Electrostatic potential acting on a point charge inside a conducting cavity

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

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The basic problem in electrostatics is to find the potential field of a given charge distribution subject to stated boundary conditions. The question asked in this type of problem is, what is the effect of the given charge distribution and the boundaries on an infinitesimal test charge. This is a standard topic of any electromagnetism text such as [1–3]. Much less discussed is the following question: given a finite point charge q inside a conducting cavity, what is the potential 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, though 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 people would write down at first sight. This problem has been discussed twice before in the American Journal of Physics [4,5], but we believe that we can still add something to its understanding. In addition we present a non-trivial example of a cubic cavity.

To make the concept clear, we start with the simplest problem of the kind: a point charge beside a grounded infinite conducting plate. See Fig. 1. This well known 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 energy of the system is

$$U = qV = \frac{q}{4\pi\epsilon_0}\left(\frac{1}{r_+} - \frac{1}{r_-}\right) \tag{1}$$

where

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

are the distances of an infinitesimal test charge 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 potential is consistent with this attractive force?

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 in distinction to 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

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

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

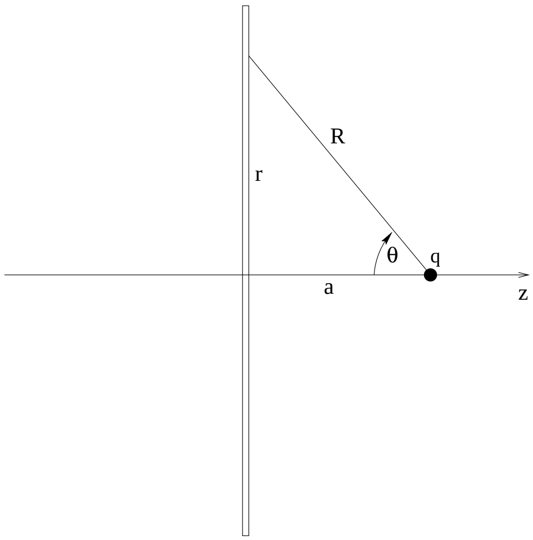

FIG. 1. Charge q at distance a from a grounded plane.

The answer must be sought in an analysis of 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. Hence the induced charge density on the surface is

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

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

$$Q = \int \sigma(R) 2\pi r dr = -q \tag{7}$$

The total electrostatic force on the charge q is the sum of the electro-static forces of the induced charges, acting on it:

$$\begin{aligned} F_z &= \frac{q}{4\pi\epsilon_0}\int_0^\infty \frac{\cos\theta\,\sigma 2\pi r dr}{R^2} = -\frac{q^2}{4\pi\epsilon_0}\int_0^\infty \frac{\cos^2\theta\, r dr}{R^4} \\ &= -\frac{q^2}{4\pi\epsilon_0(2a)^2} \end{aligned} \tag{8}$$

where θ is defined in Fig. 1, and both r and R are functions of θ. This confirms that the force derived from the image charge method is the right one. The effective potential is the negative of this force integrated over the distance a, which confirms Eq. (3).

Then what is the problem with Eq. (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:

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

This agrees with Eq. (4). This energy can be computed as the potential energy of q due to its image, or of q due to the induced charges. But here lies the difference: When we consider the total electrostatic energy of the system, we must take into account the self-energy of the induced charge, but this subtlety is obscured when the induced charge distribution is replaced by an image point charge $-q$. In other words, the image charge method conceals part of the physics in this particular problem. The total electrostatic energy is the energy of 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.

The self energy of the induced charge changes as q moves. It can be calculated by a double integration over the $z = 0$ plane:

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

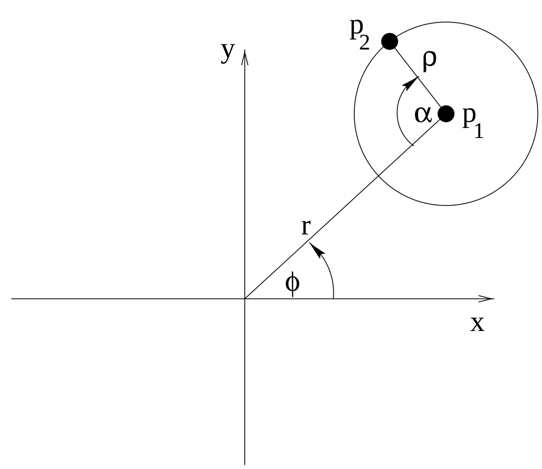

FIG. 2. Coordinates for integrating the self energy of the induced charge in the $z = 0$ plane. σ_i is the induced charge density at a point p_i.

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 $I_1 = (4\pi\epsilon_0)^{-1}\int\int \sigma_2 d\rho d\alpha$ can be regarded as the electrostatic potential due to all induced charges, at the point P_1. In order to know σ_2, we need to know the distance from P_2 to the charge q, which we call R_2:

$$R_2^2 = a^2 + r^2 + \rho^2 - 2r\rho\cos\alpha \tag{11}$$

Using Eq. (6), we have:

$$\begin{aligned} I_1 &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi}\int\int\frac{d\rho d\alpha}{(a^2+r^2+\rho^2-2r\rho\cos\alpha)^{3/2}} \\ &= \frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi}\int d\alpha \times \\ &\quad \left.\frac{\rho - r\cos\alpha}{(r^2\cos^2\alpha - a^2 - r^2)\sqrt{a^2+r^2+\rho^2-2r\rho\cos\alpha}}\right|_0^\infty \\ &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi\sqrt{a^2+r^2}}\int_0^{2\pi}\frac{d\alpha}{\sqrt{a^2+r^2}-r\cos\alpha} \\ &= -\frac{1}{4\pi\epsilon_0}\frac{aq}{2\pi\sqrt{a^2+r^2}}\frac{2\pi}{a} \\ &= -\frac{q}{4\pi\epsilon_0\sqrt{a^2+r^2}} \\ &= -\frac{q}{4\pi\epsilon_0 R_1} \end{aligned} \tag{12}$$

where R_1 is the distance from the point P_1 to the charge q (or to its image). The last integral is evaluated by a standard result in contour integration. We recognize I_1 as the electrostatic potential of the image charge at the point P_1. Continuing, the self energy is

$$\begin{aligned} U_{self} &= \frac{1}{2}\int\int\sigma_1 r dr d\phi\frac{(-q)}{4\pi\epsilon_0 R_1} \\ &= -\frac{1}{2}\frac{q}{4\pi\epsilon_0}\int_0^\infty\frac{\sigma_1\, 2\pi\, r dr}{R_1}. \end{aligned} \tag{13}$$

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

$$U_{self} = \frac{1}{4\pi\epsilon_0}\frac{q^2}{4a}. \tag{14}$$

Adding them, the total energy of the system is

$$U = -\frac{1}{4\pi\epsilon_0}\frac{q^2}{4a} \tag{15}$$

in agreement with Eq. (3).

This result is well known to surface physicists [6,8]. 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 potential: see for example [7]. Despite its simplicity, this example shows that one should be careful in applying the image charge method. This was briefly mentioned in the book by Landau and Lifshitz on the subject [9]. A more detailed discussion on the case where a point charge lies between two parallel conducting plates can be found in the recent text by J. 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 a distance r from the center, inside the sphere, has an image q' at a distance r' from the center. The charge q, its image, and the center of the sphere lie on a straight line.

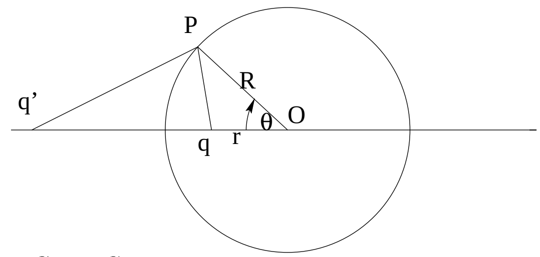

FIG. 3. Coordinates for the image charge method for a sphere.

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

$$\begin{aligned} r' &= \frac{R^2}{r} \\ q' &= -\frac{R}{r}q \end{aligned} \tag{16}$$

The force acting on q is

$$\mathbf{F} = \frac{q^2\, Rr}{4\pi\epsilon_0\,(R^2 - r^2)^2}\,\hat{\mathbf{r}}\,, \tag{17}$$

and is equivalent to a potential of the form

$$\begin{aligned} U &= -\int\mathbf{F}\cdot d\mathbf{r} = \frac{-q^2}{4\pi\epsilon_0}\int\frac{Rrdr}{(R^2-r^2)^2} \\ &= -\frac{q^2}{4\pi\epsilon_0}\frac{R}{2(R^2-r^2)} + U_0 \end{aligned} \tag{18}$$

where U_0 is a constant which can be chosen so that $U(0) = 0$. 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':

$$U_{qq'} = -\frac{q^2}{4\pi\epsilon_0}\frac{R}{(R^2-r^2)} \tag{19}$$

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 $\mathbf{r}_0$ inside a grounded cavity of arbitrary shape. We wish to find the force acting on this charge and the potential associated with it.

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

$$\nabla^2 G(\mathbf{r}-\mathbf{r}_0) = -\delta(\mathbf{r}-\mathbf{r}_0) \tag{20}$$

with Dirichlet boundary condition on the surface. This is the approach adopted by Pomer [5].

Using a complete set of real eigenmodes for the cavity, i.e., the normalized solutions of the Helmholtz equation

$$\nabla^2 \phi_n + k_n^2 \phi_n = 0 \tag{21}$$

which vanish on the boundary, the Green's function can be expanded as

$$G(\mathbf{r},\mathbf{r}_0) = \sum_n \frac{\phi_n(\mathbf{r})\phi_n(\mathbf{r}_0)}{k_n^2}\,. \tag{22}$$

V is the result of the charge q and of the induced charges. Therefore the electric potential due to the induced charge alone is

$$V_{induced}(\mathbf{r},\mathbf{r}_0) = \frac{q}{\epsilon_0}G(\mathbf{r},\mathbf{r}_0) - \frac{q}{4\pi\epsilon_0|\mathbf{r}-\mathbf{r}_0|} \tag{23}$$

This form of $V_{induced}$ shows that it is symmetrical with respect to $\mathbf{r}$ and $\mathbf{r}_0$.

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

$$V_{induced}(\mathbf{r},\mathbf{r}_0) = \oint \frac{q}{4\pi\epsilon_0|\mathbf{r}'-\mathbf{r}_0|}\nabla_{\mathbf{r}'}G(\mathbf{r}',\mathbf{r})\cdot dA' \tag{24}$$

Since Eq. (24) is just a regularized form of Eq. (23), it must also be symmetrical with respect to $\mathbf{r}$ and $\mathbf{r}_0$. The force on the charge q is

$$\mathbf{F}(\mathbf{r}_0) = -q\nabla_{\mathbf{r}}V_{induced}(\mathbf{r},\mathbf{r}_0)|_{\mathbf{r}=\mathbf{r}_0} \tag{25}$$

Defining

$$U(\mathbf{r}_0) = \frac{q}{2}V_{induced}(\mathbf{r}_0,\mathbf{r}_0) \tag{26}$$

we have

$$\begin{aligned}-\nabla_{\mathbf{r}_0}U(\mathbf{r}_0) &= -\frac{q}{2}\nabla_{\mathbf{r}}V_{induced}(\mathbf{r},\mathbf{r}_0)|_{\mathbf{r}=\mathbf{r}_0} \\ &\quad -\frac{q}{2}\nabla_{\mathbf{r}_0}V_{induced}(\mathbf{r},\mathbf{r}_0)|_{\mathbf{r}=\mathbf{r}_0} \\ &= \mathbf{F}(\mathbf{r}_0)\end{aligned} \tag{27}$$

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

So here is the recipe: For each position $\mathbf{r}_0$, solve the electrostatic problem of a point charge q at this position with Dirichlet boundary condition. Find the electric potential value at this position, excluding that generated by q itself, namely $1/(4\pi\epsilon_0|\mathbf{r}-\mathbf{r}_0|)$. Half of the resulting potential times q, as a function of $\mathbf{r}_0$, is the answer.

As an example, we computed the effective potential on an point charge inside a grounded cube. We solved Laplace's equation with boundary value $-1/|\mathbf{r}_0-\mathbf{r}|$ on a grid $41\times 41\times 41 = 68921$ 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 takes a bit less than two hours on a P-II 300MHz Linux machine. Fig. 4 shows two cross sections of the potential.

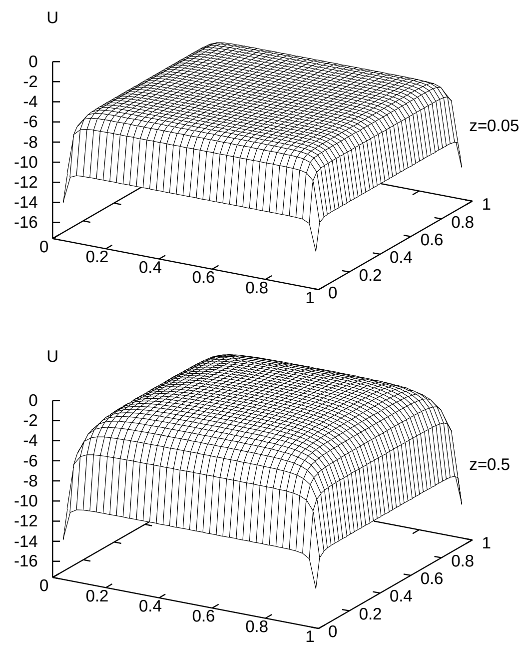

FIG. 4. Effective potential of a point charge inside a grounded cubic cavity, scaled to edge length $d = 1$. The grid size is $d/40$. The top part is the potential profile at $z = 0.05d$ while the lower part is a cut at $z = 0.5d$. The potential is in units of $q^2/(4\pi\epsilon_0 d)$.

As we can see in Fig. 4, the potential profiles at different z-values are similar in that there is a platform in the center and the potential drops quickly as we approach any surface. The difference 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:

$$\begin{aligned}\frac{4\pi\epsilon_0}{q^2}U(x) = &-\frac{1}{4}\left(\frac{1}{x}+\frac{1}{d-x}+\frac{1}{y}+\frac{1}{d-y}+\frac{1}{z}+\frac{1}{d-z}\right) \\ &+\frac{2.1}{d}+\frac{6}{d^5}\left[(\frac{d}{2}-x)^2+(\frac{d}{2}-y)^2+(\frac{d}{2}-z)^2\right]^2 \\ &+\frac{12}{d^5}\Big[(\frac{d}{2}-x)^2(\frac{d}{2}-y)^2+(\frac{d}{2}-y)^2(\frac{d}{2}-z)^2 \\ &\qquad +(\frac{d}{2}-z)^2(\frac{d}{2}-x)^2\Big]\end{aligned} \tag{28}$$

where d is the edge length. In Fig. 5 we plot the potential U (in dimensionless form, as in eq. 28) from the numerical calculation and compare it to the empirical formula.

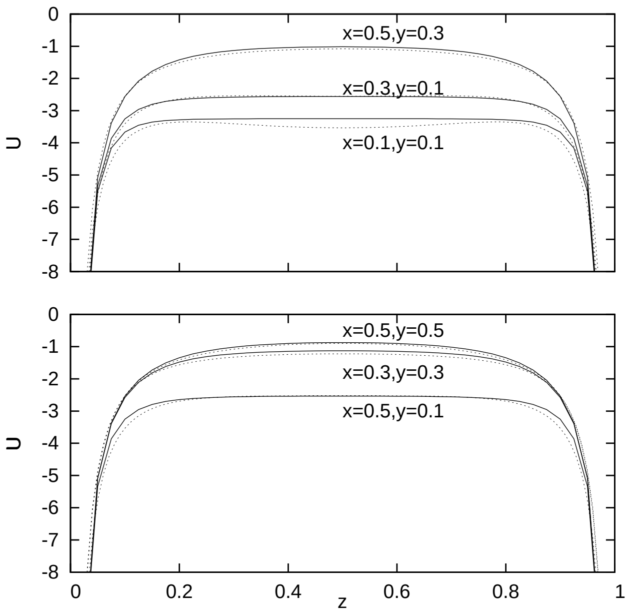

FIG. 5. Effective potential of a point charge inside a grounded cubic cavity as computed numerically (solid line) and from our empirical formula (dotted line). For selected points on the x-y plane, the potential is plotted as a function of z. The data and the energy units are as in Fig. 4.

Recent advances in nanotechnology have made it possible to confine a single electron in a quantum dot [11]. Very small Si dots enclosed in an isolating SiO_2 layer have also been fabricated [12]. These have a confining potential very different from the popular models for $GaAs$ quantum dots with electrons confined by a parabolic potential. The more appropriate hard wall confinement commonly used for silicon dots surrounded by a SiO_2 isolating layer will be reinforced by the grounded gate. As Fig. 5 shows, the potential due to the induced charge curves downward as the electron approaches the edge of the quantum dot, steepening the walls.

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

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