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# Comments on Computation of Free-Free Transitions in Atomic Physics

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**Abstract:** The amplitude T for 'free-free' processes such as bremsstrahlung or photoabsorption by an electron in the continuum in the presence of an external field, is usually written as the matrix element of the radiation operator taken between two continuum states. However, unlike the case when at least one of the states is bound, as in radiative transitions, electron capture or the photo-effect, this expression contains unphysical term, proportional to a delta function, and is not really the physical amplitude $T_{phys}$. We first give an a **priori** definition of $T_{phys}$ in terms of the scattering parts of the continuum functions, which does not have this delta function term and has an obvious interpretation in terms of time-ordered diagrams. We then show that when the formal amplitude $T$ is modified by a long-distance cutoff, the modified form $T_\alpha$ approaches $T_{phys}$ as the cutoff is removed. The modified form may be used as the basis for calculation and approximations without the need to introduce further cutoffs at a later stage.

**Keywords:** bremsstrahlung; photoabsorption; radiative transition; electron capture

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## 1. Introduction

In nonrelativistic QED the amplitude for the emission of a transverse photon by an electron, making a transition from a state |a> to a state |b>, is given, to lowest order in the coupling $e$, by

$$M = [e/(2\omega)^{0.5}]T \tag{1}$$

In the above expression, $[e/(2\omega)^{0.5}]$ describes the photon-electron interaction [1] and

$$T = \langle b|R_{op}|a\rangle \tag{2}$$

$R_{op}$ is the radiation operator, defined by

$$R_{op} = \vec{\varepsilon}\cdot\vec{p}_{op}\exp(-i\vec{k}\cdot\vec{r})/m \tag{3}$$

Here $\vec{k}$ is the 3-momentum and $\vec{\varepsilon}$ is the polarization vector of the photon, with $\vec{\varepsilon}\cdot\vec{k} = 0$. The formula has of course been used innumerable times as the starting point for the calculation of atomic processes such as radiative transitions, the photoelectric effect, and electron capture. These processes are often described as bound-bound, bound-free, and free-bound transitions, respectively. In each case, at least one of the states |a> or |b> is normalizable, with the associated coordinate wave function $\Psi_a(\vec{r}) = \langle\vec{r}|a>$ or $\Psi_b(\vec{r}) = \langle\vec{r}|b\rangle$ vanishing as $r \to \infty$. This has the consequences that the matrix element (2) is a **priori** well-defined.

However, a study of the literature indicates that the expression (2) and the attendant dipole approximation have been widely used for processes such as bremsstrahlung in the

field of an ion [2,3] and photon absorption from the continuum [4,5]. These are examples of "free-free" transitions, where neither of the states |a> and |b> is normalizable. The amplitude then contains an obviously unphysical terms, proportional to a delta function [3]. The delta function does not give rise to difficulties during modern practical calculations. For example, if the acceleration form of the dipole approximation is used there is no delta function term. In some cases, cutoff factors may be introduced a posteriori, when one encounters ill-defined integrals during calculations [6–8]. While these procedures, guided by experience and physical intuition will usually lead to correct results, it seems worthwhile to establish the relevant formulas a priori, on physical grounds, and independent of particular physical applications and/or approximations.

In Section 2.1. we give an a priori definition of a physical amplitude, $T_{phys}$, for free-free transitions which is free of the delta-function term. In Section 2.2. we introduce a cutoff form $T_a$ of formal amplitude $T$ and show that in the limit of no cutoff $T_a$ reduces to the physical amplitude $T_{phys}$. This modified form may be used as a basis for further calculation without the need to introduce cutoffs at a later stage. A concluding discussion is given in Section 3.

## 2. Analysis

### *2.1. The Physical Amplitude $T_{phys}$*

To study the problem in the simplest possible context, consider the case of bremsstrahlung in an external field, with incoming and outgoing electron of asymptotic momenta **p** and **p′**, respectively, accompanied by emission of a photon of momentum **k**. Then the wave functions associated with the states $|a\rangle$ and $|b\rangle$ have the form

$$\Psi_a(\vec{r}) = \langle \vec{r}|a\rangle = \exp(i\vec{p}\cdot\vec{r}) + \chi_a(\vec{r}) \tag{4a}$$

$$\Psi_b(r) = \langle r|b\rangle = \exp(i\vec{p}^{\,\prime}\cdot\vec{r}) + \chi_b(\vec{r}) \tag{4b}$$

where $\chi$'s denote scattered waves with appropriate boundary conditions. The physical element is properly defined by

$$T_{phys} = \langle \vec{p}^{\,\prime}|R_{op}|\chi_a\rangle + \langle\chi_b|R_{op}|\vec{p}\rangle + \langle\chi_b|R_{op}|\chi_a\rangle \tag{5}$$

In the above equation, **p** and **p′ represent incoming and outgoing momenta of the electron.** The physical interpretation of (5) is straight **forward**. The first term in (5) represents (or time ordered diagrams) in which the electron undergoes *one or more* initial-state interactions with the external potential, emits a photon and undergoes no final state interactions; in the second term the electron emits a photon first and undergoes only final-state interactions; and the last term involves both initial and final state interactions.

Note however that the insertion of (4a) and (4b) into the formal expression (2) yields four terms, the three in (5) and a fourth term which involves the matrix element of the radiation $R_{op}$ between plane waves |**p>** and |**p′>**. This term is proportional to $\delta(\vec{p}^{\,\prime} + \vec{k} - \vec{p})$ and is clearly unphysical, since it represents the electron emitting a photon without interaction with the external potential. Nevertheless, the form (2) has been used since time immemorial, at least since the *tour-de-force* paper of Sommerfeld [2], who evaluated the dipole approximation to (2) exactly for the case of an electron scattering from the nucleus (taken as infinity massive). Sommerfeld does not appear to mention the dropping of the unphysical term; we have found it difficult to pinpoint it in the context of his complicated calculations. We will now show that if a cutoff is introduced in the formal expression (2), then in the limit of no cutoff the physical amplitude is recovered.

*2.2. $T_{phys}$ as the Limit of a Regularized Form of T*

We introduce a long-distance cutoff $f_a$ ($r$), e.g., $f_a = \exp(-\alpha r)$, into the formal expression (2) and define

$$T_a = \langle b|R_{op,\alpha}|a\rangle \tag{6}$$

where

$$R_{op,\alpha} = (f_a R_{op} + R_{op} f_a)/2 \tag{7}$$

On substituting the forms (4a) and (4b) into (6) we get

$$T_a = X_a + \langle p'|R_{op,\alpha}|\chi_a\rangle + \langle \chi_b|R_{op,\alpha}|p\rangle + \langle \chi_b|R_{op,\alpha}|\chi_a\rangle \tag{8}$$

In the above equation

$$X_a = \langle p'|f_\alpha \vec{\varepsilon}\cdot\vec{p}_{op}\exp(-i\vec{k}\cdot\vec{r}) + \vec{\varepsilon}\cdot\vec{p}_{op}\exp(-i\vec{k}\cdot\vec{r})f_\alpha|p\rangle/2m \tag{9}$$

The operator $\vec{\varepsilon}\cdot\vec{p}_{op}$ in the first term of (9) commutes with the exponential and so may evidently by replaced by $\vec{\varepsilon}\cdot\vec{p}$. In the second term, because of the factor $f_\alpha$ one may integrate by parts without encountering a surface term so that the operator $\vec{\varepsilon}\cdot\vec{p}_{op}$ may be replaced by $\vec{\varepsilon}\cdot\vec{p}'$. Thus

$$X_a = \vec{\varepsilon}\cdot(\vec{p}+\vec{p}')\langle\vec{p}'|f_\alpha\exp(-i\vec{k}\cdot\vec{r})|\vec{p}\rangle/2m$$

Since, for $\vec{q} = \vec{p} - \vec{p}' - \vec{k} \neq 0$, the integral

$$\int d\vec{r} f_\alpha \exp(i\vec{q}\cdot\vec{r}) \propto \alpha/(q^2+\alpha^2)^2$$

vanishes in the limit $\alpha \to 0$, the quantity $X_a$ also vanishes in this limit. In the remaining term in (8) the limit can be taken inside the integral, because the scattered waves fall off for large $r$ as $1/r$. Thus $R_{op,\alpha}$ may be replaced by $R_{op}$ in these terms and we have shown that, as claimed,

$$T_{phys} = \lim T_\alpha|_{\alpha\to 0} \tag{10}$$

## 3. Summary and Discussion

The amplitude for free-free processes involving photon emission or absorption is usually written in the form $\langle b|R_{op}|a\rangle$ where $R_{op}$ is the radiation operator (3), $|a\rangle$ and $|b\rangle$ are continuum electron states. However, this form contains an unphysical term, proportional to a delta function, which must either be dropped by hand, as in Reference [3], or otherwise eliminated, during calculation. The main result of this paper is that the physical amplitude is more properly given by

$$T_{phys} = \lim\langle b|R_{op,\alpha}|a\rangle|_{\alpha\to 0} \tag{11}$$

where

$$R_{op,\alpha} = (f_\alpha R_{op} + R_{op} f_\alpha)/2 \tag{12}$$

is the radiation operator modified by a cutoff factor, such as $\exp(-\alpha r)$. As long as the limit is taken after integrations are carried out, no spurious delta terms arise and integration by-parts is always admissible. Although we have focused on the case of bremsstrahlung in an external field, Equation (11) may be taken over to more complicated situations, such as an electron interaction with an atom or ion. The dipole approximation (DA) in which $\exp(-i\vec{k}\cdot\vec{r})$ is replaced by unity, is frequently used. On setting $\vec{k} = 0$ in (11) we obtain the physical dipole amplitude $T^{dip}_{phys}$ for free-free transitions in the form

$$T^{dip}_{phys} = \lim\langle b|f_\alpha\vec{\varepsilon}\cdot\vec{p}_{op} + \vec{\varepsilon}\cdot\vec{p}_{op}f_\alpha|a\rangle/2m|_{\alpha\to 0} \tag{13}$$

It is straightforward to show that if the electron can be regarded as moving in an external potential $V_{ext}$ which is local, "the modified velocity form" (13) may be transformed, as expected, into a "modified into a "modified length form"

$$T_{phys}^{dip\text{-}length} = \lim i(E_b - E_a)\langle b|f_\alpha \vec{\varepsilon}\cdot\vec{r}|a\rangle|_{\alpha\to 0} \tag{14}$$

by the use of the commutation relation $\vec{p}_{op}/m = [H, \vec{r}]$. Similarly, (13) may be transformed into a "modified acceleration form" $T_{phys}^{acc}$

$$T_{phys}^{acc} = \lim -i(E_b - E_a)^{-1}\langle b|f_\alpha \vec{\varepsilon}\cdot\vec{\nabla}V_{ext}|a\rangle/m|_{\alpha\to 0} \tag{15}$$

by use of the relation $[p_{op}, H] = -i\nabla V_{ext}$. However, because of the presence of $V_{ext}$ in (15), here the limit may be taken inside the matrix element without encountering a singular integral, so that even for free-free transitions one may write

$$T_{dip}^{acc} = -i(E_b - E_a)^{-1}\langle b|\vec{\varepsilon}\cdot\vec{\nabla}V_{ext}|a\rangle/m \tag{16}$$

The acceleration form (16) is often used as a starting point for practical calculations. A remark may be made in order that the logic of its use, which seems to be implicit in the literature. As mentioned above, the situation in which at least one of the states |a> or |b> is bound the usual amplitude (2) is well-defined and so is the corresponding DA. If $V_{ext}$ may be chosen as local, this (velocity) DA may be transformed into acceleration DA, without folderol. The resulting expression (16) is then simply taken over to the free-free case. This slight-of-hand, while leading to a correct result, should not obscure the fact that the manipulations required to obtain (16) for the free-free case are suspect because the starting point, namely the expression for the dipole amplitude is not well-defined if both states are free. Starting from the modified DA amplitude (13) one obtains (16) without any ambiguity.

The exercise we have carried out in this note may strike some readers as pedantic. However, there are many examples in the literature of mathematical physics where lack of attention to issues involving delta-function leads to wrong answers. Thus it behooves one to be careful in these matters. We have considered only one-photon process, for multiphoton processes, see e.g., reference [9].

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