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Quantum electrodynamics in the presence of a dielectric

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Abstract

We discuss the formulation of quantized macroscopic electrodynamics interacting with Dirac particles. In particular, we consider the case of a dielectric half-space characterized by a constant, i.e. frequency-independent refractive index n . In contrast to perfectly reflecting boundary conditions, the matching conditions for the field strengths at the surface of the dielectric lead to the appearance of evanescent waves, and their presence modifies the representation of the photon propagator considerably. As an example of a one-loop calculation we determine the self-energy of a free electron on the vacuum side of the boundary. We find that in the limit of perfect reflectivity of the surface the self-energy disagrees with the one that emerges from calculations that assume perfect reflectivity from the outset. We develop calculational techniques for coping with problems that arise specifically due to the imperfect reflection at the surface.

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Quantum Electrodynamics is one of the fundamental theories of nature and the simplest and best studied gauge theory. In elementary particle theory it is in the simplest case formulated as a theory of electrons and photons. However in other fields—like quantum optics—a more phenomenological formulation is important. There part of matter may be represented macroscopically by a dielectric. In general this dielectric and its properties are described by a complex and frequency-dependent dielectric function satisfying Kramers–Kronig relations. Thus dispersion necessarily goes hand in hand with absorption, and the degrees of freedom that cause the absorption must be taken into account explicitly when constructing a field theory. That is why quantized theories of the electromagnetic field in the presence of a dispersive dielectric are quite complicated [1, 2], and not surprisingly even more so if one couples in another particle [3].

However, there are a broad range of problems whose physics does not depend on the dispersive properties of the dielectric material, and for those one can construct a theory of

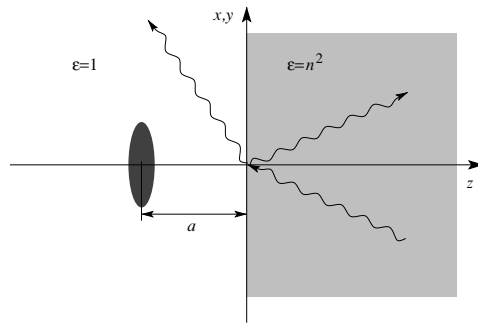


Figure 1. The left half-space is filled by vacuum, and the right by a non-dispersive dielectric. Depending on their angle of incidence, right-incident modes can be evanescent on the vacuum side. The electron is localized in a wave packet whose centre is a distance a away from the interface.

quantized macroscopic electrodynamics with less trouble by turning to a model with a non-dispersive and non-absorbing dielectric. In that case one can resort to much of the standard repertoire of quantum electrodynamics when it comes, for example, to the determination of radiative corrections or to the elimination of divergences.

While the model of a non-dispersive and non-absorbing dielectric is of course a severe and partially unphysical idealization (because any real material has to be transparent at infinite frequency), it is one step better than a perfect-reflector model in allowing for imperfect reflectivity and also for evanescent waves. However, either model can sensibly be applied only to systems and processes whose dynamics are governed by a finite frequency range for which the dielectric response of the material can be approximated by a constant. For Casimir–Polder type problems of a particle or atom located at a distance a away from a surface and interacting with it, the relevant frequencies are of order $2\pi/a$, which is normally very small since a tends to be much larger than optical wavelengths, so that only the static dielectric response matters for the interaction. Hence such problems are well suited to be studied within a non-dispersive and non-absorbing model for the dielectric.

Free field theories with a variety of dielectric or plasma surfaces as boundaries are widely discussed in Casimir-like problems [4, 5]. Our aim is to go beyond the study of the free field, and give an example of a one-loop calculation for a Dirac particle interacting with the electromagnetic field [6]. As a simple model system we consider a dielectric half-space with constant refractive index n , so that the dielectric function is a step function

$$\epsilon(\mathbf{r}) = 1 + (n^2 - 1)\Theta(z). \quad (1)$$

The classical electromagnetism of this system is treated in textbooks. Maxwell’s equations imply that the tangential components of the electric field \mathbf{E} and of the magnetic field \mathbf{H} and the normal components of the dielectric displacement \mathbf{D} and of the magnetic induction \mathbf{B} have to be continuous across the interface at $z = 0$. The two polarizations of an electromagnetic wave can then be represented as transverse electric (TE) and transverse magnetic (TM) waves, and solutions to the wave equation can be expressed in terms of an incoming and a reflected wave on one side of the interface and a transmitted wave on the other side (see figure 1). The reflection and transmission amplitudes of these waves are then the standard Fresnel coefficients.

For a quantum field theoretical treatment we need a formulation in terms of the gauge potential. As the gauge condition we use the generalized Coulomb gauge condition

$$\nabla \cdot (\epsilon \mathbf{A}) = 0, \quad (2)$$

which is widely adopted in quantum optics. Alternatively, one could adopt a generalized covariant condition [6]. The generalized Coulomb gauge may cause problems exactly on the interface, where the gauge condition is not well defined because of the discontinuity in the dielectric function. However, Barton [7] has shown that a unitary transformation can be found that resolves any such difficulties with surface-bound divergences. For the purposes of the present work it suffices to note that away from the interface the generalized Coulomb gauge is simply equivalent to the standard Coulomb gauge.

We quantize our system in terms of left-incident and right-incident waves $A^\mu = A_L^\mu + A_R^\mu$, which form an orthogonal [8] and complete [9] set of modes in Hilbert space. For example, the right-incident mode reads

$$A_R^\mu(x) = \sum_{\sigma=TE, TM, G, C} \int \frac{d^3\mathbf{k}^d \theta(-k_z^d)}{(2\pi)^{3/2} (2\omega)^{1/2}} \left\{ e_\sigma^\mu \exp(-ix^0 k^0) a_{\mathbf{k},\sigma}^R \left[\theta(z) \frac{1}{n} (\exp(i\mathbf{k}^d \cdot \mathbf{r}) + R_\sigma^R(k) \exp(i\mathbf{k}^{r,d} \cdot \mathbf{r})) + \theta(-z) T_\sigma^R(k) \exp(i\mathbf{k} \cdot \mathbf{r}) \right] + \text{h.c.} \right\}. \tag{3}$$

Here $a_{\mathbf{k},\sigma}^R$ is the photon annihilation operator of the mode, and $R_\sigma^R(k)$ and $T_\sigma^R(k)$ are its reflection and transmission coefficients.

As dictated by the laws of refraction, we have equal frequencies but different k -vectors on the two sides of the vacuum–dielectric interface. The wave vector on the vacuum side is denoted by \mathbf{k} , and the one on the dielectric side by \mathbf{k}^d . The reflected wave vectors \mathbf{k}^r and $\mathbf{k}^{r,d}$ differ from \mathbf{k} and \mathbf{k}^d , respectively, by the relative signs of their z components. The wave vector components \mathbf{k}_\parallel parallel to the interface are of course always the same within one and the same mode, just the z components differ on the two sides of the interface. Denoting the z component on the vacuum side by k_z and that on the dielectric side by k_z^d , we have

$$k_z = \begin{cases} \text{sgn}(k_z^d) \frac{1}{n} \sqrt{k_z^{d2} - (n^2 - 1)k_\parallel^2} & \text{for } k_z^{d2} - (n^2 - 1)k_\parallel^2 > 0, \\ -i \frac{1}{n} \sqrt{-k_z^{d2} + (n^2 - 1)k_\parallel^2} & \text{for } k_z^{d2} - (n^2 - 1)k_\parallel^2 < 0. \end{cases}$$

Thus, for right-incident modes the integration over \mathbf{k}^d includes imaginary values of k_z , which corresponds to modes that come from inside the dielectric, suffer total internal reflection at the interface, and are evanescent on the vacuum side.

When it comes to the quantization of the system several important points have to be taken into account:

- (i) In the generalized Coulomb gauge the mode decomposition includes just the two physical modes, i.e. the TE and TM modes, but in the generalized ‘covariant’ gauge one has to include in addition the gauge mode G and the longitudinal Coulomb mode C.
- (ii) The polarization vectors e_σ^μ are best chosen as differential operators, because this facilitates the representation of the vector field modes in terms of scalar modes.
- (iii) It is essential that the evanescent waves are included, because they are needed for the completeness of the modes.

For a perturbative treatment of the theory we need propagators and vertex factors. We assume that the electron is sufficiently far away from the dielectric so that there is no direct wavefunction overlap with the matter making up the dielectric. Then the only building block of the theory that is directly affected by the presence of the dielectric is the photon propagator. Using the mode decomposition in terms of TE and TM waves mentioned above and taking into consideration various analytical properties of the reflection and transmission coefficients,

we find [6] that the photon propagator be expressed in terms of scalar propagators $D_\sigma^c(x, x')$ for each mode:

$$D^{\mu\nu c}(x, x') = \sum_\sigma e_\sigma^\mu(\partial_x) e_{\sigma^*}^{\nu*}(\partial_{x'}) g^{\sigma\sigma} D_\sigma^c(x, x').$$

with

$$\begin{aligned} D_\sigma^c(x, x') = & - \int \frac{d^3\tilde{k}}{(2\pi)^4} e^{-i(\tilde{x}-\tilde{x}')\tilde{k}} \left\{ \theta(z)\theta(z') \int_{-\infty}^{\infty} dk_z^d [e^{ik_z^d(z-z')} + e^{-ik_z^d(z+z')} R_\sigma^R] \right. \\ & \times \frac{1}{n^2 k_0^2 - k_p^2 - k_z^{d2} + i\epsilon} \\ & + \theta(-z)\theta(-z') \left[\int_{-\infty}^{\infty} dk_z e^{ik_z(z-z')} + \int_{\mathcal{C}} dk_z e^{ik_z(z+z')} R_\sigma^L \right] \frac{1}{k^2 + i\epsilon} \\ & + \theta(z)\theta(-z') \frac{1}{n} \int_{-\infty}^{\infty} dk_z^d e^{-ik_z z' + ik_z^d z} T_\sigma^{R*} \frac{1}{k_0^2 - (k_p^2 + k_z^{d2})/n^2 + i\epsilon} \\ & \left. + \theta(-z)\theta(z') \frac{1}{n} \int_{-\infty}^{\infty} dk_z^d e^{ik_z z - ik_z^d z'} T_\sigma^R \frac{1}{k_0^2 - (k_p^2 + k_z^{d2})/n^2 + i\epsilon} \right\}, \end{aligned} \quad (4)$$

where the integrations path \mathcal{C} runs along the real axis from $-\infty$ to 0 , then down the negative imaginary axis from 0 to $-i\Gamma/n$ to the left of the square root cut, back up to the origin to the right of the cut, and then along the real axis from 0 to $+\infty$. The cut is due to $k_z^d = (n^2 k_z^2 + (n^2 - 1)k_\parallel^2)^{1/2}/n$ and extends from $k_z = +i\Gamma/n$ to $k_z = -i\Gamma/n$.

In an alternative formulation one can rewrite the photon propagator by replacing the third line of (4) by

$$\theta(-z)\theta(-z') \left[\int_{-\infty}^{\infty} dk_z e^{ik_z(z-z')} + \int_{-\infty}^{\infty} dk_z e^{ik_z(z+z')} R_\sigma^L + \int_{-\Gamma}^0 dk_z^d e^{ik_z z - ik_z^d z'} T_\sigma^{R*} T_\sigma^R \right] \frac{1}{k^2 + i\epsilon}. \quad (5)$$

With equations (4) and (5) we have obtained a closed expression for the photon propagator in terms of scalar mode-specific T functions. The evanescent modes are included either by a deformation of the integration path in the complex k_z plane, as in (4), or by explicit addition of an integral over the region of pure imaginary-valued k_z , as in (5).

Now we are in the position to start with perturbative loop calculations using standard Feynman rules: our photon propagator is more complicated than in free space and lacks translation invariance in z direction, but the vertex factor and the electron propagator are the same as in free space, since we have made the reasonable assumption that the electron does not interact with the matter making up the dielectric in any direct way³. Therefore we must assume that the electron is located outside the dielectric and at least several Compton wavelengths away from it. As an example of a 1-loop calculation we have determined the self-energy of a Dirac electron.

$$\Sigma_{\alpha\beta}^{(\text{radiative})}(x, x') = -i e^2 \gamma_{\alpha\kappa}^\mu S_{\kappa\lambda}^{(0)}(x - x') \gamma_{\lambda\beta}^\nu D_{\mu\nu}^c(x, x'). \quad (6)$$

In Coulomb gauge, where the photon propagator is made up of contributions from the TE and TM modes, this is in fact only the radiative self-energy. The electrostatic self-energy

³ If there was direct wave-function overlap between the electron and the atoms making up the dielectric then we could not use macroscopic electromagnetism, i.e. we could not describe the properties of the dielectric solely by its reaction to macroscopic fields.

must be calculated separately. This is, however, a relatively simple calculation whose result of course agrees with the classical energy of a charge and its image on the other side of the interface [10]. From equations (4) and (5) it is obvious that the photon propagator in the presence of the dielectric half-space is in fact a sum of the standard free-space propagator and a boundary-dependent correction. One also notices that divergences arise only through the free-space part, so that renormalization is the same as in the free space and loop calculations involving only the boundary-dependent part are finite if one works with already renormalized parameters. However, there can of course arise additional new divergences directly on the boundary, but these are of no relevance to the calculation of physical quantities away from the boundary.

The lack of translation invariance in z -direction is a severe technical complication. Our photon propagator and thus the self-energy depend separately on $x^3 - x'^3$ and $x^3 + x'^3$. To deal with this complication, we first note that in order to calculate physically meaningful quantities, i.e. an effective-mass correction which depends on the distance of the electron from the surface, we need to localize the electron in some sort of wave packet. If the centre of that packet is at $x^3 = -a$, we can approximate $x^3 + x'^3 \approx -2a$, while not approximating $x^3 - x'^3$. A Fourier transform of $\Sigma(x - x', x^3 + x'^3 \approx -2a)$ with respect to $x - x'$ leads to $\Sigma(p, -2a)$, which can be determined [6]. Since the distance a of the electron from the surface is supposed to be much larger than the Compton wavelength, we are in fact interested in an asymptotic expression to leading order in $1/(p_0a)$. With the electrostatic self-energy already included the result for the total self-energy is⁴

$$\Sigma(p, -2a) \simeq -\frac{e^2}{32\pi p_0a} \left[\gamma_{\parallel} \cdot \mathbf{p}_{\parallel} \frac{n^2(n^2 - 1)}{(n^2 + 1)^2} + 2\gamma_3 p_z \frac{2n^4 - n^2 - 1}{(n^2 + 1)^2} + 2\gamma_0 p_0 \frac{n^2 - 1}{n^2 + 1} \right]. \quad (7)$$

In deriving this result one encounters several issues that are characteristic of problems with imperfectly reflecting boundaries. First, one meets double integrals—effectively over the photon frequency ω and over the angle of incidence θ —whose convergence is due to factors like $\exp(4ip_0a\omega \cos\theta)$ or $\exp(-4ip_0a\omega \cos\theta)$ after Wick rotation. ω runs from 0 to ∞ , and $\cos\theta$ runs from 0 to 1. Obtaining an asymptotic approximation for large p_0a in one-dimensional integrals with this sort of factor is normally very easy; one simply integrates by parts. In the two-dimensional case this strategy does not work because integration by parts in the ω integral generates not just inverse powers of p_0a as desired but also inverse powers of $\cos\theta$ which destroy the convergence at the lower limit of the integral over $\cos\theta$. Vice versa, integration by parts in the integral over $\cos\theta$ generates unwanted inverse powers of ω which cause the resulting ω integral to diverge at the lower limit. The way out of this dilemma is to make the other parts of the integrand linear in $\cos\theta$ or ω by separating off the respective first terms in their Taylor expansions around the points $\cos\theta = 0$ or $\omega = 0$ and treating those separately [11]. The problem arises because the argument of the exponential has a saddle point in a corner of the domain of integration, and the general remedy is to subtract this point, treat it separately, and use Stokes' theorem for two-dimensional integration by parts in the remaining integral [12].

Furthermore, it is worthwhile pointing out that the limit $n \rightarrow \infty$ of our results does not agree with what one would obtain if one calculated the same quantity in a model that assumes a perfectly reflecting boundary from the outset. We have discussed this issue extensively in [13]. This discrepancy is due to the non-interchangeability of the limits $n \rightarrow \infty$ and photon frequency $\omega \rightarrow 0$. Physically it has to do with the presence of evanescent waves and the fact that the electron is unbound, which means that the integral over excitation energies of the

⁴ For a full derivation of this result by means of relativistic quantum electrodynamics see [6]; the equivalent non-relativistic derivation can be found in [13].

electron runs from zero. For e.g., an atom interacting with a surface, this problem does not arise because the transition to another atomic state has a natural IR cutoff for a bound electron. Note also that this issue is unrelated to the observation that there seem to be two ways of imposing perfectly reflecting boundary conditions, depending on one's choice of gauge and polarization vectors and interpreted as representing 'thick' or 'thin' boundaries [14].

Another important example of loop calculations for a Dirac particle near a dielectric surface are vertex corrections, which have an impact on g-2 corrections [15]. For perfect boundaries the boundary-dependent g-2 corrections are well investigated [16], but in the light of [13] one can expect different results for an unbound particle close to imperfect boundaries.

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