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Potential energy of a point charge in a grounded conducting cavity

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Abstract. The force acting on a point charge inside a grounded conducting cavity is discussed. This is a situation relevant to some quantum dot devices. We emphasize that care must be taken when applying the image-charge method to this problem.

It is a basic problem in electrostatics to find the potential field of a given charge distribution subject to stated boundary conditions. The resulting electrostatic potential gives the force acting on an infinitesimal test charge. This is a standard topic in any electromagnetism text such as [1–3]. Less often discussed is the following question: given a finite point charge q inside a conducting cavity, what is the force acting on this point charge itself? The difference from the textbook situation is that an infinitesimal test charge does not contribute to the electromagnetic field, whereas the finite charge that we consider obviously does. In addition, by asking what force acts on it, we allow that it may move.

This question generally receives less attention in texts, although it is discussed, for example, by Griffiths [2]. There is an apparent factor-of-two discrepancy between the correct answer and the one that many would write down at first sight. This problem has been discussed twice before in *American Journal of Physics* [4, 5], but we believe that this elementary discussion will add to its understanding. In addition we present a non-trivial example of a cubic cavity.

To clarify the concept, we review the simplest problem of the kind: a point charge near a grounded infinite conducting plate: see figure 1. This well-worn problem is solved by placing an opposite charge at the mirror image position. Taking the grounded plane as $z = 0$, and the point charge q at $(0, 0, a)$, the electrostatic potential function is

$$V(x, y, z) = \frac{q}{4\pi\epsilon_0}\left(\frac{1}{r_+} - \frac{1}{r_-}\right) \tag{1}$$

where

$$r_\pm = \sqrt{x^2 + y^2 + (z \mp a)^2}$$

are the distances of an infinitesimal test charge at (x, y, z) from the point charge q and its image $-q$ at $(0, 0, -a)$.

The charge q induces a surface charge distribution on the plate. These induced charges in turn attract the original charge q. The question is, what is the potential function consistent with this attractive force?

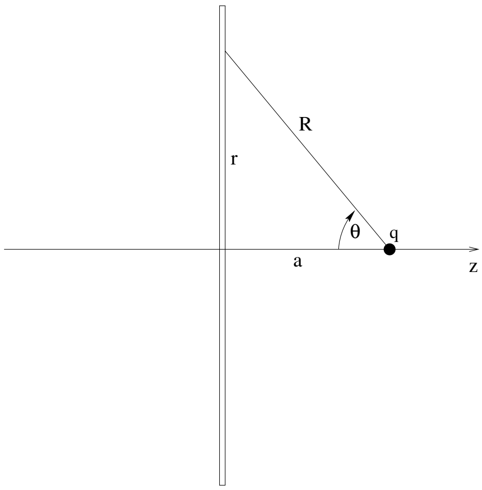

Figure 1. Charge q at distance a from a grounded plane.

On the one hand, the attractive force between q and its image is:

$$F = -\frac{q^2}{4\pi\epsilon_0(2a)^2} \tag{2}$$

for which the associated potential energy (we use the letter $U \sim qV$ to denote a potential energy as distinct from an electrostatic potential which is measured per unit charge) is

$$U = -\frac{q^2}{4\pi\epsilon_0(4a)}. \tag{3}$$

On the other hand, the electrostatic potential energy of a charge q in the presence of its image, a distance $2a$ away, is

$$\hat{U} = -\frac{q^2}{4\pi\epsilon_0(2a)} \tag{4}$$

which is twice equation (3). This is the famous factor of two. Which potential is the relevant one?

The answer is found by analysing the charge layer induced on the grounded plane, which we compute using Gauss's theorem. The electric field parallel to the plate is zero, while the normal component is

$$E_z|_{z=0} = -\frac{\partial V}{\partial z} = -\frac{aq}{2\pi\epsilon_0 R^3} \tag{5}$$

where $R = \sqrt{a^2 + x^2 + y^2}$ is the distance from a point on the plane to the charge q. This gives the induced charge density as

$$\sigma = \epsilon_0 E_z = -\frac{aq}{2\pi R^3}. \tag{6}$$

This leads to a total induced charge of $Q = -q$, as expected:

$$Q = \int \sigma(R) 2\pi r \, \mathrm{d}r = -q. \tag{7}$$

The total electrostatic force on the charge q is the sum of the forces of the induced charges:

$$F_z = \frac{q}{4\pi\epsilon_0} \int_0^\infty \frac{\cos\theta\, \sigma 2\pi r \, \mathrm{d}r}{R^2} = -\frac{q^2}{4\pi\epsilon_0} \int_0^\infty \frac{\cos^2\theta \, r \, \mathrm{d}r}{R^4} = -\frac{q^2}{4\pi\epsilon_0(2a)^2} \tag{8}$$

where θ is defined in figure 1, and both r and R are functions of θ. This confirms that the force of equation (2) derived from the image-charge method is the correct one. The effective potential is the negative of this force integrated over the distance a, confirming equation (3).

So what is the problem with equation (4)? To understand this, we first calculate the total potential energy of the charge q in the presence of the induced charges on the plane:

$$\begin{aligned} U_{q,\text{induced}} &= \frac{q}{4\pi\epsilon_0}\int_0^\infty \frac{\sigma 2\pi r\,\mathrm{d}r}{R} = -\frac{q^2}{4\pi\epsilon_0}\int_0^\infty \frac{\cos\theta\, r\,\mathrm{d}r}{R^3} \\ &= -\frac{q^2}{4\pi\epsilon_0 a}\int_0^{\pi/2}\cos\theta\sin\theta\,\mathrm{d}\theta = -\frac{q^2}{4\pi\epsilon_0(2a)}. \end{aligned} \tag{9}$$

This agrees with equation (4). This energy can be computed either as the potential energy of q due to its image, or that of q due to the induced charges. But here is the point: the total electrostatic energy is the work done in assembling the system, i.e. bringing the charge q from infinity to distance a in front of the plate, including the work done on the induced charge distribution. When you approach the solution from the image-charge viewpoint, you are likely to overlook the self-energy of the induced charges.

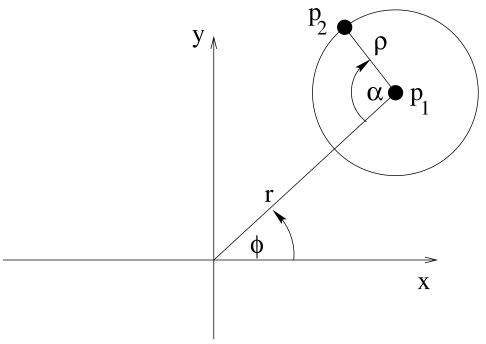

Figure 2. Coordinates for integrating the self-energy of the induced charge in the $z = 0$ plane. σ_i is the induced charge density at a point p_i.

The self-energy of the induced charge changes as q moves. It can be expressed as a double integral over the $z = 0$ plane (see figure 2):

$$\begin{aligned} U_{\text{self}} &= \frac{1}{2}\frac{1}{4\pi\epsilon_0}\int\int\int\int \frac{(\sigma_1 r\,\mathrm{d}r\,\mathrm{d}\phi)(\sigma_2\rho\,\mathrm{d}\rho\,\mathrm{d}\alpha)}{\rho} \\ &= \frac{1}{2}\int\int \sigma_1 r\,\mathrm{d}r\,\mathrm{d}\phi \frac{1}{4\pi\epsilon_0}\int\int \sigma_2\,\mathrm{d}\rho d\alpha. \end{aligned} \tag{10}$$

We relegate the details to the appendix, and quote the result

$$U_{\text{self}} = \frac{1}{4\pi\epsilon_0}\frac{q^2}{4a}. \tag{11}$$

This cancels half of equation (9), giving the total potential energy

$$U = -\frac{1}{4\pi\epsilon_0}\frac{q^2}{4a} \tag{12}$$

in agreement with equation (3).

This result is well known to surface physicists (see [6], which contains a complete discussion of the history of surface states with references to the original papers, and [7]). It is the basis for the Schottky effect, the lowering of the work function when electrons are removed from a metal surface by an applied electric field: see for example [8]. Despite its simplicity, the example shows that one should be careful in applying the image-charge method, a point which was briefly mentioned by Landau and Lifshitz [9]. A more detailed discussion of the case where a point charge lies between two parallel conducting plates can be found in the recent text by Schwinger *et al* [10]. Griffiths [2] explains the factor of two as arising from the fact that the conducting plane divides space into two halves, and the energy stored in the field is obtained by integrating over only the half space containing the charge q. This certainly works for the plane boundary, but it is less obviously helpful in our next example.

A grounded sphere is a second situation where an exact solution can be obtained by the image-charge method. A point charge q located at distance r from the centre, inside the sphere, has an image q' at distance r' from the centre. The charge q, its image, and the centre of the sphere lie on a straight line, as illustrated in figure 3.

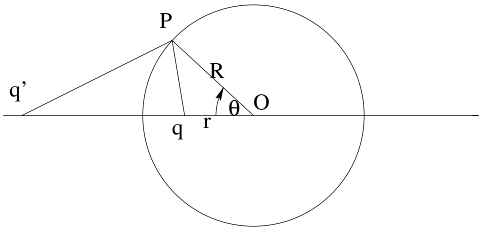

Figure 3. Coordinates for the image-charge method for a sphere.

The condition for having zero potential at any point P on the sphere yields the values

$$r' = \frac{R^2}{r} \qquad q' = -\frac{R}{r}q. \tag{13}$$

The force acting on q is

$$\boldsymbol{F} = \frac{q^2 Rr}{4\pi\epsilon_0(R^2 - r^2)^2}\hat{\boldsymbol{r}} \tag{14}$$

and is equivalent to a potential of the form

$$U = -\int \boldsymbol{F}\cdot \mathrm{d}\boldsymbol{r} = \frac{-q^2}{4\pi\epsilon_0}\int \frac{Rr\,\mathrm{d}r}{(R^2-r^2)^2} = -\frac{q^2}{8\pi\epsilon_0}\frac{R}{(R^2-r^2)} + U_0 \tag{15}$$

where U_0 is a constant of integration which can be set to zero. Note that, just as for the grounded plane problem, U is half of the potential energy of q in the presence of its image charge q':

$$U_{qq'} = -\frac{q^2}{4\pi\epsilon_0}\frac{R}{(R^2-r^2)}. \tag{16}$$

The above examples are those considered by Prato and Condat [4], who also cite some older references that we have not seen.

We now discuss the general situation of a point charge q at position $\boldsymbol{r}_0$ inside a grounded conductor of arbitrary shape. We shall find the force acting on this charge and the potential associated with it.

The electrostatic potential for this problem is $V = (q/\epsilon_0)G(\boldsymbol{r}-\boldsymbol{r}_0)$, where $G(\boldsymbol{r}-\boldsymbol{r}_0)$ is the Green's function which satisfies:

$$\nabla^2 G(\boldsymbol{r}-\boldsymbol{r}_0) = -\delta(\boldsymbol{r}-\boldsymbol{r}_0) \tag{17}$$

with Dirichlet boundary condition $G = 0$ when $\boldsymbol{r}$ lies on the surface. This is the approach adopted by Pomer [5].

Clearly, the Green's function $G(\boldsymbol{r}-\boldsymbol{r}_0)$ is symmetric under exchange of its arguments. The desired potential V is the result of the charge q and of the induced charges. Therefore, the electric potential due to the induced charge alone is

$$V_{\text{induced}}(\boldsymbol{r}, \boldsymbol{r}_0) = \frac{q}{\epsilon_0}G(\boldsymbol{r}, \boldsymbol{r}_0) - \frac{q}{4\pi\epsilon_0|\boldsymbol{r}-\boldsymbol{r}_0|} \tag{18}$$

which shows that V_{induced} also is symmetrical with respect to $\boldsymbol{r}$ and $\boldsymbol{r}_0$.

Another way to derive V_{induced} is to notice that it is the solution of Laplace's equation with boundary value $-q/[4\pi\epsilon_0|\boldsymbol{r}-\boldsymbol{r}_0|]$ on the surface. This can be constructed numerically or by means of Green's theorem:

$$V_{\text{induced}}(\boldsymbol{r},\boldsymbol{r}_0) = \oint \frac{q}{4\pi\epsilon_0|\boldsymbol{r}'-\boldsymbol{r}_0|}\nabla_{r'}G(\boldsymbol{r}',\boldsymbol{r})\cdot \mathrm{d}A'. \tag{19}$$

Since equation (19) is equivalent to equation (18), it must also be symmetrical under interchange of $\boldsymbol{r}$ and $\boldsymbol{r}_0$. The force on the charge q is

$$\boldsymbol{F}(\boldsymbol{r}_0) = -q\nabla_r V_{\text{induced}}(\boldsymbol{r},\boldsymbol{r}_0)|_{r=r_0}. \tag{20}$$

Defining

$$U(\boldsymbol{r}_0) = \frac{q}{2}V_{\text{induced}}(\boldsymbol{r}_0,\boldsymbol{r}_0) \tag{21}$$

we have

$$-\nabla_{r_0}U(\boldsymbol{r}_0) = -\frac{q}{2}\left[\nabla_r V_{\text{induced}}(\boldsymbol{r},\boldsymbol{r}_0)|_{r=r_0} + \nabla_{r_0}V_{\text{induced}}(\boldsymbol{r},\boldsymbol{r}_0)|_{r=r_0}\right] = \boldsymbol{F}(\boldsymbol{r}_0). \tag{22}$$

In the last step, we have used the symmetry property of $V_{\text{induced}}(\boldsymbol{r},\boldsymbol{r}_0)$. This shows that $U(\boldsymbol{r}_0)$ is the proper potential energy to describe the effect of the surface induced charges on the point charge itself.

So here is the recipe expressed in equations (18)–(21). For any position $\boldsymbol{r}_0$ of the point charge q, solve the electrostatic problem for a point charge q at this position with Dirichlet boundary condition. From this electric potential remove that generated by q itself, namely $q/(4\pi\epsilon_0|\boldsymbol{r}-\boldsymbol{r}_0|)$. Half of the resulting potential times q, at $\boldsymbol{r}=\boldsymbol{r}_0$, is the answer.

As an example, we computed the potential energy of a point charge inside a grounded cube. We solved Laplace's equation with boundary value $-1/|\boldsymbol{r}_0-\boldsymbol{r}|$ on a grid $41\times41\times41 = 68\,921$ points. We used a simple finite-difference plus successive over-relaxation linear equation solver. Taking into account the symmetry properties of the cube, we had to solve Laplace's equation 1540 times. It took somewhat less than two hours on a P-II 300 MHz Linux machine. Figure 4 shows two cross sections of the potential.

As one can see in figure 4, the potential profiles at different z-values are similar in that there is a plateau in the centre and the potential drops quickly as we approach any surface. The difference between the two cuts is that, for the top part of the figure, we are already very close to one surface of the box, so the platform is much lower and flatter.

Based on the observation that, as one approaches the box surface, the potential should behave as $-q^2/(4\pi\epsilon_0\,4a)$, we found the following empirical formula for it:

$$\begin{aligned}\tilde{U} = \frac{4\pi\epsilon_0}{q^2}U(x) &= -\frac{1}{4}\left(\frac{1}{x}+\frac{1}{d-x}+\frac{1}{y}+\frac{1}{d-y}+\frac{1}{z}+\frac{1}{d-z}\right)\\ &\quad+\frac{2.1}{d}+\frac{6}{d^5}\left[\left(\frac{d}{2}-x\right)^2+\left(\frac{d}{2}-y\right)^2+\left(\frac{d}{2}-z\right)^2\right]^2\\ &\quad+\frac{12}{d^5}\left[\left(\frac{d}{2}-x\right)^2\left(\frac{d}{2}-y\right)^2+\left(\frac{d}{2}-y\right)^2\left(\frac{d}{2}-z\right)^2+\left(\frac{d}{2}-z\right)^2\left(\frac{d}{2}-x\right)^2\right]\end{aligned} \tag{23}$$

where d is the edge length. In figure 5 we plot the potential $\tilde{U}$ (in dimensionless form, as in equation (23)) from the numerical calculation and compare it with the empirical formula.

Our interest in the question discussed in this paper is related to applications in nanoelectronics. A quantum dot is a structure of very small dimensions, of the order of tens of nanometres, in which a small number of electrons can be confined. Being man-made, they are often called artificial atoms. If the materials are very pure, electrons scatter only from the walls of the enclosure and can be regarded as trapped in a potential well. (Ashoori [11], for example, has described recent research on quantum dots.) Depending on the materials

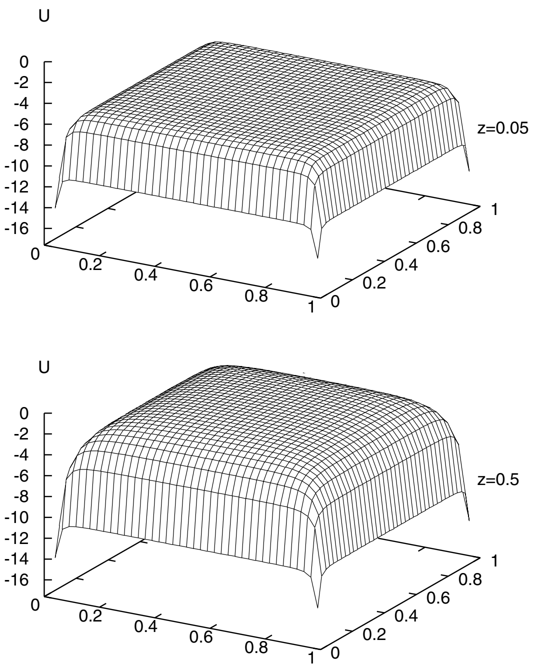

Figure 4. Effective potential of a point charge inside a grounded cubic cavity, scaled to edge length $d = 1$. The grid size is $d/40$. The top part is the potential profile at $z = 0.05d$ while the lower part is a cut at $z = 0.5d$. The potential is in units of $q^2/(4\pi\epsilon_0 d)$.

involved, the confining potential may be smooth, like an oscillator, or abrupt like a square well. For the tiny Si–SiO_2 dots fabricated in Tübingen [12], the abrupt potential well is more appropriate. The example discussed above would be a possible model for a cubic dot. As figure 5 shows, the potential due to the induced charge curves downwards as an electron approaches the edge of the quantum dot, steepening the walls.

In summary, we have clarified the question of the potential energy of a shielded charge. A recipe for constructing such a potential is given and the cubic cavity was studied as a non-trivial example.

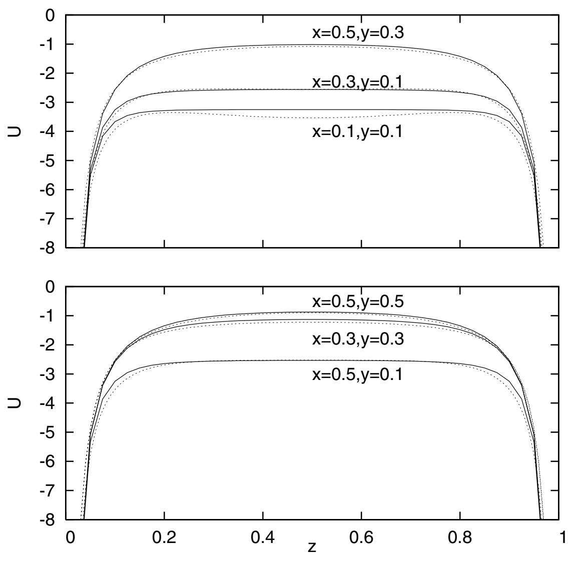

Figure 5. Effective potential of a point charge inside a grounded cubic cavity as computed numerically (solid line) and from our empirical formula (dotted line). For selected points on the x–y plane, the potential is plotted as a function of z. The data and the energy units are as in figure 4.

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Appendix. Self-energy of the induced surface charges

We choose polar coordinates (r, ϕ) for the point P_1, and relative coordinates ρ, α for the vector joining P_2 to P_1. The integral $I_1 = (4\pi\epsilon_0)^{-1}\int\int \sigma_2\,\mathrm{d}\rho\,\mathrm{d}\alpha$ can be regarded as the electrostatic potential due to all induced charges, at the point P_1. The charge density σ_2 depends on R_2, the distance from P_2 to the charge q:

$$R_2^2 = a^2 + r^2 + \rho^2 - 2r\rho\cos\alpha. \tag{A1}$$

Using equation (6), we have:

$$\begin{aligned} I_1 &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi}\int\int\frac{\mathrm{d}\rho\,\mathrm{d}\alpha}{(a^2+r^2+\rho^2-2r\rho\cos\alpha)^{3/2}} \\ &= \frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi}\int\left.\frac{(\rho - r\cos\alpha)\,\mathrm{d}\alpha}{(r^2\cos^2\alpha - a^2 - r^2)\sqrt{a^2+r^2+\rho^2-2r\rho\cos\alpha}}\right|_0^\infty \\ &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi\sqrt{a^2+r^2}}\int_0^{2\pi}\frac{\mathrm{d}\alpha}{\sqrt{a^2+r^2}-r\cos\alpha} \\ &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi\sqrt{a^2+r^2}}\frac{2\pi}{a} = -\frac{q}{4\pi\epsilon_0 R_1} \end{aligned} \tag{A2}$$

where R_1 is the distance from the point P_1 to the charge q. The integral over α was evaluated by a standard result in contour integration. We notice that I_1 is also the electrostatic potential of the image charge at the point P_1. Continuing, the self-energy is

$$U_{\mathrm{self}} = \frac{1}{2}\int\int\sigma_1 r\,\mathrm{d}r\,\mathrm{d}\phi\frac{(-q)}{4\pi\epsilon_0 R_1} = -\frac{1}{2}\frac{q}{4\pi\epsilon_0}\int_0^\infty\frac{\sigma_1\,2\pi\,r\,\mathrm{d}r}{R_1}. \tag{A3}$$

Except for a factor of $-1/2$, this is the same as (9).

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