Instituto de Física - Universidade Federal do Rio de Janeiro

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Van der Waals interaction between an atom and non-trivial conducting surfaces

W. J. M. Kort-Kamp, R. de Melo e Souza, C. Sigaud, C. Farina

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1 Introduction

Dispersive forces between atoms and surfaces are important in many physical situations, as for instance, in the adsorption of an atom at the surface of a solid or in the phenomenon of adhesion. Here, we shall focus our attention to the non-retarded interaction of a neutral, but polarizable atom, with non-trivial perfectly conducting surfaces. The assumption of perfectly conducting surfaces, though not realistic, allows us to explore analytically more interesting situations. Particularly, we will discuss the interaction between an atom and (i) an oblate ellipsoid, which case allow us to recover the results for the interaction of an atom and a sphere and an atom and a disc; (ii) a cone, which play fundamental role to understand the interaction between and atom and microscope's tip.

2 The interaction energy

Consider a polarizable atom at position $\mathbf{r}_0$ in the presence of a arbitrary perfectly conducting surface. As shown by C. Eberlein and R. Zietal [1] the non-retarded dispersive interaction energy between the atom and the surface, in first order perturbation theory, is given by

THE INTERACTION ENERGY

$$U_{NR}(\mathbf{r}_0) = \frac{1}{2\varepsilon_0}\sum_{j=1}^{3}\langle d_j^2\rangle \nabla_j\nabla_j' G_H(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'=\mathbf{r}_0} \quad (1)$$

where the atom is supposed to be in its ground state, $\langle d_j^2\rangle$ is the square mean value of the component j of the electric dipole operator and $G_H(\mathbf{r},\mathbf{r}')$ is a classical function which satisfies Laplace's equation and a appropriated boundary condition (BC) at the conducting surface,

$$\nabla^2 G_H(\mathbf{r},\mathbf{r}') = 0\,, \quad (2)$$

$$\left[\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} + G_H(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}\in S} = 0\,. \quad (3)$$

Looking at the previous equations we see that $G_H(\mathbf{r},\mathbf{r}')$ is the homogeneous solution of the non-homogeneous equation $\nabla^2 G(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}')$ which makes $G(\mathbf{r},\mathbf{r}')$ vanish at the surface. Hence, apart from a constant factor, $G_H(\mathbf{r},\mathbf{r}')$ is the contribution to the electrostatic potential at point $\mathbf{r}$ due to the surface charge density induced by a point charge located at $\mathbf{r}'$. In other words, to find the quantum dispersive force between a polarizable atom and an generic grounded conducting surface in the non-retarded regime, we just need to solve an electrostatic problem defined by equations (2) and (3).

3 Applications

3.1 Atom near a conducting oblate ellipsoid

For convenience, we will use oblate spheroidal coordinates $(\xi,\,\eta,\,\varphi)$ in which the z-axis is the revolution axis. The relation between spheroidal and cartesian coordinates has the form [2, 3]

$$\begin{aligned} x &= f\sqrt{(1+\xi^2)(1-\eta^2)}\cos\varphi\,, && 0\le\xi<\infty \\ y &= f\sqrt{(1+\xi^2)(1-\eta^2)}\sin\varphi\,, && -1\le\eta\le 1 \\ z &= f\xi\eta\,, && 0\le\varphi<2\pi \end{aligned} \quad (4)$$

where $f=\sqrt{b^2-a^2}$ is the focal distance and b and a are the ellipsoid major and minor semi-axis, respectively. The advantage of this coordinate system is because ξ = constant defines an ellipsoidal surface. To get the energy interaction we need the electrostatic potential at the position $(\xi,\,\eta,\,\varphi)$ due a charge at $(\xi',\,\eta',\,\varphi')$ near the conductor surface defined by $\xi=\xi_0$. Also, we will use that in oblate spheroidal coordinates the inverse of distance is written as [2, 3]

$$\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} = \sum_{n=0}^{\infty}\sum_{m=0}^{n} P_n^m(\eta)P_n^m(i\xi)\times \left\{\alpha_{nm}^{<}\cos m\varphi + \beta_{nm}^{<}\sin m\varphi\right\},\ \xi<\xi' \quad (5)$$

where

$$\left\{\begin{array}{c}\alpha_{nm}^{<}\\ \beta_{nm}^{<}\end{array}\right\} = \frac{i(-1)^m(2-\delta_{m0})(2n+1)}{4\pi f}\left[\frac{(n-m)!}{(n+m)!}\right]^2 \times\, \times P_n^m(\eta')Q_n^m(i\xi')\left\{\begin{array}{c}\cos m\varphi'\\ \sin m\varphi'\end{array}\right\}, \quad (6)$$

and $P_n^m(x)$, $Q_n^m(x)$ are the first and second kind Legendre polynomials, respectively. We will seek the solution of the Laplace's equation in the region $\xi_0\le\xi\le\xi'$ in the form

$$G_H(\mathbf{r},\mathbf{r}') = \sum_{n=0}^{\infty}\sum_{m=0}^{n} P_n^m(\eta)Q_n^m(i\xi)\times \left\{\alpha_{nm}^{H}\cos m\varphi + \beta_{nm}^{H}\sin m\varphi\right\}, \quad (7)$$

where α_{nm}^H and β_{nm}^H are given by

$$\left\{\begin{array}{c}\alpha_{nm}^{H}\\ \beta_{nm}^{H}\end{array}\right\} = -\frac{P_n^m(i\xi_0)}{Q_n^m(i\xi_0)}\left\{\begin{array}{c}\alpha_{nm}^{<}\\ \beta_{nm}^{<}\end{array}\right\}, \quad (8)$$

and are determined by the BC in (3).

Particularly, if the atom is on the z-axis ($\eta=\pm1$) and $\langle d_z^2\rangle \gg \langle d_x^2\rangle, \langle d_y^2\rangle$ we obtain

ATOM-ELLIPSOID INTERACTION ENERGY

$$U_{NR}^{ae}(\xi) = \frac{-i\langle d_z^2\rangle}{8\pi\varepsilon_0 f^3}\sum_{n=0}^{\infty}(2n+1)\frac{P_n(i\xi_0)}{Q_n(i\xi_0)}\left\{\frac{dQ_n(i\xi)}{d\xi}\right\}^2 \quad (9)$$

which is a monotonic function of the distance between the atom and the ellipsoid as expected and shown in figure 3.1.

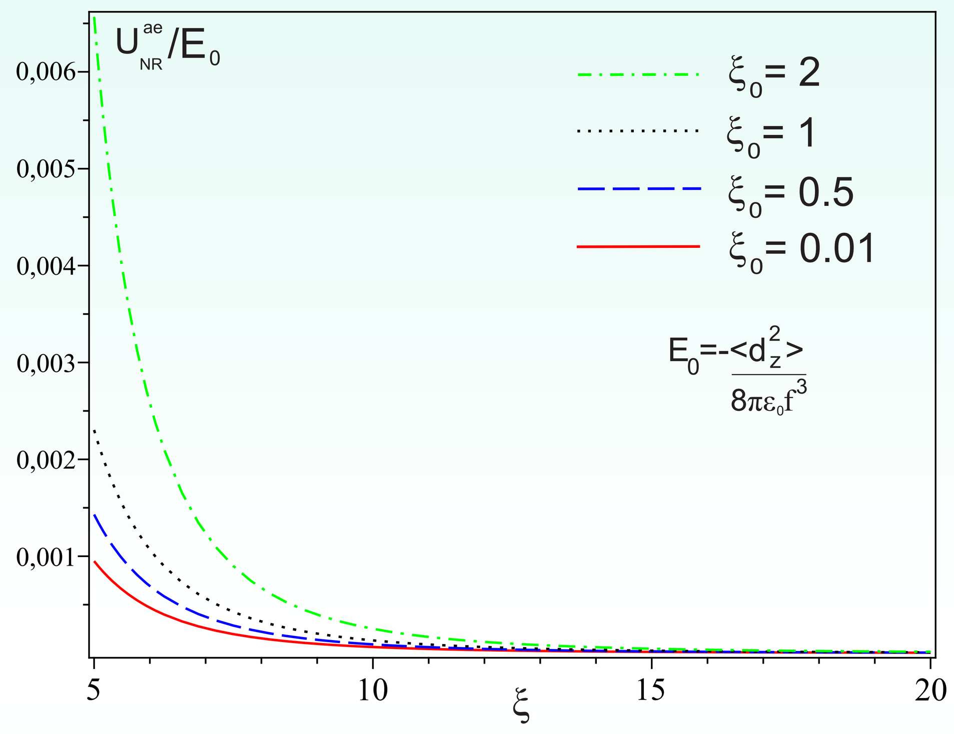

Figure 3.1

3.1.1 Sphere limit

As a particular case of equation (9) we can get the interaction between an atom and a conducting sphere with radius a just by taking the asymptotic limit $\xi_0\gg1$. In this limit the Legendre polynomials take the form [4]

$$P_n(x)\to\frac{(2n)!}{2^n n!^2}x^n\,,\quad Q_n(x)\to\frac{2^n n!^2}{(2n+1)!x^{n+1}}\quad ,x\gg1 \quad (10)$$

and it is straightforwardly show that the atom-sphere interaction is given by [5]

$$U_{NR}^{as}(r) = \frac{-\langle d_z^2\rangle}{8\pi\varepsilon_0}\left\{\frac{2a^3}{r^6}\frac{1}{(1-a^2/r^2)^3} + \frac{a}{r^4}\frac{1}{(1-a^2/r^2)^2}\right\} \quad (11)$$

3.1.2 Disc limit

Another important case to be considered here is the limit $a\to0$ which gives the interaction between an atom and a perfectly conducting disc. In terms of spheroidal coordinates this can be achieved by take $\xi_0=0$ and use the follow property of Legendre polynomials [2]

$$\frac{P_n(i\cdot0)}{Q_n(i\cdot0)} = \left\{\begin{array}{ll}0\,, & n\ \text{odd}\\ 2i/\pi\,, & n\ \text{even}\end{array}\right. . \quad (12)$$

Bear this equations in mind we arrive to

$$U_{NR}^{ad}(z) = \frac{\langle d_z^2\rangle}{4\pi^2\varepsilon_0 b^3}\sum_{n=0}^{\infty}(4n+1)\left\{\frac{dQ_{2n}(i\xi)}{d\xi}\right\}^2 \quad (13)$$

which is numerically equal to the result presented in ref. [6].

3.2 Atom near a cone

Another important example of direct application of the equation (1) is the interaction energy between an atom and a conducting cone which can be relevant in the understanding of the force on an atom due a needle of a microscope. For convenience we work in spherical coordinates with the earthed cone surface defined by the angle $\theta=\alpha$. Beside, it is possible to show that in this case the Green function at $(r,\,\theta,\,\varphi)$ due a point charge at $(r',\,\theta',\,\varphi')$ with the BC $G(\mathbf{r},\mathbf{r}')|_{\theta=\alpha}=0$ is given by [2]

$$G(\mathbf{r},\mathbf{r}') = \left\{\begin{array}{l}\displaystyle\sum_{\nu}\sum_{m=0}^{\nu}A_{\nu m}\left(\frac{r}{r'}\right)^{\nu}P_\nu^m(\mu)\cos m(\varphi-\varphi')\,, r<r'\\ \displaystyle\sum_{\nu}\sum_{m=0}^{\nu}A_{\nu m}\left(\frac{r'}{r}\right)^{\nu+1}P_\nu^m(\mu)\cos m(\varphi-\varphi')\,, r>r'\end{array}\right. \quad (14)$$

where $\mu=\cos\theta$, the coefficient $A_{\nu m}$ is written as

$$A_{\nu m} = \frac{(2-\delta_{m0})P_\nu^m(\mu')}{2\pi r'(2\nu+1)I_{\nu m}(\alpha)}\,,\ I_{\nu m}(\alpha) = \int_{\cos\alpha}^{1}[P_\nu^m(x)]^2dx\,, \quad (15)$$

and the first sum in (14) is over all ν which satisfies

$$P_\nu^m(\cos\alpha)=0. \quad (16)$$

Now, if we use (14) to determine $G_H(\mathbf{r},\mathbf{r}')$ and apply equation (1) for an atom on the z-axis and preferentially polarizable in this same direction we arrive to

ATOM-CONE INTERACTION ENERGY

$$U_{NR}^{ac}(z_0) = \frac{-\langle d_z^2\rangle}{8\pi\varepsilon_0 z_0^3}\left[\sum_{\nu}\frac{2\nu(\nu+1)x^{\nu}}{(2\nu+1)I_{\nu0}(\alpha)} - \sum_{l=0}^{\infty}l(l+1)x^{\nu}\right]_{x=1} \quad (17)$$

Among other things, our result shows that the interaction energy between an atom and a perfectly conducting cone is proportional to z_0^{-3} times a function of the geometry, which depend on α in a non-simple way. Furthermore, the geometric function is composed by two divergent functions, but the difference between them is finite. Particularly, if we take $\alpha=\pi/2$ only the odd integers values for ν satisfy (16). In this case, the sums in (17) can be evaluated analytically to get

$$\begin{aligned} U_{NR}^{aw}(z_0) &= -\frac{\langle d_z^2\rangle}{8\pi\varepsilon_0 z_0^3}\left[\frac{2x}{(x+1)^3} - \frac{2x}{(x-1)^3} - \frac{-2x}{(x-1)^3}\right]_{x=1} \\ &= -\frac{\langle d_z^2\rangle}{32\pi\varepsilon_0 z_0^3} \end{aligned} \quad (18)$$

which is just the result to the atom-wall interaction [5].

For $\alpha\neq\pi/2$ we need some approximate expressions to get the ν values which satisfy (16). As instance, for a very thin tip, $\pi-\alpha\ll1$, we have [4]

$$\nu\simeq k+\frac{2}{2\ln\left(\dfrac{2}{\pi-\alpha}\right)}\,, k=0,1,2,3,\dots \quad (19)$$

and for not very small apex angles, $\pi/6<\alpha<5\pi/6$ we can estimate the roots of (16) by [3]

$$\nu\simeq\frac{\pi}{\alpha}\left(k-\frac{1}{4}\right)-\frac{1}{2}+\frac{\cot\alpha}{8\pi k}\,, k=1,2,3,4,\dots \quad (20)$$

At the moment we are working with the approximated expressions to get numerical results for the atom-cone interaction energy in intermediary range of aperture angles.

4 Final remarks

Here we have discussed the method present in ref. [1] to calculate the interaction energy between an atom and an arbitrary earthed conducting surface. We employed it to study the interaction of an atom with an oblate ellipsoid and a cone. In the former we reobtained as limit cases the atom's interaction with a sphere and a disc. In the later we recovered the atom-wall interaction analytically as a particular case of (17) and we are working the results numerically at the moment.

References

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