equations with oscillatory time dependence $\exp(-i\omega t)$ read

$$\mathrm{rot}\,\mathbf{E} - \frac{i\omega}{c}\mathbf{B} = 0,\ \mathrm{div}\,\mathbf{B} = 0, \tag{1a}$$

$$\mathrm{rot}\,\mathbf{H} + \frac{i\omega}{c}\mathbf{D} = 0,\ \mathrm{div}\,\mathbf{D} = 0, \tag{1b}$$

where we use material equations $\mathbf{D} = \varepsilon(\omega)\mathbf{E}$ and $\mathbf{B} = \mu(\omega)\mathbf{H}$. To obtain TE -mode we express $\mathbf{B}$ from first equation and substitute in the second one

$$\mathbf{B}^{\mathsf{TE}} = -\frac{i}{\omega}\mathrm{rot}\,\mathbf{E}^{\mathsf{TE}},\ \triangle\mathbf{E}^{\mathsf{TE}} - \omega^2\mu\varepsilon\mathbf{E}^{\mathsf{TE}} = 0. \tag{2}$$

For TM mode we express $\mathbf{E}$ from second equation and substitute in the first one

$$\mathbf{E}^{\mathsf{TM}} = \frac{ic}{\omega\mu\varepsilon}\mathrm{rot}\,\mathbf{B}^{\mathsf{TM}},\ \triangle\mathbf{B}^{\mathsf{TM}} - \frac{\omega^2}{c^2}\mu\varepsilon\mathbf{B}^{\mathsf{TM}} = 0. \tag{3}$$

Then we expand solutions over spherical functions and obtain the following expressions for TE and TM ,

$$\mathbf{B}^{\mathsf{TE}}_{lm} = -\frac{ic}{\omega}\mathrm{rot}\,\mathbf{E}^{\mathsf{TE}}_{lm},\ \mathbf{E}^{\mathsf{TE}}_{lm} = f(kr)\mathbf{L}Y_{lm}, \tag{4}$$

$$\mathbf{E}^{\mathsf{TM}}_{lm} = \frac{ic}{\omega\mu\varepsilon}\mathrm{rot}\,\mathbf{B}^{\mathsf{TM}}_{lm},\ \mathbf{B}^{\mathsf{TM}}_{lm} = f(kr)\mathbf{L}Y_{lm}, \tag{5}$$

where $ck = \omega\sqrt{\mu\varepsilon}$. In spherical dribien $(e_r, e_\theta, e_\varphi)$ we obtain in manifest form

$$\begin{aligned}
\mathbf{E}^{\mathsf{TE}}_{lm} &= \left(0, \frac{if}{\sin\theta}\partial_\varphi Y_{lm}, -if\partial_\theta Y_{lm}\right), \\
\mathbf{B}^{\mathsf{TE}}_{lm} &= \left(\frac{cf}{\omega r}l(l+1)Y_{lm}, \frac{c(rf)'}{\omega r}\partial_\theta Y_{lm}, \frac{c(rf)'}{\omega r\sin\theta}\partial_\varphi Y_{lm}\right), \\
\mathbf{B}^{\mathsf{TM}}_{lm} &= \left(0, \frac{if}{\sin\theta}\partial_\varphi Y_{lm}, -if\partial_\theta Y_{lm}\right), \\
\mathbf{E}^{\mathsf{TM}}_{lm} &= -\frac{c}{\varepsilon\mu}\left(\frac{f}{\omega r}l(l+1)Y_{lm}, \frac{(rf)'}{\omega r}\partial_\theta Y_{lm}, \frac{(rf)'}{\omega r\sin\theta}\partial_\varphi Y_{lm}\right),
\end{aligned} \tag{6}$$

and the function f obeys the radial equation

$$f'' + \frac{2}{r}f' + \left(\frac{\omega^2}{c^2}\varepsilon\mu - \frac{l(l+1)}{r^2}\right)f = 0, \tag{7}$$

with solutions in the form the spherical Bessel functions $j_l(z) = \sqrt{\pi/2z}J_{l+1/2}(z),\ y_l(z) = \sqrt{\pi/2z}Y_{l+1/2}(z)$, where $z = r\omega\sqrt{\varepsilon\mu}/c$.

At the boundary, L, the matching conditions read

$$\mathbf{n}\cdot[\mathbf{B}_2-\mathbf{B}_1]_L = 0,\ \mathbf{n}\cdot[\mathbf{D}_2-\mathbf{D}_1]_L = 0, \tag{8a}$$
$$\mathbf{n}\times[\mathbf{H}_2-\mathbf{H}_1]_L = 0,\ \mathbf{n}\times[\mathbf{E}_2-\mathbf{E}_1]_L = 0, \tag{8b}$$

where $\mathbf{n} = \mathbf{r}/r$ is an unit normal to the sphere and we have to take into account that $k = \omega/c$ inside the sphere and $k = \omega\sqrt{\mu\varepsilon}/c$ outside the sphere. The square brackets above denote the coincidence limit on the $r = L$.

II. Electromagnetic fields given infinitely thin conductive surface Σ in vacuum was considered by Fetter in Ref. [21]. The application this model for vacuum fluctuations see in Refs. [22–25]. In this case the electrons of conductivity on the sphere produce currency and the Maxwell equations read

$$\mathrm{rot}\,\mathbf{E} - \frac{i\omega}{c}\mathbf{H} = 0,\ \mathrm{div}\,\mathbf{H} = 0, \tag{9a}$$
$$\mathrm{rot}\,\mathbf{H} + \frac{i\omega}{c}\mathbf{E} = 4\pi\mathbf{J},\ \mathrm{div}\,\mathbf{E} = 4\pi\rho, \tag{9b}$$

where $\rho = \delta(\mathbf{x}-\mathbf{x}_\Sigma)\sigma$, $\mathbf{J} = \delta(\mathbf{x}-\mathbf{x}_\Sigma)\mathbf{j}/c$. The equation of continuity and Newton equations give the following expressions for density and currency

$$\sigma = \frac{e^2n}{m\omega^2}\nabla_\parallel\cdot\mathbf{E}_\parallel,\ \mathbf{j} = i\frac{e^2n}{m\omega}\mathbf{E}_\parallel, \tag{10}$$

where the superscripts $\parallel$ indicates the vector components parallel to the surface Σ, e and m are a charge and mass of electron, and n is a surface density of charge.

On the conductive sphere with radius $r = R$ we have another kind of boundary conditions due to conductive electrons on the sphere

$$\mathbf{n}\cdot[\mathbf{H}_2-\mathbf{H}_1]_R = 0,\ \mathbf{n}\cdot[\mathbf{E}_2-\mathbf{E}_1]_R = \frac{\Omega}{k^2}\nabla_\parallel\cdot\mathbf{E}_\parallel, \tag{11a}$$
$$\mathbf{n}\times[\mathbf{H}_2-\mathbf{H}_1]_R = -\frac{i\Omega}{k}\mathbf{n}\times\mathbf{E}_\parallel,\ \mathbf{n}\times[\mathbf{E}_2-\mathbf{E}_1]_R = 0, \tag{11b}$$

where $k = \omega/c$ and $\Omega = 4\pi ne^2/mc^2$ is a specific wave number of plasma on the sphere. Because the sphere is infinitely thin we may consider the Maxwell equations (9) in vacuum with zero right hand side and all information about sphere will be encoded in boundary conditions (11). Interesting treatment of this boundary condition is in Ref. [27].

III. THE SOLUTION OF THE MATCHING CONDITIONS

Inside the cavity we consider a vacuum with $\mu = \varepsilon = 1$ and outside there is a media with $\mu, \varepsilon \neq 1$. We denote the radial function in the following way

$$f = \begin{cases} f_{in} &= a_{in}j_l(kr), & r < R \\ f_{out} &= a_{out}j_l(kr) + b_{out}y_l(kr), & R < r < L \\ f_\varepsilon &= a_\varepsilon h_l^{(1)}(kr), & r > L \end{cases} \tag{12}$$

where j_l, y_l and $h_l^{(1)}$ are the spherical Bessel functions.

The matching conditions (8) and (11) in manifest form read

$$\begin{aligned} [rf_{out} - rf_{in}]_R &= 0, \\ [(rf_{out})'_r - (rf_{in})'_r - \Omega(rf_{in})]_R &= 0, \\ [rf_{out} - rf_\varepsilon]_L &= 0, \\ [(rf_{out})'_r - \frac{1}{\mu}(rf_\varepsilon)'_r]_L &= 0, \end{aligned} \tag{13}$$

for TE mode, and

$$\begin{aligned} [(rf_{out})'_r - (rf_{in})'_r]_R &= 0, \\ [(rf_{out}) - (rf_{in}) + \frac{\Omega}{k^2}(rf_{in})'_r]_R &= 0, \end{aligned}$$

$$[rf_{out} - \frac{1}{\mu} rf_\varepsilon]_L \;=\; 0, \tag{14}$$
$$[(rf_{out})'_r - \frac{1}{\mu\varepsilon}(rf_\varepsilon)'_r]_L \;=\; 0,$$

for TM mode. The solutions of these equations exist if and only if the following equations are satisfied

$$\frac{1}{\sqrt{\mu\varepsilon}} H(z_\varepsilon)\Psi'_{\mathsf{TE}} - \frac{1}{\mu} H'(z_\varepsilon)\Psi_{\mathsf{TE}} \;=\; 0, \tag{15a}$$
$$-\frac{1}{\sqrt{\mu\varepsilon}} H(z_\varepsilon)\Psi'_{\mathsf{TM}} + \frac{1}{\varepsilon} H'(z_\varepsilon)\Psi_{\mathsf{TM}} \;=\; 0, \tag{15b}$$

where $z_\varepsilon = z\sqrt{\mu\varepsilon}$, $z = kL = \omega L/c$, and prime is derivative with respect the argument, and

$$\Psi_{\mathsf{TE}}(z) \;=\; J(z) + \frac{\Omega}{k} J(x)[J(x)Y(z) - J(z)Y(x)], \tag{16a}$$
$$\Psi_{\mathsf{TM}}(z) \;=\; J(z) + \frac{\Omega}{k} J'(x)[J'(x)Y(z) - J(z)Y'(x)]. \tag{16b}$$

Here $J(x) = xj_l(x),\ Y(x) = xy_l(x),\ H(x) = xh_l^{(1)}(x)$ are the Riccati-Bessel functions, and $x = kR$. Therefore the functions we need (see next section) to obtain the spectrum of the energy read (we set $\mu = 1$)

$$\Sigma_{\mathsf{TE}} \;=\; H'(z_\varepsilon)\Psi_{\mathsf{TE}} - \frac{1}{\sqrt{\varepsilon}} H(z_\varepsilon)\Psi'_{\mathsf{TE}}, \tag{17a}$$
$$\Sigma_{\mathsf{TM}} \;=\; H(z_\varepsilon)\Psi'_{TM} - \frac{1}{\sqrt{\varepsilon}} H'(z_\varepsilon)\Psi_{\mathsf{TM}}. \tag{17b}$$

For $\varepsilon = 1$ we recover the result obtained in the Ref. [25]

$$\Sigma_{\mathsf{TE}} \;=\; i\left\{1 - \frac{\Omega}{ik} J(x)H(x)\right\} = if_{\mathsf{TE}}(k), \tag{18a}$$
$$\Sigma_{\mathsf{TM}} \;=\; -i\left\{1 - \frac{\Omega}{ik} J'(x)H'(x)\right\} = -if_{\mathsf{TM}}(k), \tag{18b}$$

for real value of k, and for imaginary axis $k \to ik$ we obtain from above expressions the Jost functions in imaginary axis:

$$\Sigma_{\mathsf{TE}} \;=\; i\left\{1 + \frac{\Omega}{k} s_l(x)e_l(x)\right\} = if_{\mathsf{TE}}(ik), \tag{19a}$$
$$\Sigma_{\mathsf{TM}} \;=\; -i\left\{1 - \frac{\Omega}{k} s'_l(x)e'_l(x)\right\} = -if_{\mathsf{TM}}(ik), \tag{19b}$$

because $H(ix) = (-i)^{l+1}e_l(x)$, $J(ix) = i^{l+1}s_l(x)$ and $Y(ix) = -i^l s_l(x) - (-i)^l e_l(x)$, where

$$s_l(x) = \sqrt{\frac{\pi x}{2}} I_{l+1/2}(x),\ e_l(x) = \sqrt{\frac{2x}{\pi}} K_{l+1/2}(x) \tag{20}$$

are the Riccatti-Bessel spherical functions of the second kind. To avoid problem with $z = 0$ we multiply Σ_{TM} for z^2

$$\Sigma_{\mathsf{TE}} \;=\; -i\left\{H'(z_\varepsilon)\Psi_{\mathsf{TE}} - \frac{1}{\sqrt{\varepsilon}} H(z_\varepsilon)\Psi'_{\mathsf{TE}}\right\}, \tag{21a}$$
$$\Sigma_{\mathsf{TM}} \;=\; -iz^2\left\{H(z_\varepsilon)\Psi'_{\mathsf{TM}} - \frac{1}{\sqrt{\varepsilon}} H'(z_\varepsilon)\Psi_{\mathsf{TM}}\right\}. \tag{21b}$$

In imaginary axis $k \to ik$ we obtain

$$\Sigma_{\mathsf{TE}} \;=\; \frac{1}{\sqrt{\varepsilon}} e_l(z_\varepsilon)\Phi'_{\mathsf{TE}} - e'_l(z_\varepsilon)\Phi_{\mathsf{TE}}, \tag{22a}$$
$$\Sigma_{\mathsf{TM}} \;=\; z^2\left\{e_l(z_\varepsilon)\Phi'_{\mathsf{TM}} - \frac{1}{\sqrt{\varepsilon}} e'_l(z_\varepsilon)\Phi_{\mathsf{TM}}\right\}, \tag{22b}$$

$$\Phi_{\mathsf{TE}} = s_l(z) + \frac{Q}{x} s_l(x)[s_l(z)e_l(x) - s_l(x)e_l(z)], \tag{22c}$$

$$\Phi_{\mathsf{TM}} = s_l(z) - \frac{Q}{x} s_l'(x)[s_l(z)e_l'(x) - s_l'(x)e_l(z)], \tag{22d}$$

where $Q = \Omega R,\ z = kL,\ z_\varepsilon = z\sqrt{\varepsilon},\ x = kR$ and $\varepsilon = \varepsilon(i\omega)$. For $\varepsilon = 1$ we obtain

$$\Sigma_{\mathsf{TE}} = f_{\mathsf{TE}}(ik),\ \Sigma_{\mathsf{TM}} = z^2 f_{\mathsf{TM}}(ik) \tag{23}$$

in accordance with Ref. [25].

IV. THE ENERGY

In framework approach suggested in Ref. [28] we have the following expressions for TE and TM contributions in regularized zero-point energy ($\omega = kc$)

$$E^{\mathsf{TE}}(s) = -\frac{\hbar c \cos \pi s}{\pi} \mu^{2s} \sum_{l=1}^{\infty} \nu \int_0^\infty dk k^{1-2s} \partial_k \ln \Sigma_{\mathsf{TE}}, \tag{24}$$

$$E^{\mathsf{TM}}(s) = -\frac{\hbar c \cos \pi s}{\pi} \mu^{2s} \sum_{l=1}^{\infty} \nu \int_0^\infty dk k^{1-2s} \partial_k \ln \Sigma_{\mathsf{TM}}, \tag{25}$$

where integrand functions are give by Eqs. (22). The summations in these expressions starts from $l = 1$ because for $l = 0$ electromagnetic modes (6) are zero.

To find the expression for energy per unit atom we need for the derivative of energy with respect d ($E(s) = E^{\mathsf{TE}}(s) + E^{\mathsf{TM}}(s)$) which read in manifest form

$$\partial_d E(s) = -\frac{\hbar c \cos \pi s}{\pi} \mu^{2s} \sum_{l=1}^{\infty} \nu \int_0^\infty dk k^{1-2s} \partial_k \left\{ \frac{k(1-\varepsilon)}{\sqrt{\varepsilon}} \left[\mathcal{G}_{\mathsf{TE}}^{-1} + \mathcal{G}_{\mathsf{TM}}^{-1}\right] \right\},$$

where

$$\mathcal{G}_{\mathsf{TE}} = \frac{1}{\sqrt{\varepsilon}} \frac{\Phi_{\mathsf{TE}}'}{\Phi_{\mathsf{TE}}} - \frac{e_l'(z_\varepsilon)}{e_l(z_\varepsilon)} = \frac{\Sigma_{\mathsf{TE}}}{e_l(z_\varepsilon)\Phi_{\mathsf{TE}}},$$

$$\mathcal{G}_{\mathsf{TM}} = -\frac{\frac{\Phi_{\mathsf{TM}}'}{\Phi_{T\mathsf{TM}}} - \frac{1}{\sqrt{\varepsilon}} \frac{e_l'(z_\varepsilon)}{e_l(z_\varepsilon)}}{\frac{\Phi_{\mathsf{TM}}'}{\Phi_{\mathsf{TM}}} \frac{e_l'(z_\varepsilon)}{e_l(z_\varepsilon)} + \frac{\nu^2 - \frac14}{z^2\sqrt{\varepsilon}}} = -\frac{\Sigma_{\mathsf{TM}}}{z^2 \left[e_l'(z_\varepsilon)\Phi_{\mathsf{TM},z}' + e_l(z_\varepsilon)\Phi_{\mathsf{TM}} \frac{\nu^2 - \frac14}{z^2\sqrt{\varepsilon}}\right]}.$$

We consider now the rared media with $\varepsilon(i\omega) = 1 + 4\pi N \alpha(i\omega) + O(N^2)$, where α is polarizability of the atom and density media $N \to 0$. In this case the Casimir energy $E(s)$ is expressed in terms the energy per unite atom $E_a(s)$ by relation

$$E(s) = N \int_d^\infty E_a(s) 4\pi (R + r)^2 dr + O(N^2). \tag{26}$$

From this expression we obtain that

$$E_a(s) = -\lim_{N \to 0} \frac{\partial_d E(s)}{4\pi N (R + d)^2}, \tag{27}$$

and in manifest form

$$E_a(s) = -\frac{\hbar c \mu^{2s} \cos \pi s}{\pi (R + d)^2} \sum_{l=1}^{\infty} \nu \int_0^\infty dk k^{1-2s} \partial_k \left\{ \frac{k\alpha(i\omega)}{G_{\mathsf{TE}}} + \frac{k\alpha(i\omega)}{G_{\mathsf{TM}}} \right\}, \tag{28}$$

where

$$G_{\mathsf{TE}} = \frac{\Sigma_{\mathsf{TE}}}{e_l(z)\Phi_{\mathsf{TE}}} = \frac{f_{\mathsf{TE}}(ik)}{e_l(z)\Phi_{\mathsf{TE}}},$$

$$G_{\mathsf{TM}} = -\frac{\Sigma_{\mathsf{TM}}}{z^2 \left[e_l'(z)\Phi_{\mathsf{TM},z}' + e_l(z)\Phi_{\mathsf{TM}} \frac{\nu^2 - \frac14}{z^2}\right]} = -\frac{f_{\mathsf{TM}}(ik)}{e_l'(z)\Phi_{\mathsf{TM},z}' + e_l(z)\Phi_{\mathsf{TM}} \frac{\nu^2 - \frac14}{z^2}}.$$

By using definitions of functions Φ_{TE} and Φ_{TM} we have the following relations

$$\Phi_{\mathsf{TE}} = s_l(z) f_{\mathsf{TE}}(ik) - \frac{\Omega}{k} s_l^2(x) e_l(z),$$
$$\Phi_{\mathsf{TM}} = s_l(z) f_{\mathsf{TM}}(ik) + \frac{\Omega}{k} s'^2_l(x) e_l(z),$$

and express above formulas in slightly different form,

$$\begin{aligned} G^{-1}_{\mathsf{TE}} &= e_l(z)s_l(z) - \frac{Q}{x}\frac{s_l^2(x)e_l^2(z)}{f_{\mathsf{TE}}(ik)}, \\ G^{-1}_{\mathsf{TM}} &= -e_l'(z)s_l'(z) - e_l(z)s_l(z)\frac{\nu^2-\frac{1}{4}}{z^2} - \frac{Q}{x}\frac{1}{f_{\mathsf{TM}}(ik)}\left[s'^2_l(x)e'^2_l(z) + s'^2_l(x)e_l^2(z)\frac{\nu^2-\frac{1}{4}}{z^2}\right], \end{aligned}$$

separating the terms which do not depend on the $Q = \Omega R$. For atom in vacuum ($Q = 0$) there is no Casimir energy. For this reason for renormalization we subtract terms with $Q = 0$ and define the energy

$$E_\Omega = \lim_{s\to 0}\{E_a(s) - \lim_{\Omega\to 0} E_a(s)\}. \tag{29}$$

Then we set $s = 0$, integrate by part over k and obtain final formula ($x = kR,\ z = kL$)

$$E_\Omega = -\frac{\hbar c\Omega}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu\int_0^\infty dk\alpha(i\omega)\left\{\frac{s_l^2(x)e_l^2(z)}{f_{\mathsf{TE}}(ik)} + \frac{s'^2_l(x)e'^2_l(z) + s'^2_l(x)e_l^2(z)\frac{\nu^2-\frac{1}{4}}{z^2}}{f_{\mathsf{TM}}(ik)}\right\}, \tag{30}$$

where Jost functions on the imaginary axes read

$$f_{\mathsf{TE}}(ik) = 1 + \frac{\Omega}{k}s_l(x)e_l(x), \tag{31}$$
$$f_{\mathsf{TM}}(ik) = 1 - \frac{\Omega}{k}s_l'(x)e_l'(x). \tag{32}$$

For an atom one has

$$\alpha(i\omega) = \frac{g_a^2}{\omega^2+\omega_a^2}, \tag{33}$$

where g_a and ω_a are experimental parameters.

From the expression (30) we observe that the energy is negative because the integrand is always positive for arbitrary radius of sphere, plasmon wavevector Ω and arbitrary position of atom. The same observation was noted in Ref. [29] for ideal case. Let us consider different limits.

1) In the Boyer limit $\Omega\to\infty$ we obtain

$$E_B = -\frac{\hbar c}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu\int_0^\infty dkk\alpha(i\omega)\left\{\frac{s_l^2(x)e_l^2(z)}{s_l(x)e_l(x)} - \frac{s'^2_l(x)e'^2_l(z) + s'^2_l(x)e_l^2(z)\frac{\nu^2-\frac{1}{4}}{z^2}}{s_l'(x)e_l'(x)}\right\}. \tag{34}$$

2) We can not change the limit $R\to\infty$ with sum and integration in above expressions (30) and (34) because in this case the integrand will not depend on the l and the series will be divergent. Indeed, we have

$$\begin{aligned} 2s_l(x)e_l(z)|_{R\to\infty} &= +e^{-kd},\ 2s_l(x)e_l(x)|_{R\to\infty} = +1, \\ 2s_l'(x)e_l'(z)|_{R\to\infty} &= -e^{-kd},\ 2s_l'(x)e_l'(x)|_{R\to\infty} = -1, \\ 2s_l'(x)e_l(z)|_{R\to\infty} &= +e^{-kd}, \end{aligned}$$

and the sum over l is divergent:

$$E_\Omega = -\frac{\hbar c\Omega}{2\pi(R+d)^2}\sum_{l=1}^{\infty}\nu\int_0^\infty dk\alpha(i\omega)\frac{e^{-2kd}}{1+\frac{\Omega}{2k}} \to \infty. \tag{35}$$

To find the limit $R\to\infty$ we change the variable $k\to\nu k$ in Eq. (30)

$$E_\Omega = -\frac{\hbar c\Omega}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu^2\int_0^\infty dk\alpha(i\omega\nu)\left\{\frac{s_l^2(\nu x)e_l^2(\nu z)}{f_{\mathsf{TE}}(ik\nu)} + \frac{s'^2_l(\nu x)e'^2_l(\nu z) + s'^2_l(\nu x)e_l^2(\nu z)\frac{1-\frac{1}{4\nu^2}}{z^2}}{f_{\mathsf{TM}}(ik\nu)}\right\}, \tag{36}$$

$$E_B = -\frac{\hbar c}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu^3\int_0^\infty kdk\alpha(i\omega\nu)\left\{\frac{s_l^2(\nu x)e_l^2(\nu z)}{s_l(\nu x)e_l(\nu x)} - \frac{s'^2_l(\nu x)e'^2_l(\nu z) + s'^2_l(\nu x)e_l^2(\nu z)\frac{1-\frac{1}{4\nu^2}}{z^2}}{s'_l(\nu x)e'_l(\nu x)}\right\}, \quad (37)$$

and use the uniform expansion for Bessel functions (see Ref. [30]). We obtain

$$E_\Omega = -\frac{\hbar c\Omega}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu^2\int_0^\infty dk\alpha(i\omega\nu)e^{-2\nu[\eta(z)-\eta(x)]}\left\{\frac{xzt(x)t(z)}{4w} + \frac{1+t^2(z)}{4pxzt(x)t(z)} + \ldots\right\}, \quad (38)$$

$$E_B = -\frac{\hbar c}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu^3\int_0^\infty dkk\alpha(i\omega\nu)e^{-2\nu[\eta(z)-\eta(x)]}\left\{\frac{zt(z)}{2} + \frac{1+t^2(z)}{2zt(z)} + \ldots\right\}, \quad (39)$$

where $p = 1 + \frac{Q}{2\nu x^2 t(x)}$, $w = 1 + \frac{Qt(x)}{2\nu}$, $t(x) = 1/\sqrt{1+x^2}$, $\eta(x) = \sqrt{1+x^2} + \ln\frac{x}{1+\sqrt{1+x^2}}$ and $x = kR,\ z = kL = k(R+d)$. In the limit $R\to\infty$ both expressions coincides and the main contribution comes from the first term of expansion:

$$E = -\lim_{R\to\infty}\frac{\hbar cg^2}{\pi c^2(R+d)^2}\sum_{l=1}^{\infty}\nu^3\int_0^\infty\frac{dyy}{y^2\nu^2+q^2}\frac{e^{-2\nu[\eta(u)-\eta(y)]}}{ut(u)}, \quad (40)$$

where $u = y(1+d/R)$, $q_a = k_aR$ and we changed variable $k\to y = kR$.

The sum over l may be represented in the following form

$$\sum_{l=1}^{\infty}\frac{\nu^3 e^{-2\nu\delta}}{y^2\nu^2+q_a^2} = \frac{1}{4q_a y}\int_0^\infty\frac{27+17e^{-2(t+\delta)}+5e^{-4(t+\delta)}-e^{-6(t+\delta)}}{e^{3(t+\delta)}(e^{-2(t+\delta)}-1)^4}\sin\frac{2q_a t}{y}dt. \quad (41)$$

Taking into account this expression we change the limit $R\to\infty$ and integrals and obtain

$$E = -\frac{3\hbar c\alpha(0)}{8\pi d^4}S, \quad (42)$$

where

$$S = \frac{1}{3}\int_0^\infty dte^{-t}\left\{\frac{1+t}{1+\frac{t^2}{4v^2}} + \frac{t}{(1+\frac{t^2}{4v^2})^2}\right\}, \quad (43)$$

and $v = dk_a$. Let us consider great distance from the plate $dk_a \gg 1$. Taking the limit $v\to\infty$ we obtain $S = 1$ and therefore we have the Casimir-Polder ($\sim d^{-4}$) potential

$$E = -\frac{3\hbar c\alpha(0)}{8\pi d^4}. \quad (44)$$

For small distances $dk_a \ll 1$ we change the variable $t\to\tau = t/2v$ and take the limit $v\to 0$. We obtain in this case $S = \pi v/3$ and potential has the form $\sim d^{-3}$

$$E = -\frac{\hbar c\alpha(0)k_a}{8d^3} \quad (45)$$

as should be the case. The numerical simulation of the S as function of $v = dk_a$ is shown in Fig. 2.

3) Let us analyze the energy for great ($d\gg k_a^{-1}, d\gg R$) and small ($d\ll k_a^{-1}, d\ll R$) distances for finite Ω and R. To find expression for energy for great distance $d\to\infty$ from the shell we use the Eq. (30). We change integrand variable $k = y/d$ and take limit $d\to\infty$, then we take integrals over y and make summation over l and obtain the series over R/d:

$$E_\Omega \approx -\frac{3\hbar c\alpha(0)}{8\pi d^4}S_\Omega, \quad (46a)$$

$$S_\Omega = \frac{\pi}{3\left(\frac{R}{d}+1\right)^2}\sum_{l=1}^{\infty}\left(\frac{R}{d}\right)^{2l+1}\frac{\Gamma(l+2)\Gamma\left(2l+\frac{5}{2}\right)}{4^l\Gamma^2\left(l+\frac{1}{2}\right)\Gamma\left(l+\frac{5}{2}\right)}\left\{\frac{Q}{Q+2l+1} + \frac{(l+1)(8l^2+12l+3)}{l(4l+3)}\right\}. \quad (46b)$$

The sum may be expressed in terms of the hypergeometric functions. The main contribution comes from $l = 1$ and we arrive with expression

$$E_\Omega \approx -\frac{\hbar c\alpha(0)R^3}{8\pi(3+Q)d^7}(53Q+138). \quad (47)$$

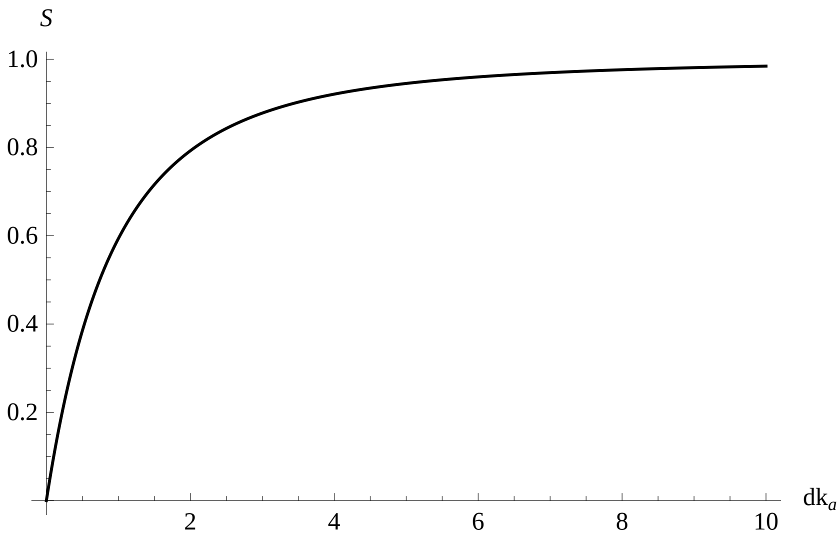

FIG. 2: The plot of S as the function of the $v = kd_a$. It tends to unit for great v ($E \sim d^{-4}$) and it is linear over v ($E \sim d^{-3}$) for small distances from plate. The relation of the energy and S is given by Eq. (42).

Comparing this expression with Casimir-Polder interaction of two atoms with polarizations α and α_f

$$E = -\frac{23}{4\pi}\frac{\hbar c\alpha(0)\alpha_f(0)}{d^7} \tag{48}$$

we observe that from this point of view conductive sphere has static polarizability

$$\alpha_f = \frac{53Q + 138}{46Q + 138}R^3. \tag{49}$$

To analyze the energy for small distances we use the following representation for series

$$\sum_{l=1}^{\infty}\frac{\nu^2}{y^2\nu^2 + q^2}\frac{e^{-2\nu\delta}}{1+\frac{a}{\nu}} = -\frac{1}{4(q^2+a^2y^2)}\int_0^\infty \left\{f^{(2)}e^{-2ax} + \frac{y}{2q}f^{(4)}\sin\frac{2qx}{y} + \frac{ay}{q}f^{(3)}\sin\frac{2qx}{y}\right\}, \tag{50}$$

where $f(x) = e^{-3(\delta+x)}/(1-e^{-2(\delta+x)})$. First and second terms give the d^3 contribution and last term give contribution $\sim d$. Taking into account this expressions we obtain the same result as above

$$E = -\frac{\hbar c\alpha(0)k_a}{8d^3} \tag{51}$$

as should be the case, because close to the sphere we observe flat surface.

V. NUMERICALS

Therefore we have the following expressions which have to be analysed numerically ($x = kR,\ z = k(R+d)$)

$$E_\Omega = -\frac{\hbar c\Omega}{\pi(R+d)^2}\sum_{l=1}^{\infty}\nu\int_0^\infty dk\alpha(i\omega)\left\{\frac{s_l^2(x)e_l^2(z)}{f_{\mathsf{TE}}(ik)} + \frac{s'^2_l(x)e'^2_l(z) + s'^2_l(x)e_l^2(z)\frac{\nu^2-\frac{1}{4}}{z^2}}{f_{\mathsf{TM}}(ik)}\right\}, \tag{52}$$

with the following formulas for the Jost functions

$$f_{\mathsf{TE}}(ik) = 1 + \frac{\Omega}{k}s_l(x)e_l(x), \tag{53}$$

$$f_{\mathsf{TM}}(ik) = 1 - \frac{\Omega}{k}s'_l(x)e'_l(x), \tag{54}$$

and polarizability of atom

$$\alpha(i\omega) = \frac{g_a^2}{\omega^2+\omega_a^2}. \tag{55}$$

In the Boyer limit $\Omega \to \infty$ we obtain

$$E_B = -\frac{\hbar c}{\pi (R+d)^2} \sum_{l=1}^{\infty} \nu \int_0^{\infty} dkk\alpha(i\omega) \left\{ \frac{s_l^2(x) e_l^2(z)}{s_l(x) e_l(x)} - \frac{s'^2_l(x) e'^2_l(z) + s'^2_l(x) e_l^2(z) \frac{\nu^2 - \frac{1}{4}}{z^2}}{s'_l(x) e'_l(x)} \right\}, \tag{56}$$

We change the integrand variable $k = y/R$,

$$E_\Omega = -\frac{\hbar g_a^2 Q}{\pi c (R+d)^2} \sum_{l=1}^{\infty} \nu \int_0^{\infty} \frac{dy}{y^2 + q_a^2} \left\{ \frac{s_l^2(y) e_l^2(z)}{f_{\mathsf{TE}}(iy)} + \frac{s'^2_l(y) e'^2_l(z) + s'^2_l(y) e_l^2(z) \frac{\nu^2 - \frac{1}{4}}{z^2}}{f_{\mathsf{TM}}(iy)} \right\}, \tag{57}$$

$$E_B = -\frac{\hbar g_a^2}{\pi c (R+d)^2} \sum_{l=1}^{\infty} \nu \int_0^{\infty} \frac{y dy}{y^2 + q_a^2} \left\{ \frac{s_l^2(y) e_l^2(z)}{s_l(y) e_l(y)} - \frac{s'^2_l(y) e'^2_l(z) + s'^2_l(y) e_l^2(z) \frac{\nu^2 - \frac{1}{4}}{z^2}}{s'_l(y) e'_l(y)} \right\}, \tag{58}$$

where $z = (1+r)y$, $q_a = \omega_a R/c$, and

$$f_{\mathsf{TE}}(iy) = 1 + \frac{Q}{y} s_l(y) e_l(y), \tag{59}$$

$$f_{\mathsf{TM}}(iy) = 1 - \frac{Q}{y} s'_l(y) e'_l(y). \tag{60}$$

Here $r = d/R$. We numerically calculate the dimensionless quantity

$$S_\Omega = \frac{8 q_a^2 Q r^4}{3(1+r)^2} \sum_{l=1}^{\infty} \nu \int_0^{\infty} \frac{dy}{y^2 + q_a^2} \left\{ \frac{s_l^2(y) e_l^2(z)}{f_{\mathsf{TE}}(iy)} + \frac{s'^2_l(y) e'^2_l(z) + s'^2_l(y) e_l^2(z) \frac{\nu^2 - \frac{1}{4}}{z^2}}{f_{\mathsf{TM}}(iy)} \right\}, \tag{61}$$

$$S_B = \frac{8 q_a^2 r^4}{3(1+r)^2} \sum_{l=1}^{\infty} \nu \int_0^{\infty} \frac{y dy}{y^2 + q_a^2} \left\{ \frac{s_l^2(y) e_l^2(z)}{s_l(y) e_l(y)} - \frac{s'^2_l(y) e'^2_l(z) + s'^2_l(y) e_l^2(z) \frac{\nu^2 - \frac{1}{4}}{z^2}}{s'_l(y) e'_l(y)} \right\} \tag{62}$$

and the energy is connected with this variable

$$E_{\Omega,B} = -\frac{3\hbar c \alpha(0)}{8\pi d^4} S_{\Omega,B}. \tag{63}$$

It is better to mesure all variables in the wave vector k_a and therefore the function S depends on the three parameters: $\Omega/k_a, q_a = Rk_a$ and dk_a. The numerical analysis of the function S for $\Omega/k_a = 2.44 \cdot 10^{-2}$ (molecule C_{60}) and $\Omega/k_a = 1$ is presented in Fig. 3.

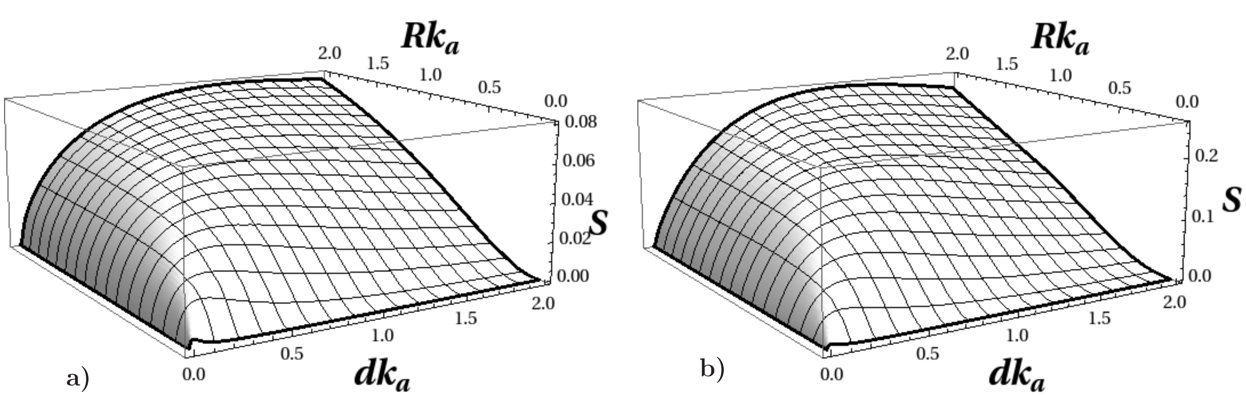

FIG. 3: The plot of S as the function of the $dk_a \in (0, 2)$ and $Rk_a \in (0.02, 2)$ for $\Omega/k_a = 2.44 \cdot 10^{-2}$ (the fig. a) and $\Omega/k_a = 1$ (the fig. b).

Let us consider above formula for molecule C_{60}. For this molecule from Ref. [22] we have $R = 3.42\text{Å} = 0.342nm$, $Q = \Omega R = 4.94 \cdot 10^{-4}$ and $\Omega/k_a = 2.44 \cdot 10^{-2}$. Polarizability of hydrogen atom reads [13, 18, 31] $\alpha_a(0) = 4.50\ a.u.$ ($1\ a.u. = 1.482 \cdot 10^{-31} m^3$) and $\omega_a = 11.65eV = 17.698 \cdot 10^{15} Hz$ ($k_a = 0.059nm^{-1}$, $\lambda_a = 106.4nm$) where $\omega/c = k = 2\pi/\lambda$. Therefore we have $q_a = k_a R = 0.0202$.

Numerically the energy for hydrogen atom has the following form

$$E_\Omega(eV) = -\frac{0.0156}{d^4(nm)} S_\Omega(q_a, r), \tag{64}$$

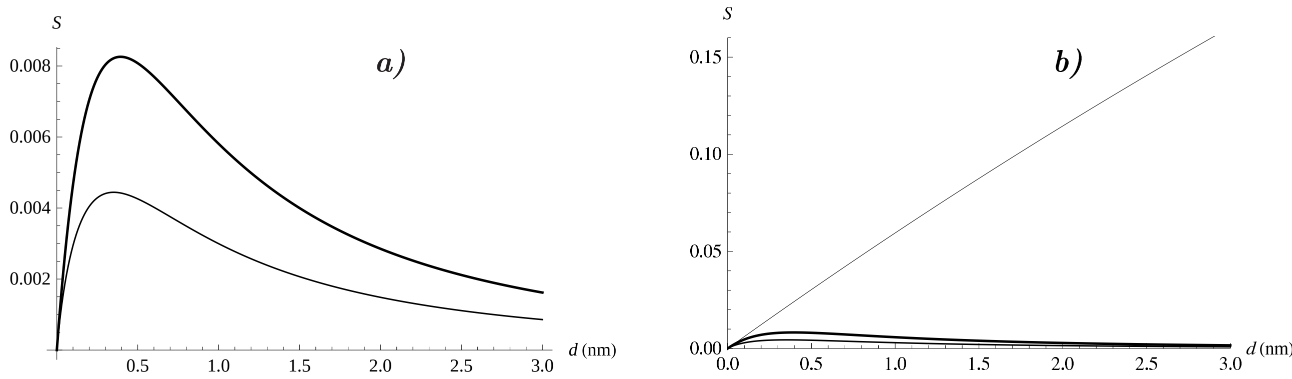

FIG. 4: The plot of S as the function of the distance d from the sphere. Thin curve is the energy for the case $R \to \infty$ (Casimir-Polder energy for plate), middle thickness curve is the case of the molecule C_{60}, and the thick curve is the case of ideal sphere ($\Omega \to \infty$). In the figure b we compare the energy for the plane with the energy in the sphere case.

where the energy is measured in the eV and the distance is measured in nanometres. The numerical simulations the function S are shown in Fig. 4 and the energy E_Ω in Fig. 5. The radius of the hydrogen atom is $r_H = 0.053nm$. For this minimal distance, $d = r_H$, we have numerically $E = 3.8eV$. In the case of plate we obtain $6.4eV$. In the interval of distances from hydrogen atom r_H up to $5r_H$ the energy is approximated by the following expression

$$E_\Omega(eV) \approx -\frac{0.00013}{d^{7/2}(nm)}. \tag{65}$$

For great distances we have from Eq. (47)

$$E_\Omega(eV) \approx -\frac{0.0095}{d^7(nm)}. \tag{66}$$

This expression approximates the exact one with error 10% starting with distance $d = 50nm$. The Eq. (49) gives the static palarizability of the fullerene $\alpha_p(0) = R^3 = 4 \cdot 10^{-29} m^3$. This expression is close to that calculated in Ref. [32] where the authors obtained $\alpha_p(0) = 7 \cdot 10^{-29} m^3$.

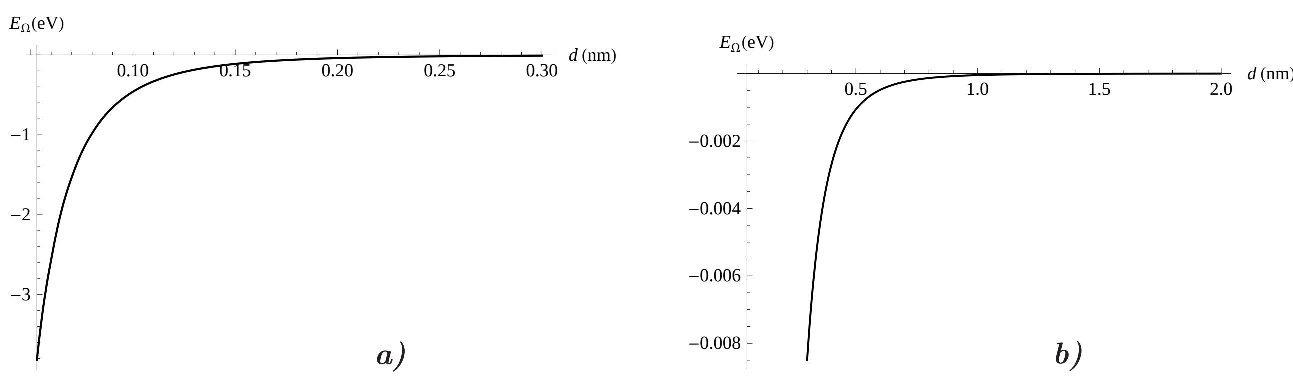

FIG. 5: The plot of the energy E_Ω as the function of the distance d from the sphere for the hydrogen atom. In the figure a) we show the energy starting from the distance $d = 0.053(nm)$ (the radius of the hydrogen atom). The figure b) shows the energy in large interval.

VI. CONCLUSION

In the foregoing, we have obtained the close expression for the Casimir-Polder (van der Waals) energy for a system which contain an atom or microparticle and conductive infinitely thin sphere which model for a fullerene. We used the zeta-regularization approach and for renormalization we used a simple physically reasonable condition – the energy should be zero without sphere. The conductive sphere with radius R is characterized by the only parameter $\Omega = 4\pi ne^2/mc^2$ with dimension wave number, where n is the surface density of electrons. The limit $\Omega \to \infty$ corresponds to the ideal case considered by Boyer [26]. The microparticle is characterized by the only parameter polarizability α.

The expression obtained reproduces in the limit $R \to \infty$ the Casimir-Polder result for the atom with plate (see Eqs. (42)-(45)). For small distances we have d^{-3} dependence and far from the plate we obtain d^{-4} due to retardation. For finite radius of the sphere we have different behavior of the energy. Close to the sphere, $d \ll 1/k_a$ and $d \ll R$, we have the same d^{-3} dependence as in the Casimir-Polder case and far from the sphere we obtained d^{-7} dependence given in Eq. (47). This expression is valid for $d \gg 1/k_a$ and $d \gg R$. For the interval $r_H < d < 5r_H$, where r_H is the radius of the hydrogen atom, the energy is approximated by $d^{-7/2}$ dependence. We also note that the finite conductivity decreases of the energy in comparison with Boyer case which may be observed in the Fig. 4.

Application to the molecule C_{60} with hydrogen atom is plotted in Fig. 5. For closest distance atom from the fullerene, which is radius of hydrogen atom r_H, the energy is $3.8eV$ which is two times smaller then for the case atom with plate. Far from the fullerene (in fact greater then $50nm$) the energy falls down as d^{-7} (see Eq. (66)) which is three order faster then for the Casimir-Polder case. This dependence corresponds to the Casimir-Polder interaction atoms for great distance. Taking into account this analogy we obtain the polarizability of fullerene ($Q = \Omega R = 4.94 \cdot 10^{-4} \ll 1$)

$$\alpha_f = \frac{53Q + 138}{46Q + 138} R^3 \approx R^3 = 4 \cdot 10^{-29} m^3.$$

Acknowledgments

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