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Exchange of Photons between Two Atoms in a 1D Waveguide. Gauge Dependent and Independent Couplings

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Abstract: Two atoms located in a one dimensional waveguide with initially one of them in the excited state interact by exchanging photons. We analyze the exchange process distinguishing between real and virtual photons contributions, and comparing between the Coulomb and Goeppert-Mayer gauges. We show that gauge-independent coupling terms can be interpreted in a simple way using the time-energy incertitude relation

Keywords: Photon exchange, Coulomb gauge, Goeppert-Mayer gauge, collective Lamb-shift, superradiance, quantum electrodynamics in waveguide, real and virtual photons

1 Introduction

The light propagation between two atoms represents an old issue that was concomitant with the development of quantum electrodynamics. It has been addressed by Fermi as earlier as 1932 [1] and represents the basic model for understanding super-radiance phenomena [2–6]. Moreover, the photon exchange is known to lead to the coupling between atoms inducing alternated transitions and light-shifts (collective Lamb-shift). Although the coupling term is finite and gauge independent, it involves the superposition of many quantum paths whose contributions are gauge-dependent and that may be divergent. For this reason, these partial quantum paths are generally considered as unphysical (unobservable) although the photon exchange process is allowed. To the best of our knowledge, no further investigation on the exact behavior of these unphysical processes has been performed. Here, we investigate the situation of atom-atom coupling in a one dimensional (1D) waveguide for both the Coulomb and Goopert-Mayer gauges. We show that each partial quantum path exhibits a finite gauge-independent part whose behavior can be understood from the time-energy incertitude and a gauge dependent contribution responsible for the unphysical behavior of these partial parts. This study represents thus an evidence for the close connection between renormalization theory and gauge formulation of quantum electrodynamics. The dynamics of atoms in 1D waveguide is a promising configuration is the realization of all-optical quantum devices [7–9] because it allows the control of the transport of the flying qubits (photon) and the realization of fundamental quantum information operations [7–14]. Even if many studies have been already achieved for the calculation of the transmission and reflection of a photon through an array of N atoms in a 1D waveguide, neither the role of photons exchanged between atoms has been realistically studied (because of the neglect of non Rotating Wave Approximation –RWA– contributions in these studies) nor the nature (real or virtual) of the photons has been established. We have addressed these considerations in a recent paper [15] stressing on the spectral and temporal modification of a photon wavepacket propagating in a 1D waveguide containing two separated atoms. Here, in this paper we focus on the physical interpretation of photons exchanged by the two atoms considering two gauges (Coulomb and Goeppert-Mayer) without performing the RWA approximation.

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2 Theory. Coupling between atoms:

We consider two identical atoms labelled $j = 1,2$ each modelized by a two-level system (ground states $|a_j>$ and excited states $|b_j>$ with eigenfrequencies 0 and ω_0 respectively). The resonant frequency is ω_0 and the interatomic distance l. We consider the case where the two atoms are localized inside an infinite lossless waveguide. The transverse dimension of the waveguide d is assumed to be much smaller than λ_0 (the resonant wavelength) and the interatomic distance l (e.g. $d \ll \lambda_0, l$) so that the electrostatic dipole-dipole interaction between the atoms is strongly inhibited in the waveguide and can be neglected [16, 17]. Moreover, the atoms no longer radiate outside the z direction and the field remains uniform in the longitudinal direction of propagation [18, 19]. We take into account here for virtual photon effects that may induce significant changes in the dynamics. Thus rotating wave approximation (rwa) is not done and the Hamiltonian of the system $\hat{H}$ can be separated into three terms $\hat{H} = \hat{H}_{atomic} + \hat{H}_{field} + \hat{H}_{inter}$. In this notation, $\hat{H}_{atomic} = \sum_{j=1}^{2} \hbar\omega_0 |b_j><b_j|$ is the Hamiltonian of the free atoms. $\hat{H}_{field} = \int_{-\infty}^{\infty} (\hbar\omega_k)\hat{a}^{\dagger}_{k_z}\hat{a}_{k_z} dk_z$ is the Hamiltonian of the free field with $\omega_k = c|k_z| = ck$ and $\hat{a}_{k_z}$ the photon annihilation operator that follows the usual bosonic commutation rules $[\hat{a}_{k_z}, \hat{a}^{\dagger}_{k'_z}] = \delta(k_z - k'_z)$. The interaction Hamiltonian depends also on the electromagnetic gauge used and can be written as $\hat{H}_{inter} = \sum_{j=1}^{2} \int_{-\infty}^{\infty} \hbar g_k \left(\tilde{i}\hat{a}_{k_z} e^{ik_z.z_j} + \tilde{i}^* \hat{a}^{\dagger}_{k_z} e^{-ik_z.z_j} \right) (\hat{\sigma}_j + \hat{\sigma}^{\dagger}_j) dk_z$ with z_j the position of atom j (with $z_2 - z_1 = l$), $\hat{\sigma}_j = |a_j><b_j|$ the lowering operator, the coupling g_k and the parameter $\tilde{i}$ depends on the gauge used. For Coulomb gauge, we have $\tilde{i} = 1$ and $g_k = g_0\sqrt{\frac{\omega_0}{\omega_k}}$ with $g_0 = \sqrt{\frac{\omega_0}{4\pi\hbar\varepsilon_0 A}} d_{ab}$ the coupling at resonance, A the effective transverse guide section and d_{ab} the dipole moment. For Goeppert-Mayer gauge, we have $\tilde{i} = -i$ and the coupling is $g_k = g_0\sqrt{\frac{\omega_k}{\omega_0}}$. When initially ($t \to -\infty$) only one atom is in the ground state, and for the second order in the interaction Hamiltonian, the wavefunction $|\psi>(t)$ of the whole system (atoms+field) can be formally expanded as:

$$
\begin{aligned}
|\psi>(t) &= \int_{-\infty}^{\infty} \alpha_{k_z}(t) e^{-i\omega_k t} |a_1, a_2, 1_{k_z}> dk_z \\
&+ \sum_{j=1}^{2} \beta_j(t) e^{-i\omega_0 t} |a_{j'\neq j}, b_j, 0> \\
&+ \int_{-\infty}^{\infty} \gamma_{k_z}(t) e^{-i(2\omega_0+\omega_k)t} |b_1, b_2, 1_{k_z}> \\
&+ \sum_{j=1}^{2} \int_{-\infty}^{\infty} dk_z \int_{-\infty}^{\infty} dk'_z \eta_{j,k_z,k'_z}(t) e^{-i(\omega_k+\omega_{k'}+\omega_0)t} |a_{j'\neq j}, b_j, 1_{k_z}, 1_{k'_z}> .
\end{aligned}
\tag{1}
$$

The two first terms corresponds to states with an excitation number equal to one. In the first term, we have states with one photon in the field and both atoms in the ground level whereas in the second term, we have states with only one atom ($j = 1,2$) in the excited state and no photon in the field. The last two terms correspond to an excitation number of three. The third term describes the situation where both atoms are excited and there is one photon in the field, whereas the last term corresponds to the situation with one excited atom (j) and two photons in the field. These states are necessary for the correct treatment of virtual photon and the collective Lamb-shift effect.

The evolution of the system is determined by the Schrödinger equation $i\hbar\frac{d|\psi>(t)}{dt} = \hat{H}|\psi>(t)$. The equations of evolution for the amplitudes obtained from the Schrödinger equation can be solved using the standard adiabatic elimination of the continuum technic [20], that holds for $\omega_0 \gg \Gamma$ where Γ is the relaxation constant given by $\Gamma = \frac{2\pi}{c} g_0^2$. Details of calculations can be found in [15]. The amplitude $\beta_j(t)$ ($j = 1,2$) follow the fundamental integro-differential equation:

$$
\dot{\beta}_j(t) = -\Gamma\beta_j - \int_{-\infty}^{t} \beta_{j'\neq j} \bar{M}(t-t') dt'. \tag{2}
$$

The first term is a relaxation term whereas the second term is a coupling between the two atoms. It depends on a memory function $\bar{M}(t-t')$ that is the sum of four contributions $\bar{M} = \bar{M}_1 + \bar{M}_2 + \bar{M}_3 + \bar{M}_4$ with:

$$
\bar{M}_1(t-t') = \int_0^{\infty} g_\omega^2 e^{i(\omega l/c)} e^{i(\omega_0-\omega_k)(t-t')} d\omega \tag{3a}
$$

$$
\bar{M}_2(t-t') = \int_0^{\infty} g_\omega^2 e^{i(\omega l/c)} e^{-i(\omega_0+\omega_k)(t-t')} d\omega \tag{3b}
$$

$$
\bar{M}_3(t-t') = \int_0^{\infty} g_\omega^2 e^{-i(\omega l/c)} e^{i(\omega_0-\omega_k)(t-t')} d\omega \tag{3c}
$$

$$
\bar{M}_4(t-t') = \int_0^{\infty} g_\omega^2 e^{-i(\omega l/c)} e^{-i(\omega_0+\omega_k)(t-t')} d\omega. \tag{3d}
$$

In these expressions, we have, $g_\omega = \frac{g_k}{\sqrt{c}}$ and the spatial term accounts for the field propagation between the two atoms. An important case is the situation where the atoms are close enough so that the interaction (exchange of photons) can be considered as instantaneous compared to the atomic dynamics. This is the case when the photon time of flight $\frac{l}{c}$ and the resonant period ($\frac{2\pi}{\omega_0}$) are smaller than the time characteristic of population amplitudes β_j that is Γ^{-1}. This is obtained for $l, \lambda_0 \ll c\Gamma^{-1}$. In this case, we can set $\beta_j(t') \simeq \beta_j(t)$ in the integral appearing in (2). Performing the integration over time first, we obtain $\int_{-\infty}^{t} \bar{M}(t'-t) = \Gamma e^{i(\omega_0 l/c)}$. Note that –as expected– the coupling term is independent of the gauge used. The equations of evolution of the β_j turn into:

$$
\dot{\beta}_j(t) = -\Gamma\beta_j(t) - \Gamma e^{i(\omega_0 l/c)} \beta_{j'\neq j}(t). \tag{4}
$$

The dependence of the coupling coefficient with the interatomic distance appears through only a phase term $e^{i(\omega_0 l/c)}$. Thus, the coupling term doesn't decrease with

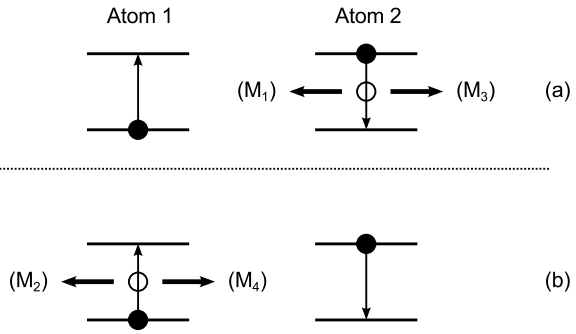

Fig. 1: Quantum paths leading to the modification of β_1, the excited state amplitude of atom1. Paths are associated with (a) relaxation of atom 2 with emission of a photon in the backward (M_1 amplitude) or forward (M_3 amplitude) directions and that interacts further with atom 1 (RWA terms), (b) excitation of atom 1 with emission of photon in the backward (M_2 amplitude) or forward (M_4 amplitude) directions and that interacts further with atom 2 (non-RWA terms). Similar photon diagrams exist for the modification of β_2.

the atomic separation in contrast with the free space situation. This is because in 1D waveguide with $l \gg d$, the propagating photons are confined along the inter atomic axis making the energy flux unchanged between atoms.

3 Photon exchange:

3.1 Quantum paths:

The photon exchange between the two atoms can be understood from equations (2, 3) by exhibiting the frequency dependence. Moreover, we proceed to integration over time in these equations. We then obtain: (with the notation $M_i = \int_{-\infty}^{t} \bar{M}_i(t-t')dt'$, $i = 1, \cdots, 4$)

$$M_1 = \pi g_\omega^2(\omega_0) e^{i(\omega_0 l/c)} + i\mathscr{P}\left(\int_0^\infty g_\omega^2(\omega)\frac{e^{i(\omega_0 l/c)}}{\omega_0-\omega}d\omega\right) \quad (5a)$$

$$M_2 = -i\int_0^\infty g_\omega^2(\omega)\frac{e^{i(\omega_0 l/c)}}{\omega_0+\omega}d\omega \quad (5b)$$

$$M_3 = \pi g_\omega^2(\omega_0) e^{-i(\omega_0 l/c)} + i\mathscr{P}\left(\int_0^\infty g_\omega^2(\omega)\frac{e^{-i(\omega_0 l/c)}}{\omega_0-\omega}d\omega\right) \quad (5c)$$

$$M_4 = -i\int_0^\infty g_\omega^2(\omega)\frac{e^{-i(\omega_0 l/c)}}{\omega_0+\omega}d\omega. \quad (5d)$$

The $\mathscr{P}$ designs the Cauchy principal part of the corresponding integrals. According to these equations, the atoms exchange photons with different frequencies and the four parts correspond to distinct quantum paths. Moreover, we represent in figure 1, the quantum paths corresponding to the photon exchange and explaining for the behavior of the field and atomic dynamic. The RWA terms (associated with M_1 and M_3) correspond to the case (a) where one -excited– atom relaxes and emits photons leading to a further absorption by the other atom. The non-RWA terms (associated with M_2 and M_4) correspond to the situation (b) where an atom in the ground state emits a photon and transits to the excited state. The emitted photon is then absorbed by the second atom that relaxes to the ground state. It's important to notice that M_1 and M_2 corresponds to an emission in the forward direction ($z > 0$) whereas M_3 and M_4 correspond to a backward emission ($z < 0$). That means that photons emitted by one of the atom in opposite direction to the other atom can also be absorbed by this latter. This is because a photon spreads "naturally" over a distance λ –although we cannot define a spatial wavefunction [21] – and cannot be considered as a point-like classical particle.

3.2 Real and virtual photons:

We distinguish in the photon exchange process between real and virtual photons. Real photons are those who appear in process that conserve the bare energy in contrast with virtual photons that doesn't conserve bare energy. Real photons contributions appear in the first terms in (5a) and (5c) that correspond to the resonant frequency in rwa terms whereas the contribution of virtual photons appear in the principal part of these terms and the whole non-rwa contributions (5b and 5d). It's worthy to notice that the sum of real photons contribution gives $\Gamma\cos(k_0 l)$ e.g. the real part of the coupling term $\Gamma e^{i(\omega_0 l/c)}$ in (4). Virtual photons that involve the remaining terms and contribute to the imaginary part of the coupling $i\Gamma\sin(k_0 l)$. The virtual photons contribute thus to only a frequency shift of the atomic resonances whereas the real photons induce atomic transitions.

We have also to distinguish between near resonance and far resonance virtual photons that influence the population behavior in different manner. Indeed, let's consider the situation where $l \gg \frac{c}{\omega_0}$ and the contribution of M_1 and M_3 terms to the coupling between atoms. In (5a-5d) we can separate the non-resonant contribution (e.g. the integral) into two parts, one corresponding to photons nearly resonant with frequencies ω located in a domain $\delta \geq \frac{c}{l}$ around ω_0 (with $\omega_0 \gg \delta$) and another part with the remaining photons. In this situation, using the relation $i\mathscr{P}\int_{\omega_0-\frac{\delta}{2}}^{\omega_0+\frac{\delta}{2}} g_\omega^2 \frac{e^{\pm i(\omega l/c)}}{\omega_0-\omega} \simeq \pm\pi g_\omega^2(\omega_0)e^{\pm ik_0 l}$, we find that the sum of M_1 and M_3 contributions gives rise to the imaginary part of the coupling $i\Gamma\sin(k_0 l)$. In other words, only nearly resonant photons contribute to the atomic coupling. Thus, the role of the remaining part (highly non resonant photons in M_1 and M_3) is to cancel the non-RWA photons contributions (M_2 and M_4).

3.3 Gauge-dependent and gauge-independent contributions:

The coupling term between the two atoms in (4) is independent from the gauge used and needs no renormalization procedure. However, the partial contribution terms M_i ($i = 1, \cdots, 4$) corresponding each to a specific quantum path are gauge-dependent and even diverges in the case of Coulomb gauge. Indeed, let's evaluate the integrals appearing in (5). We obtain the following relations:

$$i\mathscr{P}\left(\int_0^\infty g_\omega^2(\omega)\frac{e^{\pm(\omega l/c)}}{\omega_0-\omega}d\omega\right) = g_\omega^2(\omega_0)\left[\pm e^{\pm i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)+\frac{\pi}{2}\pm i\mathrm{Ci}(\omega_0 l/c)\right)-G_\pm\right] \tag{6a}$$

$$-i\int_0^\infty g_\omega^2(\omega)\frac{e^{\pm(\omega l/c)}}{\omega_0+\omega}d\omega = g_\omega^2(\omega_0)\left[\pm e^{\mp i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)-\frac{\pi}{2}\mp i\mathrm{Ci}(\omega_0 l/c)\right)+G_\pm\right]. \tag{6b}$$

With Ci and Si the cosine and sine integral functions respectively [22]. For real arguments, these functions are even and odd respectively. The asymptotic values are $\mathrm{Ci}(|x|\gg 1)=0$, $\mathrm{Si}(|x|\gg 1)=\frac{\pi}{2}$ and we have $\mathrm{Ci}(0)=\infty$. $G_\pm$ is a gauge dependent constant with $G_\pm = \mp\frac{c}{l}$ (Goeppert-Mayer gauge) and $G_\pm = \pm\frac{\pi}{2}+i\mathrm{Ci}(\varepsilon\to 0)$ (Coulomb gauge). In Coulomb gauge, these integrals diverge because of infrared singular behavior $g_k \propto \frac{1}{\sqrt{\omega}}$. Using (6a,6b) and (5), we obtain the following relations for the coupling elements:

$$M_1 = \pi g_\omega^2(\omega_0)e^{i(\omega_0 l/c)} + g_\omega^2(\omega_0)\left[e^{i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)+\frac{\pi}{2}+i\mathrm{Ci}(\omega_0 l/c)\right)-G_+\right] \tag{7a}$$

$$M_2 = g_\omega^2(\omega_0)\left[e^{-i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)-\frac{\pi}{2}-i\mathrm{Ci}(\omega_0 l/c)\right)+G_+\right] \tag{7b}$$

$$M_3 = \pi g_\omega^2(\omega_0)e^{-i(\omega_0 l/c)} + g_\omega^2(\omega_0)\left[-e^{-i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)+\frac{\pi}{2}-i\mathrm{Ci}(\omega_0 l/c)\right)-G_-\right] \tag{7c}$$

$$M_4 = g_\omega^2(\omega_0)\left[-e^{i(\omega l/c)}\left(\mathrm{Si}(\omega_0 l/c)-\frac{\pi}{2}+i\mathrm{Ci}(\omega_0 l/c)\right)+G_-\right]. \tag{7d}$$

Each coupling term M_i is the sum of a gauge-independent term and a constant part that depends on the gauge used making the interpretation of associated partial quantum paths cumbersome. However, an interpretation of the behavior of gauge-independent part is possible and is based on the report that these gauge independent parts are identical to the values of the coupling terms obtained if the coupling $g_\omega(\omega)$ was assumed constant e.g:

$$(M_i)_{G_\pm=0} = (M_i)_{g_\omega(\omega)=g_\omega(\omega_0)};\ i=1,3 \tag{8a}$$

$$(M_i)_{G_\pm=0} = (M_i)_{g_\omega(\omega)=g_\omega(-\omega_0)};\ i=2,4. \tag{8b}$$

For RWA terms (M_1 and M_3), the gauge independent terms are obtained as if the coupling parameter is the same for all the frequencies and equal to that of the central frequency. For non-RWA terms, (M_2 and M_4), the same equality exists except for the minus sign. Using these properties, the physics of some concrete situations can be highlighted. When $\omega_0 l/c \gg 1$ (e.g. $l \gg \lambda_0$), the non-RWA contributions vanish, e.g. $(M_i)_{G_\pm=0} = (M_i)_{g_\omega(\omega)=g_\omega(-\omega_0)} = 0$ ($i=2,4$) whereas for the RWA terms we have $(M_3)_{G_\pm=0} = (M_3)_{g_\omega(\omega)=g_\omega(\omega_0)} = 0$ and $(M_1)_{G_\pm=0} = (M_1)_{g_\omega(\omega)=g_\omega(\omega_0)} = \Gamma e^{i(\omega_0 l/c)}$. Only the photon exchange represented in figure 1-a with a photon emitted in the direction of the neighboring atom subsists. This behavior can explained using the time-energy incertitude relation. Indeed, a photon is present for only a time given by $|\omega-\omega_0|^{-1}$ (RWA process associated with M_1 and M_3) and $|\omega+\omega_0|^{-1}$ (non-RWA photons associated with M_2 and M_4). Except for real photons that are resonant ($\omega=\omega_0$), this lifetime is limited. All virtual photons (photons with $\omega\neq\omega_0$) travel over a finite distance that cannot exceed $c|\omega+\omega_0|^{-1}$ for non-RWA photons and $c|\omega-\omega_0|^{-1}$ for RWA photons as a consequence. Because we have $|\omega+\omega_0|^{-1} \leq \omega_0^{-1}$, it is expected that non-RWA photon can be exchanged when the interatomic distance l is larger than $\lambda_0 = \frac{c}{\omega_0}$ ($(M_i)_{G_\pm=0} = (M_i)_{g_\omega(\omega)=g_\omega(-\omega_0)}$, $i=2,4$) and only nearly resonant RWA photons such as $|\omega-\omega_0| < \frac{c}{l}$ are involved in the interaction process. In the latter case, the near-resonance frequencies give a contribution opposite to the exact resonance one (e.g. in (7c) and disregarding G_-, the first term is canceled by the second one) leading to $(M_3)_{G_\pm=0} = (M_3)_{g_\omega(\omega)=g_\omega(\omega_0)} = 0$. This result is in line with what can be deduced from figure 1-a where we see that the photon exchanged in the process involving M_3 moves away from the atoms. We then expect a vanishing contribution once the interatomic distance is larger than λ –the extension of the field on the back–. Because for significant contribution we have $c|\omega_0-\omega|^{-1} > l$, we obtain $|\omega-\omega_0| \ll \omega_0$ when $\omega\frac{l}{c} \gg 1$. The contributing frequencies are such as $\omega \simeq \omega_0$ and the spatial extension of the field on the back is given by $\lambda \simeq \lambda_0 \ll l$. Thus, the photon cannot "reach" the neighboring atom making the contribution of M_3 vanishing in this situation.

When the frequency dependence of the coupling is taking into account, the interpretation in terms of time-energy incertitude is no longer valid since the photon lifetime represents first, only an average time and secondly the rate of photon exchange doesn't depend on solely but also on the coupling parameter g_ω. This latter parameter can reach important values and even diverges. For instance, $g_\omega \to \infty$ when either $\omega \to 0$ (Coulomb

gauge) and $\omega \to \infty$ (Goeppert-Mayer gauge). The result is the appearance of the gauge-dependent constant $G_{\pm}$ that exhibits an infinite part in the case of Coulomb gauge. However, because these additional terms rule out in the final resulting coupling $\Gamma e^{i(\omega_0 l/c)}$, the interpretation in terms of time-energy incertitude relation can be considered as "effectively" valid.

Another interesting result can be obtained when gathering differently the coupling terms M_i. Indeed, for $i = 1,2$ the gauge-dependent terms are opposite (and also for $i = 3,4$). The quantity $M_1 + M_2$ is then gauge-independent and corresponds to a realistic physical situation. Indeed, if an optical-diode like device is inserted into the waveguide allowing only backward propagation of light ($k_z < 0$), the coupling term reduces to $M_1 + M_2$ and is necessarily gauge independent. Moreover, using (7a,7b), we obtain:

$$M_1 + M_2 = g_\omega^2(\omega_0)\big[\cos(\omega_0 l/c)(2\mathrm{Si}(\omega_0 l/c) + \pi) + i\sin(\omega_0 l/c)(2\pi + i\mathrm{Ci}(\omega_0 l/c))\big]. \quad (9)$$

For $\omega_0 l/c \gg 1$, we have $\mathrm{Si}(\omega_0 l/c) \simeq 1$ and $\mathrm{Ci}(\omega_0 l/c) \simeq 0$. We then obtain $M_1 + M_2 = \Gamma e^{i(\omega_0 l/c)}$, the same value of the coupling obtained in our situation where the two directions are allowed.

4 Conclusion:

The interaction between two atoms exchanging photons in a 1D waveguide has been studied in both Coulomb and Goeppert-Mayer gauges. We have shown that the photon exchange involves different quantum paths. Coupling terms between excited-state amplitudes are associated to each of these quantum paths and exhibit both gauge-independent and gauge-dependent contributions. We have clarified the physical meaning of the gauge-independent parts using the time-energy incertitude relation. The situation of two atoms interacting in a 1D waveguide turns to be very instructive to understand the interaction between atoms at the photon level. Moreover, it paves the way to an extension of these studies to the case of free space (3D) or N interacting atoms in 1D.

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