## Two definitions of the electric polarizability of a bound system in relativistic quantum theory

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## Two definitions of the electric polarizability of a bound system in relativistic quantum theory

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For the electric polarizability of a bound system in relativistic quantum theory, there are two definitions that have appeared in the literature. They differ depending on whether or not the vacuum background is included in the system. A recent confusion in this connection is clarified. © 1999 American Association of Physics Teachers.

Recently three papers appeared in this journal discussing the electric polarizability (EP) of a relativistic bound system.<sup>1–3</sup> In Refs. 1–3 it was illustrated by model calculations that the EP of a relativistic system can be negative when the interaction that binds the system is very strong. The model used in Refs. 1–3 is a particle that is bound in a given potential in one dimension and subject to the Dirac equation. Reference 3 presents interesting discussions on effects of the vacuum background on the EP on the basis of Dirac's hole theory (HT).

The purpose of this note is to point out that the definition of the EP that was assumed in Refs. 1-3 is different from the one that was used in earlier papers.<sup>4,5</sup> The two definitions differ depending on whether or not the vacuum background is regarded as part of the system. We are not going to argue that one is correct and the other is wrong but we have to be clear about the distinction between the two. Unfortunately the two definitions are apparently confused in Ref. 3; see the remark at the end of this note. As we emphasize below, if the vacuum background is included, the EP is positive no matter how strong the binding interaction is.

Consider a bound system like the hydrogen atom. When it is perturbed by an external electric field, the system is polarized and its energy shifts. Assume that the electric field  $\mathbf{E}$  is constant and weak. Then the energy shift *W* takes the form

$$W = -\frac{1}{2}\alpha \mathbf{E}^2. \tag{1}$$

This W is nothing but the second-order energy shift caused by the perturbation due to **E**. The coefficient  $\alpha$  is the EP of the system. This is how the EP is defined but there can be different definitions depending on how the system is interpreted. In Refs. 1–3 the bound system was regarded as a single particle system, a particle bound in a given potential. In quantum field theory (QFT) or equivalently in HT, in addition to the bound particle, the vacuum background is considered. When the vacuum background is interpreted as an integral part of the bound system, it is no longer a single particle system. This is how the bound system is treated in Refs. 4 and 5.

Let us elaborate on the two definitions. As a way of setting up notation, let us start with the problem as that of the singleparticle quantum mechanics. Let the Hamiltonian be

$$H = H_0 + V, \tag{2}$$

where  $H_0$  is the Dirac Hamiltonian with a binding potential and V is the external perturbation. More explicitly,  $V = -q \mathbf{E} \cdot \mathbf{r}$  where q is the charge of the particle. We take  $H_0$  as the unperturbed Hamiltonian and treat V by perturbation theory. It is understood that the solutions of the Dirac equation with  $H_0$  are known for all stationary states,

$$H_0|i\rangle = \epsilon_i|i\rangle, \quad H_0|-j\rangle = \epsilon_{-j}|-j\rangle,$$
(3)

where i=1,2,... and -j=-1,-2,.... The  $|i\rangle$ 's  $(|-j\rangle$ 's) are positive (negative) energy states;  $\epsilon_i > 0$  ( $\epsilon_{-j} < 0$ ). In particular  $|1\rangle$  is the lowest positive energy state. We are assuming that the eigenvalues are all discrete but it is straightforward to include the continuum. The  $|i\rangle$ 's and  $|-j\rangle$ 's form a complete orthonormal basis set. For the unperturbed state, let us take  $|1\rangle$ , the state of the lowest positive energy.<sup>6</sup> The secondorder energy shift  $W_{\rm QM}$  of state  $|1\rangle$  caused by perturbation V is given by

$$W_{\rm QM} = \sum_{i \neq 1} \frac{|V_{i,1}|^2}{\epsilon_1 - \epsilon_i} + \sum_j \frac{|V_{-j,1}|^2}{\epsilon_1 - \epsilon_{-j}},\tag{4}$$

where  $V_{i,1} \equiv \langle i | V | 1 \rangle$  and  $V_{-j,1} \equiv \langle -j | V | 1 \rangle$ . The suffix QM refers to single-particle quantum mechanics. The summation for *i* (*j*) is for the positive (negative) energy intermediate states. The contributions from the negative energy intermediate states can make  $W_{\text{OM}}$  positive.<sup>1–3</sup>

Let us examine the vacuum background following Ref. 3. In HT the vacuum is such that all negative energy states are occupied. We replace  $W_{OM}$  obtained above with

$$W_1 = \sum_{i \neq 1} \frac{|V_{i,1}|^2}{\epsilon_1 - \epsilon_i},\tag{5}$$

where the Pauli principle excludes the negative energy states as intermediate states. On the other hand the vacuum energy also shifts. The vacuum energy shift is given by

$$W_{\text{vac}} = \sum_{j} W_{-j}, \quad W_{-j} = \sum_{i \neq 1} \frac{|V_{i,-j}|^2}{\epsilon_{-j} - \epsilon_i}.$$
 (6)

Again the summation over i(j) is for positive (negative) energy states. The intermediate state of i=1 is excluded because it is already occupied. If we interpret that the vacuum

background is part of the system, the total energy shift is given by  $^{7}$ 

$$W_{\rm HT} = W_1 + W_{\rm vac} \,. \tag{7}$$

The  $W_1$  and  $W_{\text{vac}}$  are both negative and hence  $W_{\text{HT}}$  is negative.

As shown in Ref. 3,  $W_{\rm HT}$  can be rewritten as

$$W_{\rm HT} = W_{\rm QM} + W_{\rm vac}', \tag{8}$$

$$W'_{\text{vac}} = \sum_{j} W'_{-j}, \quad W'_{-j} = \sum_{i} \frac{|V_{i,-j}|^2}{\epsilon_{-j} - \epsilon_i}.$$
 (9)

The restriction  $i \neq 1$  has been removed in the *i*-summation for  $W'_{-j}$ . The  $W'_{vac}$  is the vacuum energy shift *in the absence* of the particle in  $|1\rangle$ . The  $W_{HT}$  of Eq. (8) contains terms that violate the Pauli principle but such terms all cancel out. This is an interesting illustration of Feynman's time-honored trick.<sup>8</sup>

In QFT no negative energy particles appear but antiparticles of positive energies appear instead. The unperturbed state that we consider is  $c_1^{\dagger} | vac \rangle$ . Here  $|vac \rangle$  is the state that contains no particles or antiparticles at all. The energy of this unperturbed vacuum is zero. The  $c_1^{\dagger}$  is an operator that creates a particle with energy  $\epsilon_1$  and wave function associated with  $|1\rangle$ . The  $|vac\rangle$  and  $c_1^{\dagger} | vac \rangle$  are the ground states of the unperturbed system within the zero-particle and one-particle sectors, respectively. Note that the particle number is a conserved quantity. The external electric field leads to creation of a particle–antiparticle pair, and so on. It turns out that HT is equivalent to QFT.

In summary, depending on what we take for the W of Eq. (1), we have different polarizabilities,

$$W_{\rm QM} = -\frac{1}{2} \alpha_{\rm QM} \mathbf{E}^2, \quad W_{\rm HT} = W_{\rm QFT} = -\frac{1}{2} \alpha \mathbf{E}^2.$$
 (10)

If we treat the system as a single-particle system, we obtain  $\alpha_{\rm QM}$  that can be negative as shown in Refs. 1–3. The  $\alpha_{\rm QM}$  corresponds to  $\alpha_{\rm pol}$  of Refs. 1 and 3 and to *P* of Ref. 2. If we include the vacuum background, we obtain  $\alpha$  that is related to  $\alpha_{\rm OM}$  by

$$\alpha = \alpha_{\rm QM} + \alpha'_{\rm vac}, \tag{11}$$

where  $\alpha'_{vac}$  is the EP of the vacuum in the absence of the particle in  $|1\rangle$ . The  $\alpha$  and  $\alpha'_{vac}$  are, respectively, equal to  $\alpha_1 + \alpha_2$  and  $\alpha_3$  of Ref. 3. The  $\alpha$  is positive because  $W_{HT} = W_{QFT}$  is negative as we have discussed. As an example, consider the hydrogen atom. The EP of the atom is  $\alpha$ . The  $\alpha'_{vac}$  is the EP of the hydrogen ion.

The notion of the EP is important in connection with the London–van der Waals force between two neutral atoms, e.g., two hydrogen atoms.<sup>9</sup> The interatomic force at large distances is proportional to  $\alpha^{2}$ .<sup>4,9</sup> This  $\alpha$  should be distinguished from  $\alpha_{QM}$ . The London–van der Waals force acts between two atoms, not just between two bound electrons. The London–van der Waals force is the long-range part of the two-photon-exchange force between atoms. Feinberg *et al.*<sup>4</sup> developed a dispersion theoretical method for the two-photon exchange process. In this method relevant matrix elements can be related to the amplitudes of Compton scattering from the atoms. The scattering is from the entire atoms

that include their vacuum background. The EP appears in the low-energy limits of the amplitudes. This EP is  $\alpha$  and not  $\alpha_{QM}$ .<sup>9</sup> In explicit calculations of the London–van der Waals force, vacuum effects are often ignored. This is because the vacuum effects are usually very small.

Finally let us mention the question raised by Sucher as to the sign of the EP.<sup>5</sup> He says that the EP defined in terms of second-order perturbation theory always gives a positive value (negative energy shift) for a system in its ground state. The EP that he refers to is, in our notation,  $\alpha$  and not  $\alpha_{OM}$ . He discussed the general validity of this result, for an arbitrary elementary system, be it atom, nucleus, or fundamental particle, within the framework of relativistic quantum theory. By using dispersion theoretical techniques, he examined the Compton scattering amplitude of which the low energy limit is related to  $\alpha$ , the EP of the target system. He argued that a possibility of negative  $\alpha$  may not be excluded as a consequence of only the most general principles of relativistic quantum theory. This has to do with the high energy limit of the scattering amplitude which in turn is related to the "compositeness" of the target system. As far as we know, this question raised by Sucher has not been clarified as yet. In discussing the EP in the sense of  $\alpha_{OM}$ . Maize *et al.*<sup>3</sup> referred to Sucher's question. They suggested that the negative  $\alpha_{OM}$ that they obtained was an answer to Sucher's question. But the EP that Sucher examined is, as we said above,  $\alpha$  rather than  $\alpha_{\rm OM}$ .

*Note added in proof.* In connection with Ref. 8, see also F. A. B. Coutinho, Y. Nogami, and L. Tomio, "Validity of Feynman's prescription of disregarding the Pauli principle in intermediate states," Phys. Rev. A **59**, 2624–2630 (1999).

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- <sup>5</sup>J. Sucher, "Sign of the static electric polarizability in relativistic quantum theory," Phys. Rev. D **6**, 1798–1800 (1972).
- <sup>6</sup>We can start with a negative energy bound state. If we do so, however, we will meet unnecessary, nonessential complications in the contexts of QFT. <sup>7</sup>This rearrangement of the terms is essentially the same as what was done in relating Eqs. (5) and (10) in Ref. 3.

<sup>9</sup>F. London, "Zur Theorie und Systematik der Molekularkräfte (On the theory and systematics of the molecular forces)," Z. Phys. **63**, 245–279 (1930); H. G. B. Casimir and D. Polder, "The influence of retardation on the London–van der Waals forces," Phys. Rev. **73**, 360–372 (1947).

<sup>&</sup>lt;sup>8</sup>R. P. Feynman, "The theory of positrons," Phys. Rev. **76**, 749–759 (1949), in particular p. 755.