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Manipulating the Coulomb interaction: a Green's function perspective

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Abstract

We present a unified framework for studying Coulomb interactions in arbitrary environments using macroscopic quantum electrodynamics on the basis of the electromagnetic Green's function. Our theory can be used to derive the Coulomb potential of a single charged particle as well as that between two charges in the presence of media, bodies and interfaces of arbitrary shapes. To demonstrate this, we reproduce the well-known screened Coulomb force, account for local-field effects and consider new cases such as a multi-layer medium, a dielectric cavity, a conducting wire and a plate with a hole.

1. Introduction

The Coulomb force is perhaps the first electromagnetic interaction encountered by a student of physics, introduced as an immutable inverse square law that delivers the force between two charged particles. The simple inverse square distance dependence is used as the basis for a wide variety of descriptions of nature, from the Hartree–Fock methods of quantum chemistry to the Derjaguin, Landau, Verwey, and Overbeek theory of colloidal dispersions [1, 2]. What is usually missing is the fact that no physical system exists in true isolation; there will always be some environment enclosing the objects of interest. A prominent example is the exponential screening of the Coulomb interaction for charges embedded in a non-local medium [3]. This appears across physics as such effects arise in materials with a high density of free or quasi-free charge carriers; these include metals (where the screening length is the Thomas–Fermi length), electrolytes (where the screening length is the Debye–Hückel length), ionic solutions or narrow-band-gap semiconductors [4–7]. One common way of arriving at these effects is to make a Thomas–Fermi approximation for a free electron gas, then solving the resulting screened Poisson equation. A small number of works in colloid physics [8] exist that extend this to charges near an interface, but these rely on a linearised Poisson–Boltzmann equation in which several assumptions must be made.

A more fundamental and flexible point of view is provided by macroscopic quantum electrodynamics (QED), where the Coulomb interaction involves the emission and reabsorption of a photon. For example, the interaction between two charges is mediated by a photon that is emitted from one charge and subsequently absorbed by the other. On the way, this photon may interact with its environment, for example it may reflect off a macroscopic body or be travelling through some bulk medium. This leads to an environment-dependent Coulomb force, which is the subject of this work. We will write the Coulomb force in terms of a version of the dyadic Green's function, well-known from the formalism known as macroscopic QED [9, 11]. The special case of bulk media will, as we shall see, reproduce the screening effects discussed above, but the unified formalism we use is much more general. It provides a link between medium-assisted Coulomb interactions and the considerable literature on dyadic Green's functions [12, 13]. We will demonstrate this by considering general expressions as well as several particular geometries that demonstrate the power of the toolbox we are presenting.

In general, environment-dependent effects may be described by the dielectric function, so if this can be engineered the Coulomb interaction can be controlled. One simple way to do this is by varying macroscopic geometric parameters [14], but an increasingly relevant class of media are those whose microscopic structure is

designed to generate a desired permittivity. Control of the Coulomb interaction is particularly important in many solid-state devices like solar cells, where an increase of screening allows for a stronger separation of excitons into electrons and holes [15]. Moreover trapped atomic ions can be used as a collection of qubits where quantum information is transferred between the ions thorough their mutual Coulomb interaction [16, 17].

An interesting related problem, which is of particular interest in colloid physics, is the Coulomb interaction between two charged particles near non-translational-invariant media, like for example a planar multilayer system. This is distinct from the screening imposed by bulk media, and is much less well-studied, though in the formalism we present here it may be studied in exactly the same way as screening effects. Charged particles near macroscopic objects induce a polarisation-charge density on the surface of those objects, which in turn affects their Coulomb interaction. These polarisation effects are particularly important at the interfaces between media with very different dielectric permittivities. This problem is usually treated by the method of images, where the medium is replaced by a set of image charges in order to satisfy a relevant set of boundary conditions on the surfaces. Sometimes, however, in complex geometries (such as a wedge) it is not clear where to place the image charges so one must resort to complex calculations of potentials for particular systems, which may be of limited applicability. Here we will express all Coulomb forces in terms of the dyadic Green's function, which is a very well-studied object in a large number of different geometries. The interaction between two atoms near the relatively simple system of an infinite dielectric slab or metal has been studied [18–21] and, in the metallic case, extended to include spatial dispersion. The result shows that the Coulomb interaction must be corrected for distances shorter in comparison with the Thomas–Fermi screening length in the dispersive case [22]. Similarly, the Coulomb interaction between a charged moving particle and a plasma has been studied in the literature [23].

Although some disparate particular cases have been investigated, to our knowledge no general expression of the medium-assisted Coulomb interaction is known in the literature. As stated earlier, the aim of this work is to study the Coulomb interaction in generic environments that are described by the dyadic Green's tensor. The interaction will be described in the framework of macroscopic QED as a one-photon exchange process, where the photon propagator is governed by the electromagnetic environment.

After deriving some general formulae, we will demonstrate the power of the method by firstly considering a set of examples that reproduce well-known results, the novelty arising from their unification within the same framework. These will include the screening for spatially dispersive media, the interaction between two charges near a planar interface between two dielectrics and the interaction between a charge and a polarisable particle. Following this we also apply our general results to new, non-trivial settings, namely local-field effects, a multi-layer medium, a dielectric cavity, a conducting wire and a conducting plate with a hole. Our approach can be applied to every case where the Green's tensor is known or can be calculated by analytical or numerical means. As already mentioned, there is a vast literature on the subject of the dyadic Green's tensor—the calculations presented here represent a means to reliably translate this wealth of results to the language of the Coulomb interaction in a rigorous and transparent way.

2. Coulomb interaction in the presence of dielectrics

To study the Coulomb interaction between two charged particles, we use field quantisation in linear absorbing and non-local media [9, 10, 24, 25], using the Coulomb gauge. Here and throughout we take the medium to be non-magnetisable (i.e. with unit relative permeability), so that the electric field can be expanded in terms of the creation and annihilation operators $\hat{\mathbf{f}}^\dagger(\mathbf{r}, \omega)$, $\hat{\mathbf{f}}(\mathbf{r}, \omega)$ for electric excitations labelled by frequency ω and position \mathbf{r} ;

$$\hat{\mathbf{E}}(\mathbf{r}, \omega) = \int d^3s \mathbf{G}_e(\mathbf{r}, \mathbf{s}, \omega) \cdot \hat{\mathbf{f}}(\mathbf{s}, \omega). \quad (1)$$

The tensors \mathbf{G}_e are mode-tensors that depend on the imaginary parts of the electric permittivity of the absorbing medium:

$$\mathbf{G}_e(\mathbf{r}, \mathbf{r}', \omega) = i \frac{\omega^2}{c^2} \sqrt{\frac{\hbar}{\pi \varepsilon_0}} \text{Im} \varepsilon(\mathbf{r}', \omega) \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) \quad (2)$$

and on the classical Green tensor of the Helmholtz equation $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$ [9, 10]:

$$\left[\nabla \times \nabla \times - \frac{\omega^2}{c^2} \varepsilon(\mathbf{r}, \omega) \right] \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}') \mathbb{I}, \quad (3)$$

where \mathbb{I} is the identity matrix.

An important relation involving these mode-tensors is:

$$\int d^3s \mathbf{G}_e(\mathbf{r}, \mathbf{s}, \omega) \cdot \mathbf{G}_e^{*\top}(\mathbf{r}', \mathbf{s}, \omega) = \frac{\hbar\mu_0}{\pi} \omega^2 \text{Im } \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega), \quad (4)$$

where $^\top$ denotes the transpose.

Charged particles interact with the radiation field through the scalar and vector potentials, not directly via the electric field. The scalar potential $\hat{\phi}$ is related to the longitudinal part of the electric field via $\hat{\mathbf{E}}^\parallel = -\nabla\hat{\phi}$. The longitudinal part \mathbf{f}^\parallel of a general vector-valued function \mathbf{f} can be calculated using the longitudinal delta function $\delta^\parallel(\mathbf{r}) = -\nabla\nabla(4\pi|\mathbf{r}|)^{-1}$ via:

$$\mathbf{f}^\parallel(\mathbf{r}) = \int d^3s \delta^\parallel(\mathbf{r} - \mathbf{s}) \cdot \mathbf{f}(\mathbf{s}). \quad (5)$$

Hence the scalar potential satisfies the equation:

$$\nabla\hat{\phi}(\mathbf{r}, \omega) = -\int d^3s \mathbf{G}_e^\parallel(\mathbf{r}, \mathbf{s}, \omega) \cdot \hat{\mathbf{f}}(\mathbf{s}, \omega), \quad (6)$$

where \mathbf{G}_e^\parallel is the left-longitudinal component of \mathbf{G}_e :

$$\mathbf{G}_e^\parallel(\mathbf{r}, \mathbf{r}', \omega) = \int d^3s \delta^\parallel(\mathbf{r} - \mathbf{s}) \cdot \mathbf{G}_e(\mathbf{s}, \mathbf{r}', \omega). \quad (7)$$

The scalar potential can hence be derived performing a line integral of a vector field:

$$\hat{\phi}(\mathbf{r}, \omega) = -\int d^3s \int_{\mathbf{r}_0}^{\mathbf{r}} d\mathbf{r}' \cdot \mathbf{G}_e^\parallel(\mathbf{r}', \mathbf{s}, \omega) \cdot \hat{\mathbf{f}}(\mathbf{s}, \omega). \quad (8)$$

We assume that the point \mathbf{r}_0 may be placed at infinity ($|\mathbf{r} - \mathbf{r}_0| \rightarrow \infty$) and take the scalar potential to be defined relative to this; $\hat{\phi}(\mathbf{r}_0, \omega) = 0$. As expected, the potential at a point \mathbf{r} is proportional to the work done by the longitudinal electric field in order to move the charge from infinity to that point. Analogously the vector potential can be expressed in terms of the bosonic excitation operators ($\hat{\mathbf{E}}^\perp = -\hat{\mathbf{A}}$):

$$\hat{\mathbf{A}}(\mathbf{r}, \omega) = \frac{1}{i\omega} \int d^3s \mathbf{G}_e^\perp(\mathbf{r}, \mathbf{s}, \omega) \cdot \hat{\mathbf{f}}(\mathbf{s}, \omega), \quad (9)$$

where \mathbf{G}_e^\perp is the left-transverse component of \mathbf{G}_e :

$$\mathbf{G}_e^\perp(\mathbf{r}, \mathbf{r}', \omega) = \int d^3s \delta^\perp(\mathbf{r} - \mathbf{s}) \cdot \mathbf{G}_e(\mathbf{s}, \mathbf{r}', \omega) \quad (10)$$

and $\delta^\perp(\mathbf{r}) = \nabla \times (\nabla \times \mathbb{I})(4\pi|\mathbf{r}|)^{-1}$ is the transverse delta function.

3. Energy shift

We consider the interaction between two charged particles assisted by a polarisable medium. The distances between the particle and any interfaces of the medium are considered to be large enough that the interface may be regarded as a macroscopic surface, i.e. its microscopic structure is not resolved. This means that we are far enough away to exclude such effects as Pauli repulsion and covalent bonding.

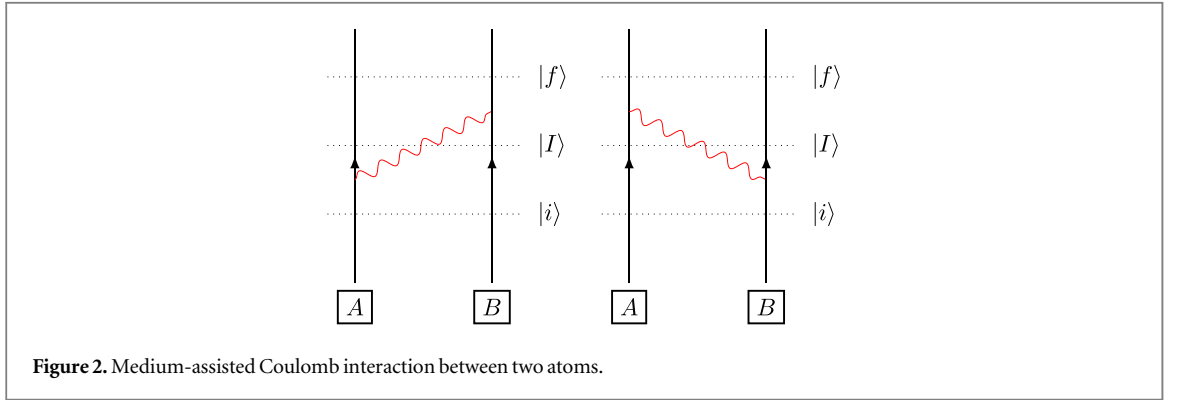
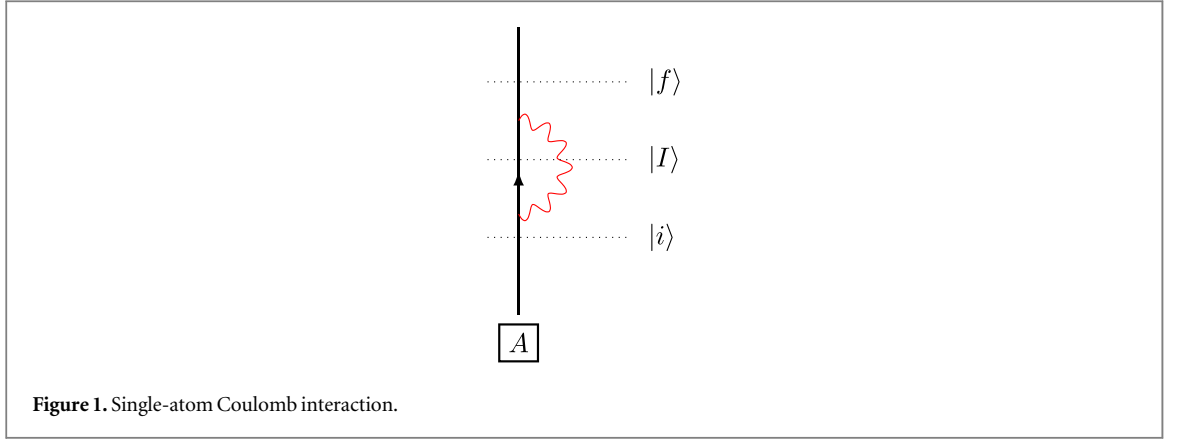
As mentioned in the introduction, the Coulomb interaction may be pictured as arising from the emission and absorption of one virtual photon. There are three processes which can contribute to the interaction, which can be conveniently represented through Feynman diagrams. One diagram involves the photon being emitted and reabsorbed by the same particle as shown in see figure 1. This photon may be affected by the medium, causing a position-dependent shift—hence this process describes the interaction between a single charged particle and a polarisable medium.

The other two diagrams involve the exchange of a single virtual photon between the two charges (see figure 2), and describe the Coulomb interaction between the pair. In all three of these diagrams the interaction is affected by the medium because the photon can be reflected by the body's surface, and hence can be considered emitted by a fictitious image charge.

The energy shift describing the Coulomb interaction can be obtained from second order perturbation theory

$$\Delta E = \langle i | \hat{H}_{\text{int}} | i \rangle - \sum_{I \neq i} \frac{\langle i | \hat{H}_{\text{int}} | I \rangle \langle I | \hat{H}_{\text{int}} | i \rangle}{E_I - E_i}, \quad (11)$$

and \hat{H}_{int} is the Hamiltonian for a set of charges q_α of momentum \mathbf{p}_α minimally coupled to the electromagnetic scalar and vector potentials $\hat{\phi}$ and $\hat{\mathbf{A}}$;



$$\hat{H}_{\text{int}} = \sum_{\alpha=A,B} q_{\alpha} \hat{\phi}(\mathbf{r}_{\alpha}) - \sum_{\alpha=A,B} \frac{q_{\alpha}}{m_{\alpha}} \hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{A}}(\mathbf{r}_{\alpha}) + \sum_{\alpha=A,B} \frac{q_{\alpha}^2}{2m_{\alpha}} \hat{\mathbf{A}}^2(\mathbf{r}_{\alpha}). \quad (12)$$

The second term is absent when one considers charges fixed in space ($\mathbf{p}_{\alpha} = 0$). The intermediate state $|I\rangle$ corresponds to a state in which one virtual photon is present: $|I\rangle \equiv |\{1(\mathbf{r}, \omega)\}\rangle = \hat{\mathbf{f}}^{\dagger}(\mathbf{r}, \omega) |\{0\}\rangle$, $E_I - E_i = \hbar\omega$, while the initial state corresponds to a state without photons $|i\rangle \equiv |\{0\}\rangle$. Using equations (8), (9), the expectation value

$$\langle \{0\} | \hat{\mathbf{f}}(\mathbf{r}, \omega) \hat{\mathbf{f}}^{\dagger}(\mathbf{r}', \omega') | \{0\} \rangle = \delta(\mathbf{r} - \mathbf{r}') \delta(\omega - \omega') \mathbb{I} \quad (13)$$

and the integral relation (4), the matrix elements of the individual terms that make up equation (11) read;

$$\langle i | q_{\alpha} \hat{\phi}(\mathbf{r}_{\alpha}) | I \rangle = -q_{\alpha} \int_{\mathbf{r}_0}^{\mathbf{r}_{\alpha}} d\mathbf{r}' \cdot \mathbb{G}_e(\mathbf{r}', \mathbf{r}, \omega), \quad (14)$$

$$\langle i | \frac{q_{\alpha}^2}{2m_{\alpha}} \hat{\mathbf{A}}^2(\mathbf{r}_{\alpha}) | i \rangle = \frac{\hbar\mu_0 q_{\alpha}^2}{2\pi m_{\alpha}} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_{\alpha}, \mathbf{r}_{\alpha}, \omega) \}, \quad (15)$$

where we have introduced the two-sided-transverse component of \mathbf{G}

$$^{\perp} \mathbf{G}^{\perp}(\mathbf{r}, \mathbf{r}', \omega) = \int d^3s \int d^3s' \delta^{\perp}(\mathbf{r} - \mathbf{s}) \cdot \mathbf{G}(\mathbf{s}, \mathbf{s}', \omega) \cdot \delta^{\perp}(\mathbf{s}' - \mathbf{r}'). \quad (16)$$

where δ^{\perp} is the transverse delta function defined below equation (10). Using this and the integral relation (4), the total energy shift reads:

$$\begin{aligned} \Delta E = & -\frac{\mu_0}{\pi} \sum_{\alpha,\beta=A,B} q_{\alpha} q_{\beta} \int_0^{\infty} \frac{d\omega}{\omega} \omega^2 \int_{\mathbf{r}_0}^{\mathbf{r}_{\alpha}} \int_{\mathbf{r}_0}^{\mathbf{r}_{\beta}} d\mathbf{r} \cdot \text{Im} \mathbb{G}^{\parallel}(\mathbf{r}, \mathbf{r}', \omega) \cdot d\mathbf{r}' \\ & + \frac{\hbar\mu_0}{\pi} \sum_{\alpha=A,B} \frac{q_{\alpha}^2}{2m_{\alpha}} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_{\alpha}, \mathbf{r}_{\alpha}, \omega) \}, \end{aligned} \quad (17)$$

where we have introduced the two-sided-longitudinal component of \mathbf{G} :

$$\mathbb{G}^{\parallel}(\mathbf{r}, \mathbf{r}', \omega) = \int d^3s \int d^3s' \delta^{\parallel}(\mathbf{r} - \mathbf{s}) \cdot \mathbf{G}(\mathbf{s}, \mathbf{s}', \omega) \cdot \delta^{\parallel}(\mathbf{s}' - \mathbf{r}'), \quad (18)$$

where $\delta^{\parallel} = \nabla \otimes \nabla (4\pi|\mathbf{r}|)^{-1}$ is the longitudinal delta function. Here we have used a property of the Green's tensor under transposition; $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)^{\top} = \mathbf{G}(\mathbf{r}', \mathbf{r}, \omega)$. We use the Schwarz reflection principle;

$$\mathbf{G}^*(\mathbf{r}, \mathbf{r}', \omega) = \mathbf{G}(\mathbf{r}, \mathbf{r}', -\omega) \quad (19)$$

to extend the frequency integral (17) to the whole real axis:

$$\begin{aligned} \Delta E = & -\frac{\mu_0}{2\pi i} \sum_{\alpha, \beta=A,B} q_{\alpha} q_{\beta} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \omega^2 \int_{\mathbf{r}_0}^{\mathbf{r}_{\alpha}} \int_{\mathbf{r}_0}^{\mathbf{r}_{\beta}} d\mathbf{r} \cdot \mathbf{G}^{\parallel}(\mathbf{r}, \mathbf{r}', \omega) \cdot d\mathbf{r}' \\ & + \frac{\hbar\mu_0}{\pi} \sum_{\alpha=A,B} \frac{q_{\alpha}^2}{2m_{\alpha}} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_{\alpha}, \mathbf{r}_{\alpha}, \omega) \}. \end{aligned} \quad (20)$$

The tensor $\omega^2 \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$ is analytic in the upper half of the complex plane (including the real axis), and it is also finite at the origin. This means we close the path with an infinitely large half-circle in the upper complex half-plane and deal with the singular point $\omega = 0$ using the principal value prescription. The integral along the infinite semi-circle vanishes for $\mathbf{r} \neq \mathbf{r}'$ because:

$$\lim_{|\omega| \rightarrow \infty} \omega^2 \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)|_{\mathbf{r} \neq \mathbf{r}'} = 0. \quad (21)$$

Calculating the residue at $\omega = 0$, the energy shift reads:

$$\begin{aligned} \Delta E = & -\frac{1}{2\varepsilon_0} \sum_{\alpha, \beta=A,B} q_{\alpha} q_{\beta} \int_{\mathbf{r}_0}^{\mathbf{r}_{\alpha}} \int_{\mathbf{r}_0}^{\mathbf{r}_{\beta}} d\mathbf{r} \cdot \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot d\mathbf{r}' \\ & + \frac{\hbar\mu_0}{\pi} \sum_{\alpha=A,B} \frac{q_{\alpha}^2}{2m_{\alpha}} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_{\alpha}, \mathbf{r}_{\alpha}, \omega) \}, \end{aligned} \quad (22)$$

where we have defined the static Green tensor

$$\mathbf{G}(\mathbf{r}, \mathbf{r}') = \lim_{\omega \rightarrow 0} \frac{\omega^2}{c^2} \mathbf{G}^{\parallel}(\mathbf{r}, \mathbf{r}', \omega) = \lim_{\omega \rightarrow 0} \frac{\omega^2}{c^2} \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega). \quad (23)$$

The last equality follows from the fact that for zero frequency the Green's tensor is purely longitudinal [9].

The energy shift (22) consists of two parts. Firstly there are the single-particle terms which describe the interaction with the surface;

$$U(\mathbf{r}_A) = -\frac{q_A^2}{2\varepsilon_0} \int_{\mathbf{r}_0}^{\mathbf{r}_A} \int_{\mathbf{r}_0}^{\mathbf{r}_A} d\mathbf{r} \cdot \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot d\mathbf{r}' + \frac{\hbar\mu_0 q_A^2}{2\pi m_A} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_A, \mathbf{r}_A, \omega) \} \quad (24)$$

and secondly the medium-assisted Coulomb interaction between the two particles, which reads:

$$U(\mathbf{r}_A, \mathbf{r}_B) = -\frac{q_A q_B}{\varepsilon_0} \int_{\mathbf{r}_0}^{\mathbf{r}_A} \int_{\mathbf{r}_0}^{\mathbf{r}_B} d\mathbf{r} \cdot \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot d\mathbf{r}' \quad (25)$$

as is well-known for arbitrary charge distributions [26]. Combining the single-particle and two-particle terms one has;

$$\Delta E = U(\mathbf{r}_A) + U(\mathbf{r}_A, \mathbf{r}_B). \quad (26)$$

Note that the single-particle shift $U(\mathbf{r}_A)$ contains an infinite contribution which comes from the free Coulomb interaction; however this shift does not depend on the position of the particle and does not lead to any observable force. Note that our results (24) and (25) remain valid for non-local media where the mode tensor (2) involves a convolution over the non-local permittivity [25].

In equation (24) the first term represents the classical interaction while the second term is a quantum correction that vanishes in the classical limit $\hbar \rightarrow 0$. The single-particle shift represents a correction to the force if the charge is situated in an environment. In general the expressions for such a correction are very complicated, but it is in fact possible to estimate the order of magnitude of this term by direct inspection of equation (24).

Firstly we rewrite (24) in terms of the Compton wavelength $\lambda_A = 2\pi\hbar/(m_A c)$

$$U(\mathbf{r}_A) = -\frac{q_A^2}{2\varepsilon_0} \left[\int_{\mathbf{r}_0}^{\mathbf{r}_A} \int_{\mathbf{r}_0}^{\mathbf{r}_A} d\mathbf{r} \cdot \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot d\mathbf{r}' - \frac{\lambda_A}{2\pi^2 c} \int_0^{\infty} d\omega \text{Tr} \{ \text{Im}^{\perp} \mathbf{G}^{\perp}(\mathbf{r}_A, \mathbf{r}_A, \omega) \} \right]. \quad (27)$$

We begin by noting that the Green's tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$ typically has an order of magnitude of r^{-1} where r represents the typical distance between the charge and the surface of the medium. Then, equation (23) tells us that the static Green's tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}')$ has an order of magnitude of r^{-3} . Hence, the ratio between the second and first term of (27) is of order of magnitude λ_A/r . An electron has $\lambda_A \approx 10^{-12}$ m, this should be contrasted with the fact that the description of the surface as a macroscopic body breaks down at distances of around 10^{-9} m. Thus for all distances for which the basic assumptions of this work hold, the second term of equation (27) can safely be discarded.

This analysis is backed up by the detailed evaluation of both terms previously carried out in [23], where the problem was analysed in both the non-retarded and the retarded regimes for a plasma surface. There, it is found that the ratio of the second term to the first term is equal to $\lambda_A \lambda_p / (2\pi\sqrt{2} r^2)$ in the non-retarded regime, and $\lambda_A / (\pi r)$ in the retarded regime, where λ_p is the plasma wavelength. Since for real materials the plasma wavelength is in the visible range we recognise also in this case that the first term of (27) dominates the second.

4. Energy shift in terms of the scalar Green's function

The Coulomb interaction depends on the static Green tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}')$ as defined in equation (23), which is related to the scalar Green function $g(\mathbf{r}, \mathbf{r}')$ from electrostatics defined via [26]:

$$\nabla \cdot [\varepsilon(\mathbf{r}) \nabla g(\mathbf{r}, \mathbf{r}')] = -\delta(\mathbf{r} - \mathbf{r}'). \quad (28)$$

Note that the scalar Green's function is symmetric, $g(\mathbf{r}, \mathbf{r}') = g(\mathbf{r}', \mathbf{r})$, see [26].

In order to show the connection between the two quantities $\mathbf{G}(\mathbf{r}, \mathbf{r}')$ and $g(\mathbf{r}, \mathbf{r}')$ consider equation (3), which defines the full, frequency-dependent dyadic Green's tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$. Taking the divergence of both sides of (3) and considering the static limit $\omega \rightarrow 0$ one has:

$$\nabla \cdot [\varepsilon(\mathbf{r}) \mathbf{G}(\mathbf{r}, \mathbf{r}')] = -\nabla \delta(\mathbf{r} - \mathbf{r}'), \quad (29)$$

where $\varepsilon(\mathbf{r}) \equiv \varepsilon(\mathbf{r}, \omega \rightarrow 0)$ is the static permittivity and $\mathbf{G}(\mathbf{r}, \mathbf{r}')$ the static Green's tensor, see equation (23).

Applying the operator ∇' to both sides of equation (28) and comparing the result to equation (29) we see that:

$$\mathbf{G}(\mathbf{r}, \mathbf{r}') = -\nabla \nabla' g(\mathbf{r}, \mathbf{r}'). \quad (30)$$

Using the well-known relation

$$\int_{\mathbf{r}_0}^{\mathbf{r}} d\mathbf{r}' \cdot \nabla' f(\mathbf{r}') = f(\mathbf{r}) - f(\mathbf{r}_0), \quad (31)$$

to replace g by \mathbf{G} in equations (24) and (25), we find:

$$\begin{aligned} U(\mathbf{r}_A) &= \frac{q_A^2}{2\varepsilon_0} g(\mathbf{r}_A, \mathbf{r}_A) \\ U(\mathbf{r}_A, \mathbf{r}_B) &= \frac{q_A q_B}{\varepsilon_0} g(\mathbf{r}_A, \mathbf{r}_B), \end{aligned} \quad (32)$$

where we have additionally used the property $g(\mathbf{r}, \mathbf{r}') \rightarrow 0$ for $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$. It is worth noting that, apart from the quantum correction, the Coulomb interaction between two charge distributions ρ_A, ρ_B was already described by, for example, Schwinger [26] as:

$$\Delta U = \frac{1}{2\varepsilon_0} \int d^3r \int d^3r' \rho_A(\mathbf{r}) g(\mathbf{r}, \mathbf{r}') \rho_B(\mathbf{r}'). \quad (33)$$

In free space we obtain the well-known Coulomb potential since $g^{(0)}(\mathbf{r}_A, \mathbf{r}_B) = 1/(4\pi|\mathbf{r}_A - \mathbf{r}_B|)$. In general the Green's function is the sum of the free-space contribution $g^{(0)}$ and the scattering part $g^{(1)}$ which accounts for reflections from any surfaces that may be present. In the rest of this work we subtract from $U(\mathbf{r}_A)$ the divergent free-space contribution, as our main focus is the corrections to this stemming from the electromagnetic environment, thus we will work with the following pair of equations;

$$U^{(1)}(\mathbf{r}_A) = \frac{q_A^2}{2\varepsilon_0} g^{(1)}(\mathbf{r}_A, \mathbf{r}_A), \quad (34)$$

$$U(\mathbf{r}_A, \mathbf{r}_B) = \frac{q_A q_B}{\varepsilon_0} g(\mathbf{r}_A, \mathbf{r}_B). \quad (35)$$

The Green's function $g(\mathbf{r}, \mathbf{r}')$ represents the propagator of the field, describing the amplitude for a photon emitted at \mathbf{r}' to be absorbed at \mathbf{r} . Hence equation (34) represents an emission and absorption of a photon by the charge, with a reflection from the surface. In fact the reflected photon can be thought of as emitted by a fictitious image charge. Equation (35) represents a back-and-forth excitation exchange between the two charges (with possible reflection).

Formulae (34) and (35) together with (30) constitute a recipe that takes a dyadic Green's tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$ as input, and produces Coulomb potentials $U^{(1)}(\mathbf{r}_A)$ and $U(\mathbf{r}_A, \mathbf{r}_B)$. As mentioned in the introduction, a proper account of this process allows one to calculate Coulomb interactions in exotic situations by exploiting the huge literature on dyadic Green's functions.

For transitionally invariant media the Green's function depends only on the difference between the two points: $g(\mathbf{r}_A, \mathbf{r}_B) = g(\mathbf{r}_A - \mathbf{r}_B)$. In this kind of system the forces acting on the two charges would be equal and

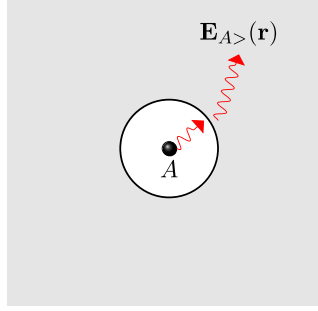


Figure 3. Cavity model: the guest charges in a medium are separated by small, vacuum-filled spherical cavities of radius R . $E_{A>}(\mathbf{r})$ is the electric field transmitted by the cavity's surface into a point \mathbf{r} outside the cavity.

opposite, which is just a consequence of the action–reaction principle. However when the translational invariance is broken and local-field corrections are taken into account the two forces are not equal and opposite. This is not a violation of action–reaction since the interface between two different media takes some momentum to restore the balance.

Finally, we note that we can give an interpretation of the classical shift in terms of the work needed to bring the static charges from infinity and assemble them in the required positions. The medium-assisted Coulomb electric field produced by the charge A , with position \mathbf{r}_A , using equation (30), is:

$$\mathbf{E}_A(\mathbf{r}) = \frac{q_A}{\varepsilon_0} \int_{\mathbf{r}_0}^{\mathbf{r}_A} d\mathbf{r}' \cdot \mathbf{G}(\mathbf{r}', \mathbf{r}) = -\frac{q_A}{\varepsilon_0} \nabla g(\mathbf{r}, \mathbf{r}_A). \quad (36)$$

Hence the potential in \mathbf{r} due to both charges is:

$$\phi(\mathbf{r}) = -\int_{\mathbf{r}_0}^{\mathbf{r}} d\mathbf{r}' \cdot (\mathbf{E}_A(\mathbf{r}') + \mathbf{E}_B(\mathbf{r}')). \quad (37)$$

The work W required to assemble the charges is

$$W = \frac{1}{2} \sum_{\alpha=A,B} q_\alpha \phi(\mathbf{r}_\alpha), \quad (38)$$

which coincides with the classical energy shift derived previously in equation (32).

5. Local-field corrections to the Coulomb interaction

In section 4 we derived the Coulomb interaction between two charges placed within a generic environment. It was assumed that the local electromagnetic field acting on the two particles is the macroscopic field. However this assumption is not satisfied in optically dense media, where local field corrections are important [27, 28]. One way to introduce the local-field correction is via the real-cavity model. There, the charges are considered to be surrounded by small, empty, spherical cavities of radius R and are hence well-separated from the neighbouring atoms of the media.

We consider first the electric field transmitted by the cavity's surface into a point \mathbf{r} outside the cavity, where the surrounding medium is infinite, see figure 3. The Green's function of the infinite body with the cavity, for $r > R$, $r_A < R$, reads [29]:

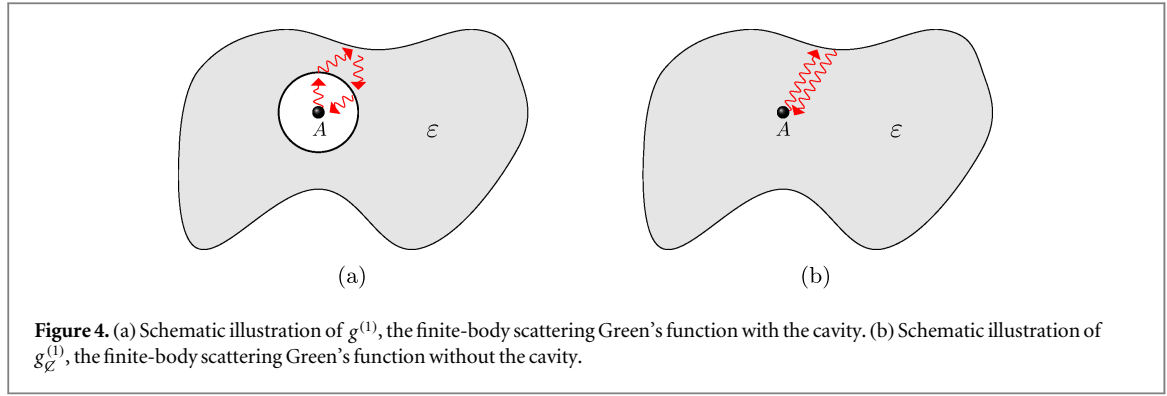
$$g_C^{(0)}(\mathbf{r}, \mathbf{r}_A) = \sum_{l=0}^{\infty} \frac{1}{\varepsilon(l+1) + l} \frac{r_A^l}{r^{l+1}} \sum_{m=-l}^l Y_{lm}(\theta, \phi) Y_{lm}^*(\theta_A, \phi_A), \quad (39)$$

where Y_{lm} are the spherical harmonics. The Green's tensor of the infinite body without the cavity ($r > R$, $r_A < R$) is:

$$g^{(0)}(\mathbf{r}, \mathbf{r}_A) = \frac{1}{4\pi\varepsilon} \frac{1}{|\mathbf{r} - \mathbf{r}_A|} = \sum_{l=0}^{\infty} \frac{1}{\varepsilon(2l+1)} \frac{r_A^l}{r^{l+1}} \sum_{m=-l}^l Y_{lm}(\theta, \phi) Y_{lm}^*(\theta_A, \phi_A). \quad (40)$$

Hence the electric field $\mathbf{E}_{A>}$ transmitted through the cavity surface to a point \mathbf{r} outside the cavity is equal to the field that would be transmitted to the same point in the absence of the cavity ($\mathbf{r}_A = 0$):

$$\mathbf{E}_{A>}(\mathbf{r}) = -\frac{q_A}{\varepsilon_0} \nabla g_C^{(0)}(\mathbf{r}, \mathbf{r}_A) = -\frac{q_A}{\varepsilon_0} \nabla g^{(0)}(\mathbf{r}, \mathbf{r}_A). \quad (41)$$



Moreover:

$$\nabla_A g_C^{(0)}(\mathbf{r}_A, \mathbf{r}) = \frac{3\epsilon}{2\epsilon + 1} \nabla_A g^{(0)}(\mathbf{r}_A, \mathbf{r}). \quad (42)$$

This means that the electric field transmitted through the cavity surface to the point inside the cavity \mathbf{r}_A is equal to the field that would be transmitted to the same point in the absence of the cavity, multiplied by a global factor $3\epsilon/(2\epsilon + 1)$. However the medium can have a finite size and the electric field can be reflected from the outer surface of the medium. The scattering of the field from the outer surface is taken into account by replacing the infinite-body Green's function $g^{(0)}$ with the finite-body Green's scattering function $g^{(1)}$, see figure 4. The electric field transmitted through the cavity surface, reflected from the outer body surface and finally retransmitted into the cavity reads:

$$\mathbf{E}_{A<}^{(1)}(\mathbf{r}) = -\frac{q_A}{\epsilon_0} \nabla g_C(\mathbf{r}, \mathbf{r}_A) = -\frac{3\epsilon}{2\epsilon + 1} \frac{q_A}{\epsilon_0} \nabla g^{(1)}(\mathbf{r}, \mathbf{r}_A), \quad (43)$$

where $g^{(1)}$ is the scattering Green's function of the finite-body with the cavity, see figure 4.

The local-field corrected force acting on A reads:

$$\mathbf{F}_A(\mathbf{r}_{A,B}) = q_A \mathbf{E}_{A<}^{(1)}(\mathbf{r}_A) = -\frac{3\epsilon}{2\epsilon + 1} \frac{q_A^2}{\epsilon_0} \nabla g^{(1)}(\mathbf{r}, \mathbf{r}_A)|_{\mathbf{r}=\mathbf{r}_A}. \quad (44)$$

Note that we should consider the electric field reflected at the surface of the cavity as well; however using the Green's function in [29] it is simple to show that this contribution vanishes. We can generalise our results when the dielectric constant of the medium is not homogeneous; the local field corrected force acting on A reads:

$$\mathbf{F}_A(\mathbf{r}_{A,B}) = q_A \mathbf{E}_{A<}^{(1)}(\mathbf{r}_A) = -\frac{3\epsilon(\mathbf{r}_A)}{2\epsilon(\mathbf{r}_A) + 1} \frac{q_A^2}{\epsilon_0} \nabla g^{(1)}(\mathbf{r}, \mathbf{r}_A)|_{\mathbf{r}=\mathbf{r}_A}. \quad (45)$$

We now focus on the local-field corrected interaction between two charges. Charge B will produce some field which is experienced by charge A . Following the same previous steps we find that the force experienced by the charge A is:

$$\mathbf{F}_A(\mathbf{r}_A, \mathbf{r}_B) = q_A \mathbf{E}_{B<}(\mathbf{r}_A) = -\frac{3\epsilon(\mathbf{r}_A)}{2\epsilon(\mathbf{r}_A) + 1} \frac{q_A q_B}{\epsilon_0} \nabla_A g(\mathbf{r}_A, \mathbf{r}_B). \quad (46)$$

Both the scattering and the bulk contributions of the Green's tensor contribute, leading to enhancement of the force. For example, water has a static permittivity of approximately 80 leading to an enhancement factor of about 1.49. To our knowledge the local-field corrected Coulomb force calculated in this section is a new result, which could find applications in the physics of ions suspended in solvents.

6. Applications

To demonstrate the use of our general results (34), (35) and their generalisations (45), (46) including local-field effects, we apply them to several geometries.

6.1. Homogeneous non-local medium

As an initial example to check the consistency of our method we consider a translationally invariant medium, which is also spatially dispersive. Spatial dispersion is the dependence of the permittivity on the wave vector (rather than simply its magnitude), which means that the electric induction \mathbf{D} at some point is caused by the electric field \mathbf{E} at one or more displaced points. In a bulk medium the Green's function must be translation-invariant, which means that it can only depend on the difference between the coordinates:

$$\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \mathbf{G}(\mathbf{r} - \mathbf{r}', \omega). \quad (47)$$

In this case the Green's dyadic is often Fourier transformed:

$$\mathbf{G}(\mathbf{r} - \mathbf{r}', \omega) = (2\pi)^{-3} \int d^3k e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \mathbf{G}(\mathbf{k}, \omega), \quad (48)$$

where the Fourier transform can be given in terms of the transverse and longitudinal permittivities, $\varepsilon_{\perp}(k, \omega)$ and $\varepsilon_{\parallel}(k, \omega)$ [30]:

$$\mathbf{G}(\mathbf{k}, \omega) = - \left[\frac{\omega^2}{c^2} \varepsilon_{\perp}(k, \omega) - k^2 \right]^{-1} \left(\mathbb{I} - \frac{\mathbf{k}\mathbf{k}}{k^2} \right) - \frac{c^2}{\omega^2 k^2 \varepsilon_{\parallel}(k, \omega)} \mathbf{k}\mathbf{k}. \quad (49)$$

Here \mathbb{I} is the identity matrix. Hence the Green's function reads:

$$g(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^3} \int d^3k \frac{1}{k^2 \varepsilon_{\parallel}(k, 0)} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}. \quad (50)$$

Substituting the Fourier-transformed Green's function (50) into the two-body Coulomb potential given by equation (35), we find (using $\int d\Omega e^{i\mathbf{k} \cdot \mathbf{r}} = 4\pi \sin(kr)/kr$):

$$U(\mathbf{r}_A, \mathbf{r}_B) = \frac{q_A q_B}{(2\pi)^3 \varepsilon_0} \int d^3k \frac{1}{k^2 \varepsilon_{\parallel}(k, 0)} e^{i\mathbf{k} \cdot (\mathbf{r}_A - \mathbf{r}_B)} = \frac{q_A q_B}{4\pi^2 \varepsilon_0 i} \int_{-\infty}^{\infty} dk \frac{1}{\varepsilon_{\parallel}(k, 0)} \frac{e^{ikr}}{kr}, \quad (51)$$

where $\mathbf{r} \equiv \mathbf{r}_A - \mathbf{r}_B$.

The longitudinal and transverse non-local permittivity of a real medium can be described by the hydrodynamic Drude model, which can be considered a limiting case of the Hopfield model [31–33]:

$$\varepsilon_{\parallel}(k, \omega) = 1 + \frac{\tilde{\omega}_p^2}{\omega_0^2 - \omega(\omega + i\Gamma)} + \frac{\omega_p^2}{\beta^2 k^2 - \omega(\omega + i\gamma)}. \quad (52)$$

The first term represents the dielectric function for bound electrons and the second one that for conduction electrons. The plasma frequencies are defined by $\omega_p = \sqrt{ne^2/m_e \varepsilon_0}$, $\tilde{\omega}_p = \sqrt{Ne^2/m \varepsilon_0}$, where n, m, m_e are respectively the number density, effective mass of the free electrons and bound electrons and the N is the density of bound electrons. Finally, ω_0 is a transition frequency and $\Gamma, \gamma > 0$ are damping constants that govern absorption in the medium. For a free electron gas $\beta^2 = 3v_F^2/5$, with v_F the Fermi velocity [34].

Inserting the longitudinal permittivity (52) into the energy shift (51) and evaluating the residua of the poles in the upper part of the complex plane we find;

$$U(r) = \frac{q_A q_B}{4\pi \varepsilon_0 \varepsilon} \frac{e^{-k_s r}}{r} \quad (53)$$

with $\varepsilon = 1 + \tilde{\omega}_p^2/\omega_0^2$ and $k_s = \omega_p/(\beta\sqrt{\varepsilon})$. This is a screened Coulomb potential where both bound and free electrons contribute to the screening [7, 34]. In particular, bound electrons reduce the interaction by a factor $1/\varepsilon$, where ε represents the associated permittivity; free electrons are responsible for the exponential suppression $e^{-k_s r}$.

6.2. Dielectric slab

In the previous section we considered a homogeneous medium. However in many interesting cases translational symmetry is broken, for example in planar multilayer systems. Here we consider two point charges embedded in a semi-infinite dielectric medium of dielectric constant ε_1 , which has a planar interface with a material of dielectric constant ε_2 (see figure 5)

The Green's function satisfies equation (28), with the boundary conditions that g and the normal component of the displacement vector \mathbf{D} are continuous across the interface between two media. Its expression for source position $z' > 0$ reads [26]:

$$g(\mathbf{r}, \mathbf{r}') = \begin{cases} \frac{1}{\varepsilon_1} \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} + \frac{1}{\varepsilon_1} \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'^*|}, & \text{if } z > 0 \\ \frac{2}{\varepsilon_1 + \varepsilon_2} \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|}, & \text{if } z < 0 \end{cases}, \quad (54)$$

where $\mathbf{r}^* = (x, y, -z)$ is the position of an image charge that corresponds to a real charge placed at \mathbf{r} . We can first derive the single-particle Coulomb term ($z_A > 0$):

$$U(z_A) = - \frac{q_A^2}{8\pi \varepsilon_0 \varepsilon_1} \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + \varepsilon_1} \frac{1}{|\mathbf{r}_A - \mathbf{r}_A^*|} = - \frac{q_A^2}{16\pi \varepsilon_0 \varepsilon_1} \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + \varepsilon_1} \frac{1}{z_A} \quad (55)$$

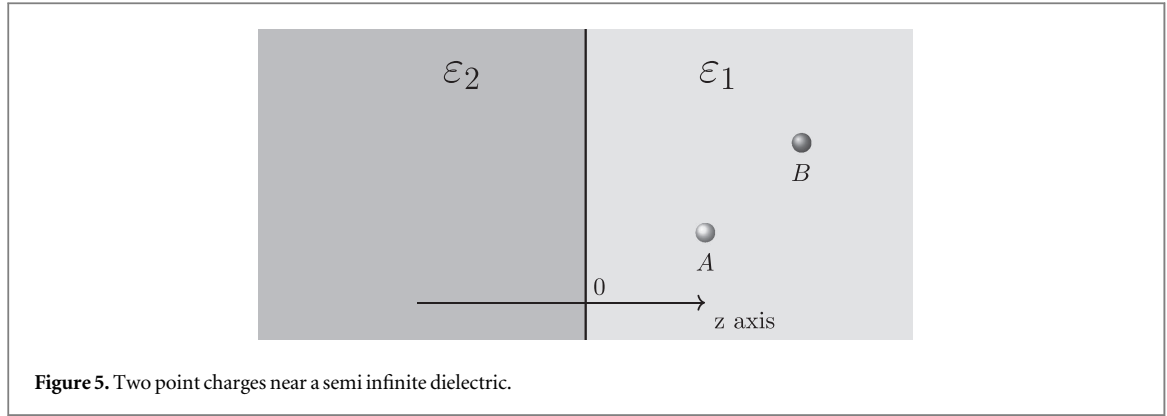


Figure 5. Two point charges near a semi infinite dielectric.

and the related corrected force:

$$F_A(z_A) = -\frac{q_A^2}{16\pi\epsilon_0\epsilon_1} \frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} \frac{3\epsilon_1}{2\epsilon_1 + 1} \frac{\hat{z}}{z_A^2}. \quad (56)$$

This can be interpreted in terms of the interaction between the real charge A and its image. The factor $1/2$ arises because the image charge is not a real charge, but rather an induced one.

Inserting the Green's function (54) into (35) we obtain the following Coulomb interaction between the two charges ($z_A, z_B > 0$):

$$U(\mathbf{r}_A, \mathbf{r}_B) = \frac{q_A q_B}{4\pi\epsilon_0\epsilon_1} \left(\frac{1}{|\mathbf{r}_A - \mathbf{r}_B|} - \frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} \frac{1}{|\mathbf{r}_A - \mathbf{r}_B^*|} \right), \quad (57)$$

where $\mathbf{r}_B^* = (x_B, y_B, -z_B)$ is the position of the image of charge B . The first term represents the free Coulomb interaction, while the second one represents the interactions between the real charge A and the image charge B^* .

The result (57) is well-known, however using our formalism we can introduce local-field effects at the level of the Green's function as described in section 5. The local-field corrected force on A reads:

$$\mathbf{F}_A(\mathbf{r}_A, \mathbf{r}_B) = -\frac{q_A q_B}{4\pi\epsilon_0\epsilon_1} \frac{3\epsilon_1}{2\epsilon_1 + 1} \nabla_A \left(\frac{1}{|\mathbf{r}_A - \mathbf{r}_B|} - \frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} \frac{1}{|\mathbf{r}_A - \mathbf{r}_B^*|} \right). \quad (58)$$

We also briefly comment on the case where one charge is embedded in a medium of dielectric constant ϵ_1 and the other charge embedded in the medium of dielectric constant ϵ_2 . In this case:

$$U(\mathbf{r}_A, \mathbf{r}_B) = \frac{q_A q_B}{2\pi\epsilon_0} \frac{1}{\epsilon_1 + \epsilon_2} \frac{1}{|\mathbf{r}_A - \mathbf{r}_B|}. \quad (59)$$

In particular if one medium is a perfect conductor (e.g. $\epsilon_1 \rightarrow \infty$), the two charges do not interact, since any photon emitted by one charge is completely reflected by the interface and does not reach the other charge. The local-field corrected force reads:

$$\mathbf{F}_A(\mathbf{r}_A, \mathbf{r}_B) = -\frac{q_A q_B}{2\pi\epsilon_0} \frac{1}{\epsilon_1 + \epsilon_2} \frac{3\epsilon_1}{2\epsilon_1 + 1} \nabla_A \frac{1}{|\mathbf{r}_A - \mathbf{r}_B|}. \quad (60)$$

The above results can easily be generalised to the case of a multi-layer medium. For the Green's function g_1 in the rightmost layer of an n -layer ($n - 1$ interface) stack whose layers are indexed by j one has (see, for examples, [9, 35]):

$$g_1(\rho, z, z') = \frac{1}{\epsilon_1} \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} - \frac{1}{4\pi\epsilon_1} \int_0^\infty dk R_1 e^{-k(z+z')} J_0(k\rho), \quad (61)$$

where J_0 is the zeroth-order Bessel function of the first kind, $\rho = \sqrt{(x - x')^2 + (y - y')^2}$, and the reflection coefficient R_1 is defined recursively via:

$$R_j = \frac{(\epsilon_{j+1} - \epsilon_j) + (\epsilon_{j+1} + \epsilon_j)e^{-2kL_{j+1}}R_{j+1}}{(\epsilon_{j+1} + \epsilon_j) + (\epsilon_{j+1} - \epsilon_j)e^{-2kL_{j+1}}R_{j+1}}, \quad (62)$$

where $j = 1 \dots n - 1$, and L_j is the thickness of layer j . The recursion is stopped by imposition of the termination condition $R_n = 0$, physically corresponding to there being no interface to reflect from (i.e. a zero-reflectivity boundary) after the final interface. For $n = 2$ it is trivial to reproduce the Green's function (54), and the recursive reflection coefficient allows large numbers of layers to be systematically taken into account.

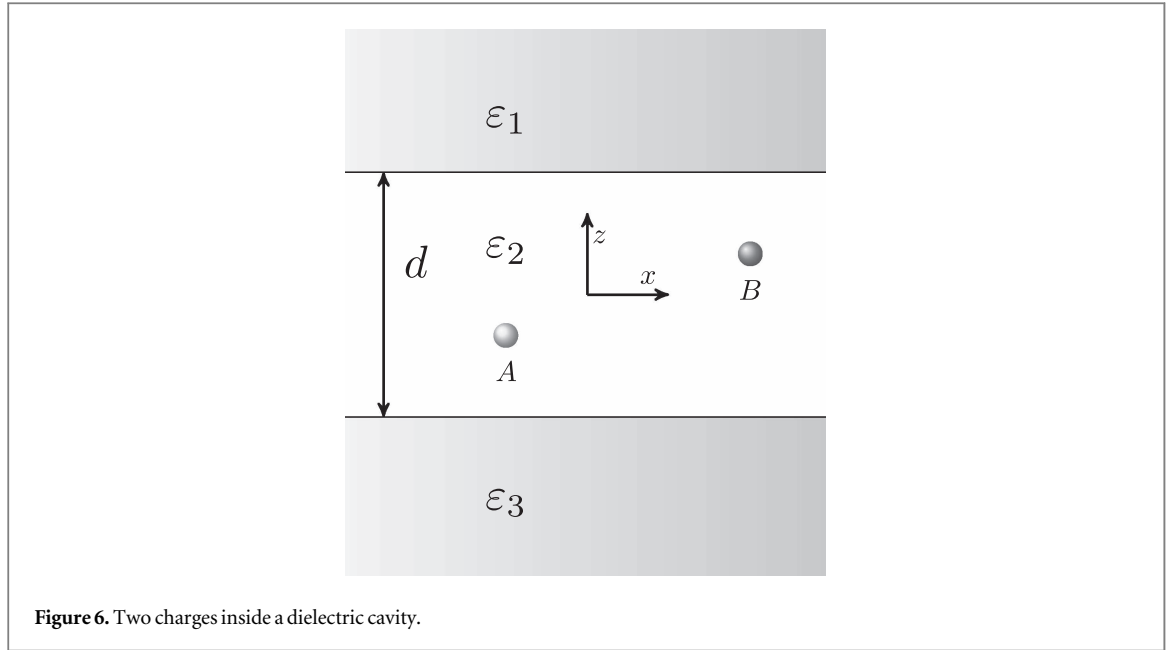


Figure 6. Two charges inside a dielectric cavity.

6.3. Cavity

Our next example is the Coulomb interaction between two charges in a cavity. We suppose that two charges are embedded in a medium with dielectric constant ε_2 and are near two other parallel semi-infinite dielectrics with relative permittivity ε_1 and ε_3 . The plane $z = 0$ is equidistant from the two dielectric surfaces, which are separated by a distance d , as shown in figure 6

At the midpoint between the plates ($z_A = z_B = 0$), the Green's function (see [appendix](#)) reads

$$g_2(\rho) = \frac{1}{4\pi\varepsilon_2} \int_0^\infty dk \frac{(1 - e^{-kd}R_1)(1 - e^{-kd}R_3)}{1 - e^{-2kd}R_1R_3} J_0(k\rho), \quad (63)$$

where R_1 and R_3 are the reflection coefficients for the two media bounding region 2;

$$R_1 = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}, \quad R_3 = \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 + \varepsilon_2} \quad (64)$$

and $\rho = \sqrt{(x_A - x_B)^2 + (y_A - y_B)^2}$. We can expand the denominator of (63) in a power series $(1 - e^{-2kd}R_1R_3)^{-1} = \sum_{n=0}^\infty (R_1R_3 e^{-2kd})^n$, which can then be integrated term-by-term

$$g_2(\rho) = \frac{1}{4\pi\varepsilon_2\rho} + \frac{1}{4\pi\varepsilon_2} \sum_{n=1}^\infty \frac{2(R_1R_3)^n}{\sqrt{d^2(2n)^2 + \rho^2}} - \frac{1}{4\pi\varepsilon_2} \sum_{n=0}^\infty \frac{(R_1R_3)^n(R_1 + R_3)}{\sqrt{d^2(2n+1)^2 + \rho^2}}. \quad (65)$$

Each term here can be interpreted as what one would have obtained using the image method, but the method outlined here and in the [appendix](#) is more convenient as in this case we would have to deal with an infinite series of images corresponding to multiple reflections.

Formula (65) is a new result, valid for arbitrary values of reflectivities R_1, R_3 , position ρ and cavity size d . To make contact with previous results [36, 37], we consider an asymptotic limit where the left and right surfaces are perfect conductors: $R_1 = R_3 = 1$, and the charges are separated by a much larger distance than that between the plates $\rho \gg d$, finding

$$g_2(\rho \gg d, R_1 = R_3 = 1) = \frac{1}{4\pi\varepsilon_2} \sqrt{\frac{8}{\rho d}} e^{-\pi\rho/d} \quad (66)$$

in agreement with [36, 37].

Since both charges are equidistant from the conducting surfaces ($z_A = z_B = 0$) the interaction between the charges and the surfaces vanishes, as one would expect from symmetry considerations. However the interaction between the two charges does not vanish. In particular for $\rho \gg d$, according to equation (35) the interaction reads:

$$U(\rho \gg d) = \frac{q_A q_B}{4\pi\varepsilon_0\varepsilon_2} \sqrt{\frac{8}{\rho d}} \exp\left(-\frac{\pi\rho}{d}\right). \quad (67)$$

Hence the cavity exponentially suppresses the Coulomb interaction at large distances. At small ρ (or equivalently large d) the interaction is just the Coulomb potential between two isolated charges

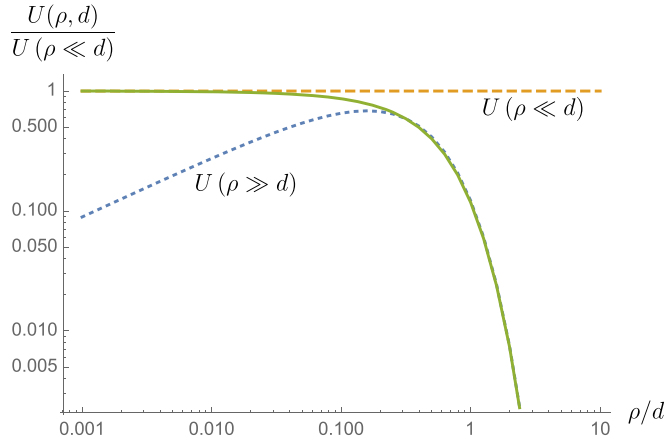


Figure 7. Coulomb interaction between two charges in vacuum at the midpoint of a perfectly reflecting cavity. At small distances the interaction is equal to the standard Coulomb result (68), and at large distances it is equal to the asymptotic result (67) where the interaction is exponentially suppressed.

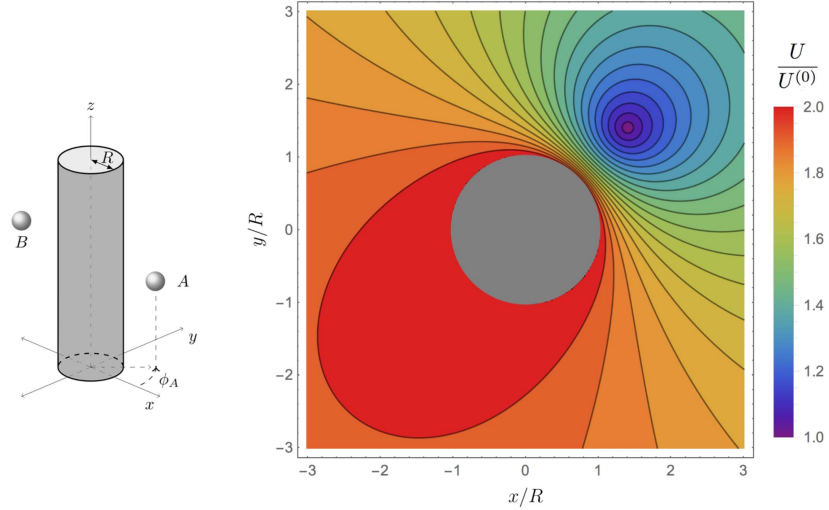


Figure 8. Left; two charges located near a perfect conducting cylinder of radius R . Right; Coulomb potential U of charge A in the xy plane. The charge B is placed at $\mathbf{r}_B/R = \{3/2, 3/2, 0\}$, and the resulting potential is scaled to that for the interaction potential $U^{(0)}$ of two charges in free space.

$$U(\rho \ll d) = \frac{q_A q_B}{4\pi\epsilon_0\epsilon_2\rho}, \quad (68)$$

which we plot in figure 7, alongside the large-distance asymptotic result (67) and the result obtained from numerical evaluation of (35) using (65). Finally, if the region inside the cavity has $\epsilon_2 \neq 1$, the local-field corrected force reads:

$$\mathbf{F}_A(\rho \gg d) = \frac{q_A q_B}{4\pi\epsilon_0\epsilon_2} \frac{3\epsilon_2}{2\epsilon_2 + 1} \frac{\sqrt{2}}{(\rho d)^{3/2}} \exp\left(-\frac{\pi\rho}{d}\right) (d + 2\pi\rho) \hat{\rho}. \quad (69)$$

6.4. Interaction between charges placed near a conducting wire

We now consider the Coulomb interaction near an infinitely long conducting wire of radius R , as shown in the left panel of figure 8. The scalar scattering Green's function g for such a setting is found (in agreement with [38]) to be;

$$g^{(1)}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{1}{2\pi^2} \sum_{m=-\infty}^{\infty} \int_0^{\infty} d\kappa \, e^{im(\phi_A - \phi_B) + i\kappa(z_A - z_B)} \frac{I_m(\kappa R)}{K_m(\kappa R)} K_m(\kappa\rho_A) K_m(\kappa\rho_B), \quad (70)$$

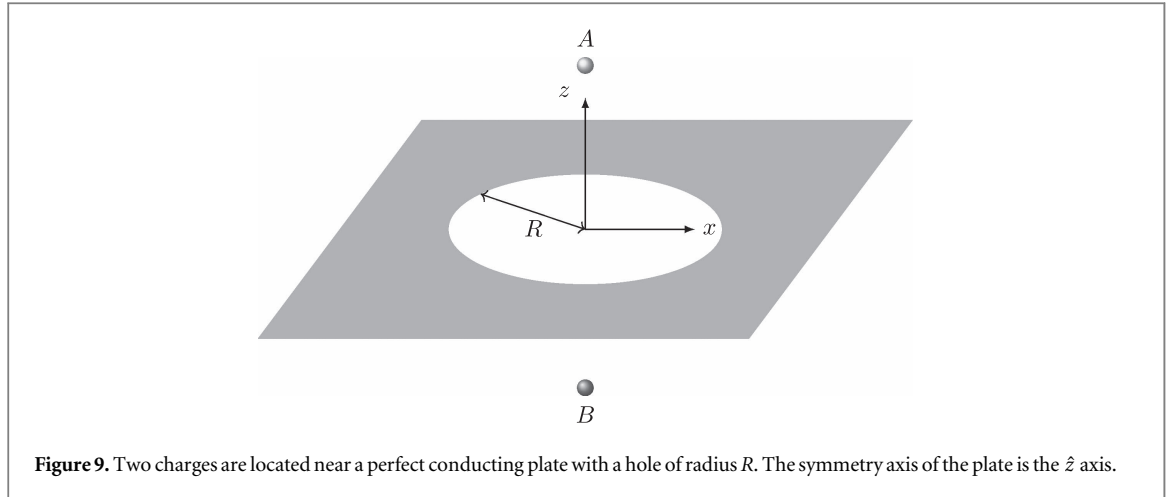


Figure 9. Two charges are located near a perfect conducting plate with a hole of radius R . The symmetry axis of the plate is the \hat{z} axis.

where $\rho = \sqrt{x^2 + y^2}$, $x = x_A - x_B$, $y = y_A - y_B$ and I_m, K_m are the m th modified Bessel functions of the first and second kind, respectively. The remaining coordinates are defined as shown in figure 8, where the Coulomb potential in the xy plane is plotted as a function of the position of charge B .

6.5. Plate with a hole

Finally we consider a more involved example, namely a perfect conducting plate with a hole of radius R , as shown in figure 9. Analogous problems involving the plate with a hole have been considered in the literature [39, 40]. This case is interesting from a technical point of view since it is not obvious how to locate the image charges to satisfy the boundary conditions, and interesting from an applied point of view due to its relevance to membranes. A hole or pore in the membrane of a biological cell can allow a variety of possibly ionised particles to enter [41]. The required Green's function may be obtained from the Kelvin inversion from the Green's function of the semi-infinite half-plane [38, 42]. However the expression obtained in [42] is valid for \mathbf{r} and \mathbf{r}' lying on the same side of the plate: $z, z' > 0$. Here we generalise the Green's function to include the case $z > 0, z' < 0$ as well, finding:

$$g(\mathbf{r}, \mathbf{r}') = \frac{1}{8\pi} \left\{ \frac{1}{D_-} \left[1 + \frac{2\lambda_-}{\pi} \arctan\left(\frac{F_-}{D_-}\right) \right] - \frac{1}{D_+} \left[1 + \frac{2\lambda_+}{\pi} \arctan\left(\frac{F_+}{D_+}\right) \right] \right\}, \quad (71)$$

where:

$$F_{\pm} = \frac{1}{\sqrt{2}R} \{ (\rho^2 + z^2 - R^2)(\rho'^2 + z'^2 - R^2) \mp 4R^2 z z' + \sqrt{(z^2 + (\rho - R)^2)(z^2 + (\rho + R)^2)} \times \sqrt{(z'^2 + (\rho' - R)^2)(z'^2 + (\rho' + R)^2)} \}^{1/2}, \quad (72)$$

$$D_{\pm} = \sqrt{\rho^2 + \rho'^2 - 2\rho\rho' \cos(\phi - \phi') + (z \pm z')^2}, \quad (73)$$

$$\lambda_{\pm} = \begin{cases} \text{sgn}[z'(\rho^2 + z^2 - R^2) + z(\rho'^2 + z'^2 - R^2)], & \text{if } z > 0, z' > 0, \\ -1, & \text{if } z > 0, z' < 0, \\ 1, & \text{if } z < 0, z' > 0, \\ \text{sgn}[z'(\rho^2 + z^2 - R^2) - z(\rho'^2 + z'^2 - R^2)], & \text{if } z < 0, z' < 0 \end{cases} \quad (74)$$

and (ρ, ϕ, z) represents the coordinates of \mathbf{r} in a cylindrical system where the symmetry axis of the hole is the z axis and the origin is at the centre of the hole. We will initially focus on the case where both charges are on the symmetry axis, and firstly quote the single-particle result found via equation (34)

$$U(z_A) = -\frac{q_A^2}{32\pi\epsilon_0 z_A} + \frac{q_A^2}{16\pi^2\epsilon_0 z_A} \arctan\left[\frac{R}{2z_A} - \frac{z_A}{2R}\right]. \quad (75)$$

The resulting interaction is shown in figure 10, where we have scaled with respect to the free interaction ($U^{(0)}(z_A) = -q_A^2/16\pi\epsilon_0 z_A$, i.e. the interaction for large distances).

The interaction is always attractive and vanishes in the limit $z_A \rightarrow 0$ for finite R , which is also clear from symmetry considerations. In the full-plate case ($R = 0$) the force diverges as $z_A \rightarrow 0$ since there we can construct the image charge which approaches the real charge. Hence in the limit $z_A \ll R$, for d finite, the

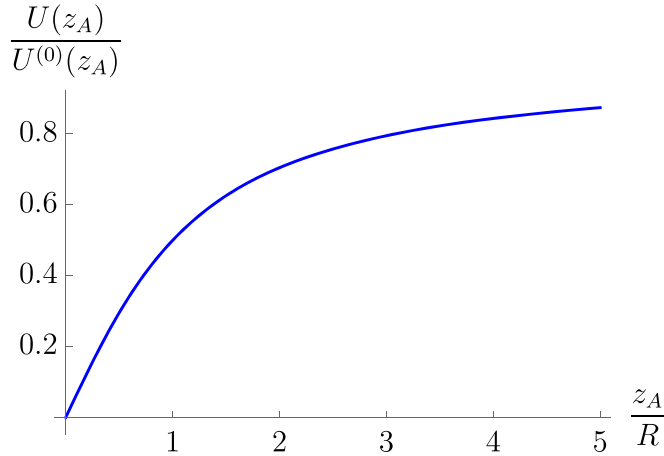


Figure 10. Coulomb interaction between an on-axis electron and the plate for $R \neq 0$. The interaction is scaled with respect to the function $U^{(0)}(z_A) = -q_A^2/16\pi\epsilon_0 z_A$.

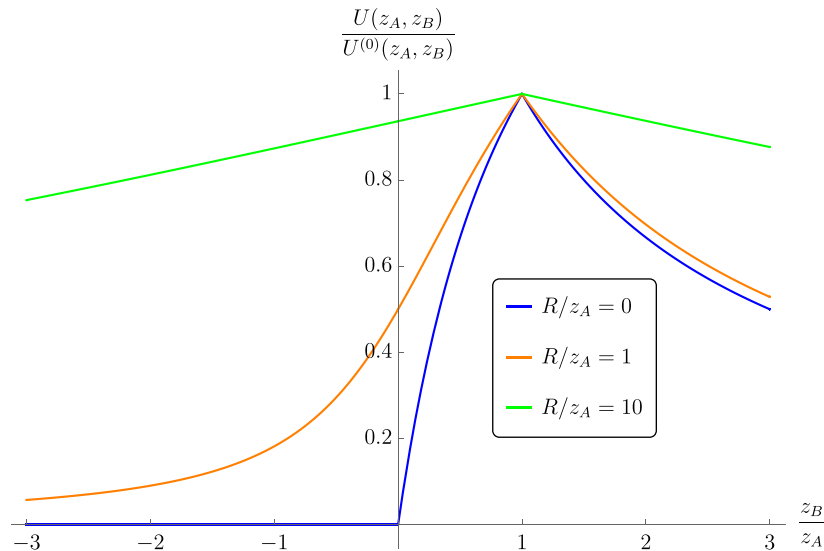


Figure 11. Coulomb interaction between two on-axis charges assisted by the plate. The interaction is scaled with respect to the free interaction $U^{(0)}(z_A, z_B) = 1/4\pi|z_A - z_B|$. We consider three different values of the radius: $R/z_A = 0, 1, 10$.

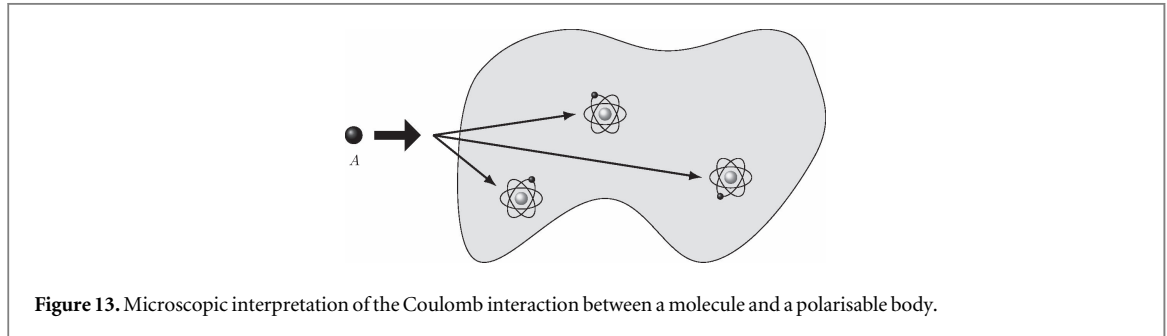
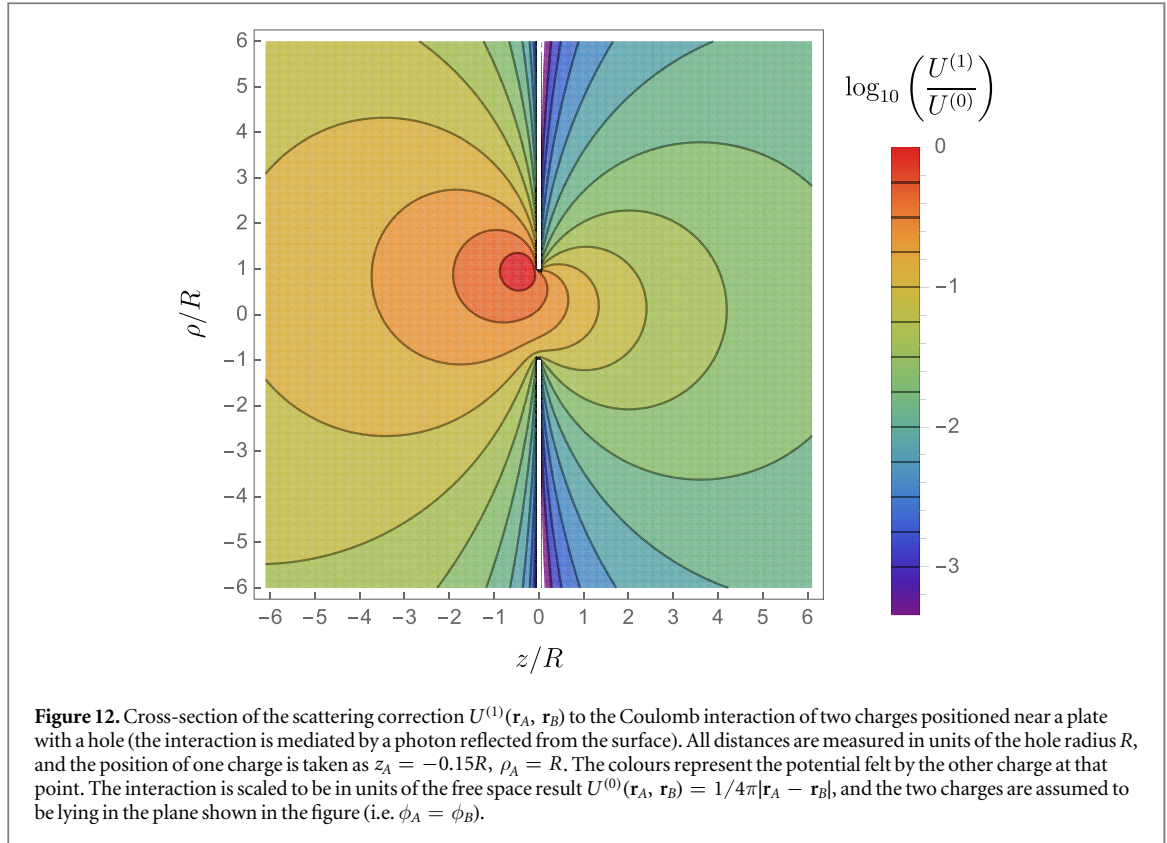
interaction with the surface can be neglected and we can focus only on the medium-assisted interaction between the two charges.

To calculate the interaction potential between the charges we suppose that one charge is on one side of the plate and we vary the position of the other charge. If the two charges are lying on the z axis on opposite sides of the plate: $z_A > 0$, $z_B < 0$ and $R \rightarrow 0$ we have $F_{\pm}/D_{\pm} \rightarrow +\infty$ and $\lambda_{\pm} = -1$, meaning that the interaction vanishes. This is to be expected since the plate is a perfect conductor, so any photon emitted by one charge is completely reflected by the surface, so the charges do not see each other. If R is finite a photon can travel from one side to the other, so we expect a non-vanishing interaction. In figure 11 we plot the this interaction energy for different value of the radius of the hole. The interaction is scaled with respect to the free interaction $U^{(0)}(z_A, z_B) = 1/4\pi|z_A - z_B|$. For a finite hole radius R there is a non-vanishing weak interaction also when $z_B < 0$.

To demonstrate the power and general applicability of our method we consider now the interaction between charges A and B when each charge may be located at any position. Directly using (35) in (71) we can produce the full three-dimensional interaction potential, which we show a slice of in figure 12;

6.6. Interaction between a charged particle and a polarisable molecule

Finally we consider what happens when a charged particle is placed near a polarisable medium, in which case the Coulomb field of the charged particle will polarise the molecules that constitute the medium. In the dilute limit



the Coulomb interaction between the charge and the surface can be described in microscopic terms, as arising from the Coulomb interaction of the charge and the individual molecules, as shown in figure 13.

It is well-known that for a dilute medium a Born expansion of the scattering Green tensor can be performed [10]:

$$\mathbf{G}^{(1)}(\mathbf{r}, \mathbf{r}', \omega) = \mu_0 \omega^2 \int d^3 r_B \eta(\mathbf{r}_B) \bar{\mathbf{G}}(\mathbf{r}, \mathbf{r}_B, \omega) \cdot \boldsymbol{\alpha}_B(\omega) \cdot \bar{\mathbf{G}}(\mathbf{r}_B, \mathbf{r}', \omega) + \dots, \quad (76)$$

where $\bar{\mathbf{G}}$ is the background Green's tensor, i.e. the Green's tensor in the absence of the dilute medium (which could be yet another medium), η is the number density and the integration is over the volume of the polarisable medium. Using equations (23), (30) we can write the Born expansion in terms of the scalar background Green's function \bar{g} :

$$g^{(1)}(\mathbf{r}, \mathbf{r}') = -\frac{1}{\varepsilon_0} \int d^3 r_B \eta(\mathbf{r}_B) \nabla_B \bar{g}(\mathbf{r}, \mathbf{r}_B) \cdot \boldsymbol{\alpha}_B(0) \cdot \nabla_B \bar{g}(\mathbf{r}_B, \mathbf{r}') + \dots \quad (77)$$

We substitute this expansion into the single-particle Coulomb interaction, equation (34):

$$U(\mathbf{r}_A) = \int d^3 r_B \eta(\mathbf{r}_B) U_{q-\alpha}(\mathbf{r}_A, \mathbf{r}_B), \quad (78)$$

where $U_{q-\alpha}(\mathbf{r}_A, \mathbf{r}_B)$ is the electrostatic interaction between a charged particle and a polarisable molecule in the presence of arbitrary media as background (with the background Green's function now denoted as g):

$$U_{q-\alpha}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{q_A^2}{2\varepsilon_0^2} \nabla_B g(\mathbf{r}_A, \mathbf{r}_B) \cdot \boldsymbol{\alpha}_B(0) \cdot \nabla_B g(\mathbf{r}_B, \mathbf{r}_A). \quad (79)$$

In free space, since $g^{(0)}(\mathbf{r}_A, \mathbf{r}_B) = 1/4\pi|\mathbf{r}_A - \mathbf{r}_B|$ we find:

$$U_{q-\alpha}^{(0)}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{q_A^2}{32\pi^2\varepsilon_0^2} \frac{\mathbf{r} \cdot \boldsymbol{\alpha}_B(0) \cdot \mathbf{r}}{r^6} \quad (80)$$

and $\mathbf{r} = \mathbf{r}_A - \mathbf{r}_B$. This expression is well-known in the literature for the special case of isotropic particles [43], in which case one has;

$$U_{q-\alpha}^{(0)}(r) = -\frac{q_A^2 \alpha_B(0)}{32\pi^2\varepsilon_0^2 r^4}. \quad (81)$$

Our result (79) generalises this to anisotropically polarised particles, as well as being applicable to any geometry. For example, the interaction between a charged particle and a polarisable molecule near a perfectly conducting surface can be found by using in equation (79) the result of an image construction $g(\mathbf{r}_A, \mathbf{r}_B) = g^{(0)}(\mathbf{r}_A, \mathbf{r}_B) + g^{(1)}(\mathbf{r}_A, \mathbf{r}_B)$, where $g^{(1)}(\mathbf{r}_A, \mathbf{r}_B) = -1/4\pi|\mathbf{r}_A - \mathbf{r}_B^*|$, $\mathbf{r}_B^* = (x_B, y_B, -z_B)$. The scattering Green's function $g^{(1)}$ corresponds to the interaction between the charge and the image dipole of the polarisable molecule. In fact in equation (79) the interaction can be easily interpreted: the photon propagates from the charge A to the polarisable molecule B , directly or after a reflection (these processes being described with the propagator $g(\mathbf{r}_B, \mathbf{r}_A)$), is reflected by the polarisable molecule, and finally absorbed by the charge A . Hence the interaction between the charge and the polarisable molecule is a two-photon process.

7. Conclusions and outlook

In this article we have developed a systematic and unified description of Coulomb interactions of charges in non-trivial environments. The presence of the environment is included via the classical Green's tensor, or also in a simpler fashion in terms of the Green's function.

Our approach can be applied to non-trivial geometries where it is not possible or practical to find the suitable image charges, we have demonstrated this via the examples of the plate with a hole and a wire. Using the same framework, we have shown examples where the environment significantly changes the interaction, for example by exponentially suppressing it in the dielectric cavity geometry. We have quantified how the Coulomb interaction can be significantly tuned by changing the geometric and dielectric parameters of the environment, many more cases of which could be investigated, all within the formalism presented here.

Thus the outlook from this work is to apply the formalism to important practical examples. For example, we have considered only neutral environments here, while without much extra complication one could consider environments which carry a net charge, like for example ionic solutions. We have also considered only stationary charges, in which case there is no real complication associated with the instantaneous nature of the Coulomb interaction. A time-dependent model could be developed to include retardation effects thereby satisfying causality requirements and opening up our work to the study of moving charges.

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Appendix. Green's function of a cavity

We consider the cavity configuration in figure 6. The dielectric constant is:

$$\varepsilon(z, \rho) = \begin{cases} \varepsilon_1, & \text{if } z < -d/2 \\ \varepsilon_2, & \text{if } -d/2 < z < d/2, \\ \varepsilon_3, & \text{if } z > d/2 \end{cases} \quad (A.1)$$

where ρ is the radial component of a cylindrical co-ordinate system. A point charge is placed at $z = z_0$ in the central region, which induces surface charges at the interfaces. The corresponding source-term of the Green function is:

$$\frac{1}{4\pi\epsilon_2|\mathbf{r} - \mathbf{r}_0|} = \frac{1}{4\pi\epsilon_2} \int_0^\infty dk J_0(k\rho) e^{-k|z-z_0|}, \quad (\text{A.2})$$

where J_n is the n th Bessel function of the first kind. In the central region the Green's function consists in a superposition of rising and falling exponentials, as well a term stemming from the point source:

$$g_2(\rho, z, z_0) = \frac{1}{4\pi\epsilon_2} \int_0^\infty dk J_0(k\rho) (a(k)e^{-k(z-z_0)} + b(k)e^{k(z-z_0)} + e^{-k|z-z_0|}), \quad (\text{A.3})$$

where $a(k)$ and $b(k)$ are coefficients to be found. In the left region we have only rising exponential since the Green's function must vanish for $z \rightarrow -\infty$:

$$g_1(\rho, z, z_0) = \frac{1}{4\pi\epsilon_2} \int_0^\infty dk J_0(k\rho) c(k) e^{k(z-z_0)} \quad (\text{A.4})$$

while in the right region:

$$g_3(\rho, z, z_0) = \frac{1}{4\pi\epsilon_2} \int_0^\infty dk J_0(k\rho) d(k) e^{-k(z-z_0)}, \quad (\text{A.5})$$

where $c(k)$ and $d(k)$ are coefficients not yet determined. In order to find the four unknown coefficients $a(k)$, $b(k)$, $c(k)$, $d(k)$ we impose the condition from Maxwell's equations that the Green's function and the normal component of the displacement vector \mathbf{D} are continuous across the interface between the media:

$$\begin{aligned} g_1(0, -d/2, z_0) &= g_2(0, -d/2, z_0) \\ \epsilon_1 \partial g_1 / \partial z(0, -d/2, z_0) &= \epsilon_2 \partial g_2 / \partial z(0, -d/2, z_0) \\ g_2(0, d/2, z_0) &= g_3(0, d/2, z_0) \\ \epsilon_2 \partial g_2 / \partial z(0, d/2, z_0) &= \epsilon_3 \partial g_3 / \partial z(0, d/2, z_0). \end{aligned} \quad (\text{A.6})$$

Solving the resulting system of equations allows one to eliminate the four unknowns, the result for the Green's function in the central region is, for $z \geq z_0$:

$$g_2(\rho, z, z_0) = \frac{1}{4\pi\epsilon_2} \int_0^\infty dk e^{-k(z-z_0)} \frac{(1 - e^{-k(d+2z_0)} R_1)(1 - e^{-k(d-2z)} R_1)}{(1 - e^{-2kd} R_1 R_3)} J_0(k\rho), \quad (\text{A.7})$$

where R_1 and R_3 are the reflection coefficients for the left and right media, as shown in equation (64).

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