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PAPER

Emergent causality and the *N*-photon scattering matrix in waveguide QED

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Abstract

In this work we discuss the emergence of approximate causality in a general setup from waveguide QED—i.e. a one-dimensional propagating field interacting with a scatterer. We prove that this emergent causality translates into a structure for the *N*-photon scattering matrix. Our work builds on the derivation of a Lieb–Robinson-type bound for continuous models and for all coupling strengths, as well as on several intermediate results, of which we highlight: (i) the asymptotic independence of space-like separated wave packets, (ii) the proper definition of input and output scattering states, and (iii) the characterization of the ground state and correlations in the model. We illustrate our formal results by analyzing the two-photon scattering from a quantum impurity in the ultrastrong coupling regime, verifying the cluster decomposition and ground-state nature. Besides, we generalize the cluster decomposition if inelastic or Raman scattering occurs, finding the structure of the S-matrix in momentum space for linear dispersion relations. In this case, we compute the decay of the fluorescence (photon–photon correlations) caused by this S-matrix.

1. Introduction

Causality is expected to hold in every circumstance. The causality principle states that two experiments which are space-like separated, such that no signal traveling at the speed of light can connect them, must provide uncorrelated results [1]. In quantum field theory (QFT), strict causality imposes that two operators $A(x,\ t)$ and $B(y,\ t')$ acting on two space-like separated points (x, t) and $(y,\ t')$, must commute,

$$[A(x,\ t),\ B(y,\ t')] = 0 \text{ if } |x-y| - c|t-t'| > 0, \tag{1}$$

where c is the speed of light (we restrict ourselves to $1+1$ dimensions). Another consequence of causality in QFT appears in the study of scattering events or collisions: scattering matrices describing causally disconnected events must 'cluster', or decompose into a product of independent scattering matrices [2]. In fact, all acceptable QFT interactions must result in S-matrices fulfilling such a decomposition [3].

Nonrelativistic quantum mechanics is an effective theory which allows signals to propagate arbitrarily fast, but which may give rise to different forms of emergent approximate causality. The typical examples are low-energy models in solid state, where quasiparticle excitations have a maximum group velocity. In this case, there exists an approximate light cone, outside of which the correlations between operators are exponentially suppressed. This emergent causality was rigorously demonstrated by Lieb and Robinson [4] for spin-models on lattices with bounded interactions that decay rapidly with the distance. Lieb–Robinson bounds not only imply causality in the information-theoretical sense [5], but lead to important results in the static properties of many-body Hamiltonians, such as the clustering of correlations, locality in the dynamics of lattices of harmonic oscillators, and the area law in gapped models [6–8].

In this work we demonstrate the existence and explore the consequences of emergent causality in the nonrelativistic framework of waveguide QED [9–13]. Theses systems consist of photons propagating in low-dimensional environments—waveguides, photonic crystals, etc—interacting with local quantum systems. Such models do not satisfy Lorentz or translational invariance, they are typically dispersive, and the photon-matter interaction may become highly non-perturbative. Experimental implementations include dielectrics [14, 15], cavity arrays [16], metals [17], diamond structures [18, 19], and superconductors [20–24] interacting with atoms, molecules, quantum dots, color centers in diamond or superconducting qubits. The focus of waveguide QED is set on quantum processes involving few photons and scatterers. In this regard, it is not surprising that there exists an extensive theoretical literature for waveguide-QED systems [13], which develops a variety of analytical and numerical methods for the study of the N-photon S-matrix [25–36].

The main result in this work is the structure of the N-photon S-matrix in waveguide QED, rigorously deduced from emergent causality constraints. Our result builds on a general model of light–matter interactions, *without* any approximations such as the rotating-wave approximation (RWA), the Markovian limit, or weak light–matter coupling. To derive the S-matrix decomposition we are assisted by several intermediate and important results, of which we remark: (i) the freedom of wave packets far away from the scatterer, (ii) Lieb–Robinson-like independence relations and approximate light-cones for propagating wave packets, (iii) a characterization of the ground state correlation properties, and (iv) a proper definition and derivation of scattering input and output states.

We illustrate our results with two representative examples. The first one is a numerical study of scattering in the ultrastrong coupling limit [35, 37], where we demonstrate the clustering decomposition and the nature of the ground state predicted by our intermediate results. The second is an analytical study of a non-dispersive medium interacting with a general scatterer, which admits exact calculations. Here, we find the shape of the S-matrix from general principles, including the inelastic processes. We recover the nontrivial form computed by Xu and Fan for a particular case in [38] and find the generalization of the standard cluster decomposition to the waveguide-QED model given by equation (2), with several ground states.

The paper has the following organization. Section 2 presents the nonrelativistic Hamiltonian that models the interaction between propagating photons and quantum impurities, the concept of wave packet, a review of the scattering theory needed, and two conditions necessary for the validity of our results. Section 3 summarizes our formal theory arriving to the general N-photon scattering compatible with causality. Section 4 presents the examples applying the theory. We close this work with further comments and outlooks. Intermediate lemmas, theorems, and technical issues are discussed in the appendices.

2. Model and scattering theory

2.1. Waveguide QED model

The simplest model that describes a waveguide-QED setup consists of a one-dimensional bosonic medium and a scatterer. Using units such that $\hbar = 1$, it reads

$$H = H_0 + H_{\mathrm{sc}} + \int (g_k G^\dagger a_k + g_k^* G a_k^\dagger)\mathrm{d}k. \tag{2}$$

The first term stands for the free-Hamiltonian of the photons

$$H_0 = \int \omega_k\, a_k^\dagger a_k \mathrm{d}k, \tag{3}$$

with frequency ω_k for momentum k, which is created (annihilated) by the corresponding Fock operator a_k ($a_k^\dagger$), satisfying $[a_k, a_{k'}^\dagger] = \delta(k - k')$. The last two terms are the Hamiltonian H_{sc} of the finite-dimensional system, which is the scatterer, and the dipolar interaction term described by the bounded operators G and the coupling strengths g_k. We assume that the coupling strengths in position space

$$g_x = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k\ \mathrm{e}^{\mathrm{i}kx} g_k \tag{4}$$

have a finite support centered around $x_{\mathrm{sc}} = 0$. The model (2) is not exactly solvable in general. For instance, if the scatterer is a two-level system, $H_{\mathrm{sc}} \propto \sigma_z$ and $G = \sigma_x$ the model is the celebrated spin-boson model [39], which results in a nontrivial ground state with localized photonic excitations around the scatterer.

The discussion below assumes a single photonic band $\omega_k \in [\omega_{\min}, \omega_{\max}]$ and typically a chiral medium $k \geqslant 0$, $\partial_k \omega_k \geqslant 0$. This is a rather standard simplification which does not affect the generality and applicability of our results. We generalize our results to nonchiral media in appendix E. The structure for S^0 is essentially identical in that case, so the conclusions of the paper also hold for nonchiral media. Anyway, chiral waveguides can be realized experimentally, for instance with photonic crystals [40, 41], or nanofibers coupled to nanoparticles or atoms [14, 42]. Besides, we can consider more generic dispersion relations by introducing additional degrees of freedom in the photons (band index, etc) and keeping track of those quantum numbers in a trivial extension of our results.

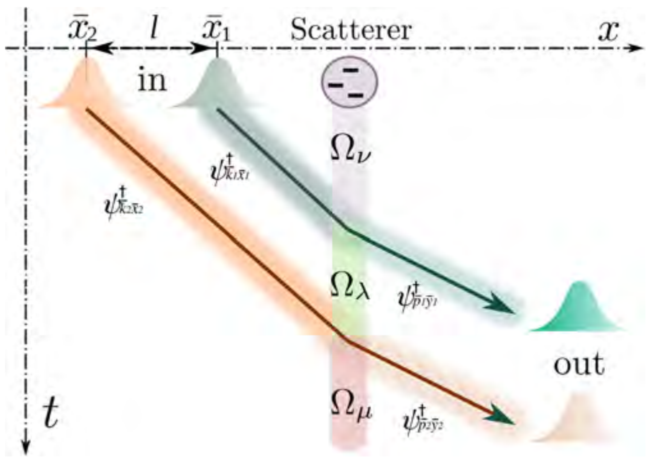

Figure 1. Two incoming photons with average momenta $\bar{k}_1$ (red) and $\bar{k}_2$ (green), initially centered around distant points $\bar{x}_1$ and $\bar{x}_2$ ($l \to \infty$), scatter against a general quantum object. The scatterer-field can have several bound states (localized and not propagating). In the figure, the scatterer-field is in one of those bound states $|\Omega_\nu\rangle$ (gray region). If the first incoming photon leaves the scattering region in another localized eigenstate $|\Omega_\lambda\rangle$ the second photon *meets* the interaction region in a different state, found by the first wave packet. If this occurs (see main text) the scattering matrix cannot be just a product, it must differentiate the order in which both events happen.

Our model is lossless. Losses are negligible in several experimental platforms, such as superconducting transmission lines interacting with superconducting qubits [21, 22]. Besides, the one-dimensional approximation is valid for all the implementations considered in the references we included above.

2.2. Localized wave packets

In order to talk about causality, we introduce a set of localized wave packets to which an approximate position can be ascribed. As we will see below, approximate localization becomes essential in the discussion, allowing us to discuss the order in which photons interact with the scatterer.

Let us introduce the creation operator $\psi_{\bar{k}\bar{x}}(t)^\dagger$ for a wave packet as

$$\psi_{\bar{k}\bar{x}}(t - t_0)^\dagger = \int \mathrm{e}^{\mathrm{i}k\bar{x} - \mathrm{i}\omega_k(t-t_0)} \phi_{\bar{k}}(k) a_k^\dagger \, \mathrm{d}k. \tag{5}$$

The wavefunction $\phi_{\bar{k}}(p) = \phi(p - \bar{k}) \in \mathcal{L}^2$ is normalized and centered around the average momentum $\bar{k}$. The exponential factor $\mathrm{e}^{ik\bar{x}}$ ensures the wave packet is centered around $\bar{x}$ in position space at time $t = t_0$.

As wave packets we will use both Gaussian

$$\phi_{\bar{k}}(k) = \frac{1}{\sqrt[4]{2\pi}\sqrt{\sigma}} \exp[-(k - \bar{k})^2/4\sigma^2], \tag{6}$$

and Lorentzian envelopes

$$\phi_{\bar{k}}(k) = \sqrt{\frac{\sigma}{\pi}} \frac{1}{k - \bar{k} + \mathrm{i}\sigma}. \tag{7}$$

These wave functions are only approximately localized in the sense that the probability of finding a photon decays exponentially far away from the center $\bar{x}$. The width σ in momentum space implies a localization length $1/\sigma$ in position space.

Figure 1 illustrates the collision of two approximately localized wave packets against a quantum impurity in a chiral medium. The average momentum of the wave packets $\bar{k}_1$ or $\bar{k}_2$ determines the group velocity at which the photons move $v_g(k) = \partial_k \omega_k$. The wave packets may be distorted due both to the dispersive nature of the medium and the interaction with the scatterer.

2.3. Scattering operator

In the typical scattering geometry, the interaction occurs in a finite region. Besides, it is assumed that asymptotically far away from that region the field is a linear combination of free-particle states (generated via creation operators on the non-interacting vacuum) even in the presence of the scatterer-waveguide interaction.

A sufficient condition for this is that both the ground state and any non-propagating excited state accessible by scattering $|\Omega_\mu\rangle$ are indistinguishable from the vacuum state $|\mathrm{vac}\rangle$ far away from the scatterer. Mathematically this occurs when

$$\lim_{\bar{x}\to\pm\infty}\langle\Omega_\mu|O(\bar{x},\,\Delta)|\Omega_\mu\rangle = \langle\mathrm{vac}|O(\bar{x},\,\Delta)|\mathrm{vac}\rangle, \tag{8}$$

where $O(\bar{x},\,\Delta)$ is an operator with compact support in the finite interval $\bar{x} - \Delta/2 < x < \bar{x} + \Delta/2$ and the vacuum state $|\mathrm{vac}\rangle$ is such that $a_k|\mathrm{vac}\rangle = 0\ \forall\, k$.

Besides, the free particle states must satisfy the asymptotic condition [43]:

$$\| U(t)|\Psi\rangle - U^0(t)|\Psi_{\mathrm{in/out}}\rangle \| \overset{t\to\mp\infty}{\longrightarrow} 0, \tag{9}$$

with $U(t)$ the evolution operator of the full Hamiltonian (2) and $U^0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$ the free-evolution operator.

The scattering operator S relates the amplitude of the output and input fields through

$$|\Psi_{\mathrm{out}}\rangle = S\,|\Psi_{\mathrm{in}}\rangle, \tag{10}$$

which, using (9), has the formal expression:

$$S = \lim_{t_\pm\to\pm\infty} U_I(t_+,\,t_-). \tag{11}$$

Here, $U_I(t_+,\,t_-) = \mathrm{e}^{\mathrm{i}H_0 t_-}\,\mathrm{e}^{-\mathrm{i}H(t_+-t_-)}\,\mathrm{e}^{-\mathrm{i}H_0 t_+}$ is the evolution operator in the interaction picture. Using again equation (9) leads to $|\Psi_{\mathrm{in}\ /\mathrm{out}}\rangle = U_0^\dagger(t_{-/+})U(t_{-/+})|\Psi\rangle \equiv |\Psi(t_{-/+})\rangle_I$, which shows that the input and output fields are represented in the interaction picture.

Related quantities are the scattering *amplitudes*. For example, the single-photon amplitude is defined as:

$$A \equiv \langle\Omega_\mu|\psi^{\mathrm{out}}(t_+)S\psi^{\mathrm{in}}(t_-)^\dagger|\Omega_\nu\rangle \tag{12}$$

with $\psi^{\mathrm{in}}(t_-)^\dagger = \psi_{\bar{k}\bar{x}}(t_-)^\dagger$ and an analogous definition for $\psi^{\mathrm{out}}(t_+)$ and the photon mean position $\bar{x}$ being well separated from the scatterer.

One of the goals of this work is to find the most general form for the amplitude A compatible with causality, thus providing a more clear understanding of the structure of the scattering matrix.

2.4. Sufficient conditions for having a well-defined scattering theory

Given a general Hamiltonian (2), it is not generally known whether the condition (8) is satisfied. Thus, the existence of scattering states must be assumed. In this work, we provide a further evidence of the validity of this assumptions by demonstrating a limited version of equation (8) (see appendix A) for the unique ground state of Hamiltonian (2), which reads

$$\langle\Omega_0|\psi_{\bar{k}\bar{x}}^\dagger\psi_{\bar{k}\bar{x}}|\Omega_0\rangle \leqslant \mathcal{O}(|\bar{x}|^{-n}),\quad |\bar{x}| \to \infty \tag{13}$$

provided that: (i) for all k, $|g_k/\omega_k| < \infty$ and (ii) that the correlators $C_{kp} = \langle\Omega_0|a_k^\dagger a_p|\Omega_0\rangle$ are n-differentiable functions.

Unfortunately, this result is insufficient for treating the most general case. It is well known that the Hamiltonian (2) may support excited eigenstates which are localized around the scattering center [34, 35, 44, 45], which in the literature are usually referred as *ground states*. Two paradigmatic examples of scatterer with multiple ground states are the three-level Λ atom, with two electronic ground state, and a two-level system coupled to a cavity array in the ultrastrong coupling regime [35].

However, we have been unable to find a general proof that (8) is satisfied (and thus that input and output states can be defined) for non propagating excited states that appear in these systems. In order to make any progress, and as usual in the literature, we have instead assumed a plausible *first condition*: the Hamiltonian (2) has a finite set of ground states, $\{|\Omega_\mu\rangle\}$, which are localized in the sense of equation (8). Notice that with this assumption (2) has a well defined theory (see appendix B.3). This condition allows the expression of the elements of S in the momentum basis:

$$(S_{\mathbf{pk}})_{\mu\nu} = \left\langle \Omega_\mu|\prod_i a_{p_i} S \prod_j a_{k_j}^\dagger|\Omega_\nu \right\rangle. \tag{14}$$

In this paper we will also assume a *second condition*: the N-photon scattering process conserves the number of flying photons in the input and output states. We only provide results for the sector of the scattering matrix that conserves the number of excitations, excluding us from considering other scattering channels, such as downconversion processes. Notice, however, that a large number of systems fulfill this condition. For instance, the unbiased spin-boson model (where $H_{\mathrm{sc}} \propto \sigma_z$ and $G = \sigma_x$) exactly conserves the number of excitations within the RWA, which is valid when the coupling strength is much smaller than the photon energy. But even in the ultrastrong coupling regime, when counter-rotating terms are important, numerical simulations have shown that the scattering process conserves the number of flying excitations within numerical uncertainties (see [35, 37, 46] and section 4.1).

3. Causality and the N-photon scattering matrix

3.1. Approximate causality

We are describing waveguide QED using nonrelativistic models for which strict causality (1) does not apply. However, as a foundational result we have been able to prove that the waveguide-QED model (2) supports an approximate form of causality. This form states that there exists an approximate light cone, defined by the maximum group velocity, $c = \max(\partial_k \omega_k)$. Two wave-packet operators which are outside their respective cones and far away from the scatterer approximately commute.

To be precise, we define the distance $d(x-y, t-t') = |\bar{x} - \bar{y}| - c|t-t'|$ and prove in appendix B that

$$\|[\psi_{\bar{k}\bar{x}}(t), \psi_{\bar{p}\bar{y}}(t')^\dagger]\| = \mathcal{O}\left(\frac{1}{|D|^n}\right) + \mathcal{O}\left(\frac{1}{|D_0|^{n-1}}\right), \tag{15}$$

with $D \equiv d(x-y, t-t')$ and $D_0 \equiv \min\{d(\bar{x}, t), d(\bar{x}, t_0), d(\bar{y}, t), d(\bar{y}, t_0)\}$ the distance between the packets and the minimum distance between them and the scatterer respectively. The power n stands because we use that the dispersion relation is n-times differentiable. A sketch of the proof is as follows. First, we prove (15) for free fields, i.e. for wave packets moving under H_0. In the Heisenberg picture, the phases $\mathrm{i}k(\bar{x}-\bar{y}) - \mathrm{i}\omega_k(t-t')$ can be bounded by the distance $d(x-y, t-t')$. Using the Riemann–Lebesgue lemma ($\int \mathrm{e}^{\mathrm{i}kz} f(k)\,\mathrm{d}k \to 0$, as $z \to \infty$) we find the power law decay, $|D|^{-n}$. Causality is thereby linked to the cancellation or averaging of fast oscillations in the unitary dynamics. Applying a similar technique to the interaction term in (2) allows us to prove that packets away the *influence* of the scatterer evolve freely, producing the second algebraic decay term $|D_0|^{1-n}$. This leads the second decay $|D_0|^{1-n}$. If their evolution can be approximated by the evolution under H_0, what we found for the commutator of free-evolving packets holds also in the interacting part.

This result is analogous to Lieb–Robinson-type bounds that were initially developed for a lattice of locally interacting spins [4], and which were later generalized to finite-dimensional models, (an)harmonic oscillators, master equations, and spin-boson lattices [6, 7, 47–51]. It is important to remark that the approximate causality in equation (15) is not obtained for the free theory, but for the *full* waveguide-QED model. As a consequence, it can be used to derive important results on the photon-scatterer interaction.

3.2. Causality and the scattering matrix

Causality imposes restrictions on the S-matrix [3], among which is the cluster decomposition that we summarize here. For now, let us consider the case of a unique ground state and split the S-matrix into a free part S^0 and an interacting part T, both in momentum space

$$S_{\mathbf{pk}} = S^0_{\mathbf{pk}} + \mathrm{i}T_{\mathbf{pk}}. \tag{16}$$

The interacting part T accounts for processes in which two or more photons coincide and interact simultaneously with the scatterer. Causality is then invoked to argue that they cannot influence each other if the input events are space-like separated. Thus, T does not contribute to the scattering amplitude as wave packets fall apart $|\bar{x}_i - \bar{x}_j| \to \infty$. This, together with energy conservation, imposes the constraint $\mathrm{i}T_{\mathbf{pk}} = \mathrm{i}C_{\mathbf{pk}}\delta(E_{\mathbf{p}} - E_{\mathbf{k}})$ [1]. In this limit the only term contributing to the scattering amplitude is the free part, S^0. In QFT (typically) occurs momentum conservation which implies that

$$S^0_{\mathbf{pk}} = \frac{1}{N!}\left(\prod_{n=1}^{N} S_{p_n k_n} + \text{permutations}[k_n \leftrightarrow k_m, p_n \leftrightarrow p_m]\right), \tag{17}$$

with $S_{p_n k_n} \propto \delta(\omega_{p_n} - \omega_{k_n})$ the one-photon S-matrix. In order to clarify the notation permutations$[k_n \leftrightarrow k_m, p_n \leftrightarrow p_m]$, let us write the two-photon S matrix:

$$S^0_{\mathbf{pk}} = \frac{1}{2}(S_{p_1k_1}S_{p_2k_2} + S_{p_2k_1}S_{p_1k_2} + S_{p_2k_2}S_{p_1k_1} + S_{p_1k_2}S_{p_2k_1}) = S_{p_1k_1}S_{p_2k_2} + S_{p_2k_1}S_{p_1k_2}. \tag{18}$$

This is nothing but the cluster decomposition. Fourier transforming $S^0_{\mathbf{pk}}$, this structure also holds

$$S^0_{\mathbf{yx}} = \frac{1}{N!}\left(\prod_{n=1^N} S_{y_n x_n} + \text{permutations}[x_n \leftrightarrow x_m, y_n \leftrightarrow y_m]\right). \tag{19}$$

This shall be relevant in the following section, where we will work in position space.

3.3. Generalized cluster decomposition

Our goal is to explain how approximate causality (15) implies a cluster decomposition for the S-matrix. We will also show that in waveguide QED the photon momenta need not be conserved and that S^0 may not have the structure given by equation (17).

To understand how causality fixes the form of S^0 we refer to our figure 1 where two well separated wave packets interact with a scatterer. The scattering amplitude is,

$$A = \langle \Omega_\mu | \prod_{m=1}^{2} \psi^{\rm out}_{\bar{p}_m \bar{y}_m}(t_+) \prod_{n=1}^{2} \psi^{\rm in}_{\bar{k}_n \bar{x}_n}(t_-)^\dagger | \Omega_\nu \rangle.$$

Note that for a sufficiently large separation of the wave packets, the output state of the first packet must be causally disconnected. This implies that the input operator for the first wave packet must commute with the output operator for the second packet (see equation (15)). Notice that the second output and the first input will not commute in general. We can then approximate, at any degree of accuracy, the above amplitude as,

$$A \simeq \langle \Omega_\mu | \psi^{\rm out}_{\bar{p}_2 \bar{y}_2}(t_+) \psi^{\rm in}_{\bar{k}_2 \bar{y}_2}(t_-)^\dagger \psi^{\rm out}_{\bar{p}_1 \bar{x}_1}(t_+) \psi^{\rm in}_{\bar{k}_1 \bar{x}_1}(t_-)^\dagger | \Omega_\nu \rangle. \tag{20}$$

Let us know insert the identity between the operators $\psi^{\rm in}_{\bar{k}_2 \bar{x}_2}(t_-)^\dagger$ and $\psi^{\rm out}_{\bar{p}_1 \bar{y}_1}(t_+)$. Recalling the conditions discussed in section 2.4, namely the localized nature for the ground states together with the fact that there is not particle creation, just $\{|\Omega_\lambda\rangle\}_{\lambda=0}^{M-1}$ will contribute to the identity. The final result is:

$$A_{12} = \sum_{\lambda=0}^{M-1} A_{1,\nu\to\lambda} A_{2,\lambda\to\mu}, \tag{21}$$

with $A_{1,\nu\to\lambda} = \langle \Omega_\lambda | \psi^{\rm out}_{\bar{p}_1 \bar{y}_1}(t_+) \psi^{\rm in}_{\bar{k}_1 \bar{x}_1}(t_-)^\dagger | \Omega_\nu \rangle$ and similarly for $A_{2,\lambda\to\mu}$. We can generalize this expression to N photons, with initial average positions $\bar{x}_1 > \bar{x}_2 > \ldots > \bar{x}_N$ and asymptotic ground states $\lambda_0 := \nu$ and $\lambda_N := \mu$

$$A = \sum_{\lambda_1,\ldots,\lambda_{N-1}=0}^{M-1} \prod_{n=1}^{N} A_{n,\lambda_{N+1-n}\to\lambda_{N-n}}, \tag{22}$$

with

$$A_{n,\lambda_{N+1-n}\to\lambda_{N-n}} = \langle \Omega_{\lambda_{N-n}} | \psi^{\rm out}_{\bar{p}_n \bar{y}_n}(t_+) \psi^{\rm in}_{\bar{k}_n \bar{x}_n}(t_-)^\dagger | \Omega_{\lambda_{N+1-n}} \rangle. \tag{23}$$

The sketched constructive demonstration (a complete demonstration is given in appendix C) has confirmed that causality imposes that the amplitude can be built from single photon events whenever those are well separated. Inelastic processes yield the sum over intermediate states. If only one ground state is considered, the amplitude is the product $A = \Pi_n A_n$. In this case, the S-matrix in momentum space recovers the typical structure in QFT (see equation (17)). However, when inelastic-scattering events occur, the sum in (22) leads to a particular structure for the free part of the scattering matrix S^0 that we discuss now.

We now find the structure for S^0 in position space compatible with the amplitude (22). For the sake of simplicity, we work with chiral waveguides and a monotonously growing dispersion relation, $\partial_k \omega_k \geqslant 0$. Therefore, we can order the events using step functions, eliminating unphysical contributions (e.g. the wave packet $\psi_{\bar{k}_2 \bar{x}_2}$ arriving before than $\psi_{\bar{k}_1 \bar{x}_1}$, see figure 1). Some algebra, fully described in appendix D yields that S^0 has the following structure

$$(S^0_{\mathbf{yx}})_{\mu\nu} = \sum_{\lambda_1\ldots\lambda_{N-1}=0}^{M-1} \prod_{n=1}^{N} (S_{y_n x_n})_{\lambda_{N+1-n}\lambda_{N-n}} \prod_{m=1}^{N-1} \theta(y_{m+1} - y_m) + \text{permutations}[x_n \leftrightarrow x_m, y_n \leftrightarrow y_m]. \tag{24}$$

The sum over intermediate states and the Heaviside functions are a direct consequence of causality, since they order the different wave packets and keep track of the state of the scatterer for each arrival. Nevertheless, if the ground state is unique ($M = 1$), the step functions cancel out and we recover the structure described by (19). However, strikingly, for $M > 1$ this S-matrix cannot be written as a product of one-photon scattering matrices, up to permutations, due to the Heaviside functions. In order to shed light on this, it is convenient to move to momentum space. Although $(S^0_{\mathbf{pk}})_{\mu\nu}$ cannot be analytically calculated for a general dispersion relation, a mathematical expression can be found for a linear one. This calculation will be presented in section 4.2. The final result is that $(S^0_{\mathbf{pk}})_{\mu\nu}$ cannot be written as a product of one-photon S-matrices. This has been recently pointed out in the particular example of a Λ atom coupled to a waveguide within the RWA and Markovian approximations with point-like coupling by Xu and Fan [38] using the input–output formalism [27].

As we said in the introduction, the generalization to nonchiral waveguides is straightworward. We explain the details in appendix E.

4. Applications

The set of previous theorems and conditions create a framework that describes many useful problems and experiments in waveguide QED. We are now going to illustrate two particular problems which are amenable to numerical and analytical treatment, and which highlight the main features of all the results.

The first problem consists of a two-level system that is *ultrastrongly* coupled to a photonic crystal. The scattering dynamics has to be computed numerically. The simulations fully conform to our our framework,

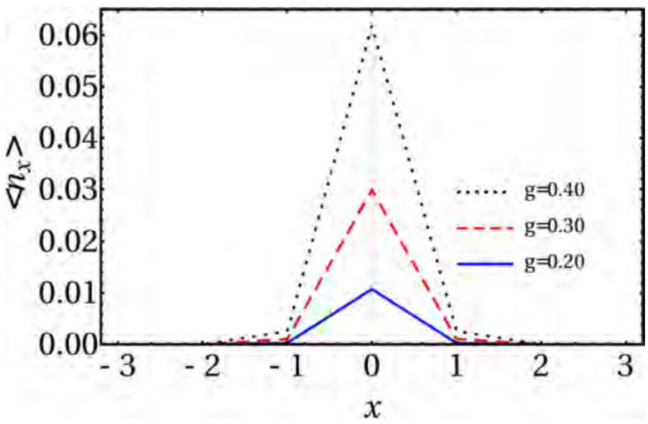

Figure 2. Number of excitations in position space of the minimum-energy state of (25) for $\epsilon = 1$, $J = 1/\pi$, and $\Delta = 1$, varying g. The coordinate x is dimensionless, since we are working in units such that the lattice spacing b is 1.

showing the fast decay of photon-qubit dressing with the distance, the independence of space-like separated wave packets, and the decomposition of the two-photon scattering amplitude as a product (for the chosen parameters, the one-photon scattering is elastic).

The second problem consists of a general scatterer with several ground states that is coupled to a *non-dispersive* medium and it serves to illustrate the breakdown of the S-matrix decomposition in momentum space.

4.1. Ultrastrong scattering

Let us consider a system described by the following Hamiltonian

$$H = \Delta\sigma^+\sigma^- + \epsilon\sum_x a_x^\dagger a_x - J\sum_x (a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x) + g(\sigma^- + \sigma^+)(a_0 + a_0^\dagger). \tag{25}$$

The scatterer is a two-level system described by the ladder operators $\sigma^\pm$ and the level splitting Δ. The lattice tight-binding Hamiltonian, describes an array of identical cavities with frequency ϵ, cavity–cavity coupling J, and bosonic modes $[a_x, a_y^\dagger] = \delta_{xy}$. We work in units such that the lattice spacing is the unit of length.

The lattice model (second and third terms of the Hamiltonian) is diagonalized in momentum space, giving raise to a cosine-shaped dispersion relation, $\omega_k = \epsilon - 2J\cos k$. Some recent implementations of such cosine-shaped dispersion are superconducting coupled resonators and photonic crystals (see [23, 40, 41] respectively).

The scatterer-waveguide interaction, which is described by the last term, is point-like and g is the coupling constant.

The light–matter interaction term can be expressed as a sum of the RWA part, $g(\sigma^+ a_0 + \sigma^- a_0^\dagger)$, and the so-called counter-rotating terms, $g(\sigma^- a_0 + \sigma^+ a_0^\dagger)$. The latter can be neglected if g is small enough compared to the other energies of the full system. This is known as the RWA. It is well known that the RWA simplifies the problem because: (i) the new effective model conserves the number of excitations and (ii) the ground state is the trivial vacuum $|\text{vac}\rangle$ with $\sigma^-|\text{vac}\rangle = a_x|\text{vac}\rangle = 0\ \forall x$. However, when the coupling strength is large enough—the so-called ultrastrong coupling regime—the RWA fails to describe the dynamics and one has to use the full Rabi model (25). This regime not only represents an interesting and challenging problem where we can test our theoretical framework, but it describes a family of current experiments [24, 52–54] for which the following simulations are of interest. An important remark is that, despite the fact that the number of excitations $\hat{N} = \sum_x a_x^\dagger a_x + \sigma^+\sigma^-$ is not a good quantum number, i.e. $[H, \hat{N}] \neq 0$, numerical simulations indicate that the total number of flying photons is asymptotically conserved throughout the simulation [35, 37]. Therefore, the second condition needed for proving our results is fulfilled (see section 2.4).

We have studied this model using the matrix-product-state variational ansatz, a celebrated method for describing the low-energy sector of one-dimensional many-body systems [55–58], which has been recently adapted to the photonic world in [35, 37, 59]. Using this ansatz, we computed the nontrivial minimum-energy state [35], which consists of a photonic cloud exponentially localized around the qubit, see figure 2. This result confirms our theoretical predictions from equation (13) and implies that the minimum-energy state $|\Omega_0\rangle$ can be approximated by the vacuum far away from the qubit.

According to the previous result, we can generate free wave packets, such as input and output states of equations (C1) and (C2) by inserting photons far away from the scatterer. We have used the MPS ansatz to study the evolution of input states which consist of a pair of photons, see equation (C1), with $|\Omega_\nu\rangle = |\Omega_0\rangle$. Both wave packets will be Gaussians, equation (6), with mean momentum $\bar{k}$ and width σ. The numerical simulations show that the scattering is elastic for the chosen parameters ($\epsilon = 1$, $J = 1/\pi$, $\Delta = \epsilon = 1$, and $g = 0.3$) [35].

We have also demonstrated numerically that the correlation between output photons vanish as the separation between the input wave packet increases. Our study aimed at computing the two-photon wave function in momentum space, $\phi_{p_1,p_2}(t) = \langle \Omega_0 | \, a_{p_1} a_{p_2} | \Psi(t) \rangle$. This was used to compute the fluorescence F at time t_+, the number of output photons whose energy and momentum differ from the input wave packets. More precisely

$$F = \int \mathrm{d}p_1 \mathrm{d}p_2 \, |\phi_{p_1,p_2}(t_+)|^2, \tag{26}$$

with p_1 and p_2 such that $\omega_{p_1} + \omega_{p_2} = 2(\omega_{\bar{k}} \pm \sigma_\omega)$ and $\omega_{p_1}, \omega_{p_2} \not\in (\omega_{\bar{k}} - \sigma_\omega, \omega_{\bar{k}} + \sigma_\omega)$, being σ_ω the width of the input wave packets in energy space. Figure 3(g) shows F as function of the distance between the incident wave packets. When the wave packets are close enough the fluorescence maximizes and the output wave function shows a nontrivial structure, with $\phi_{p_1,p_2}(t_+) \neq 0$ even though $|p_1| \neq \bar{k}$ or $|p_2| \neq \bar{k}$ (see panels (a) and (c)). The wave function has also a rich structure in position space, with antibunching in the reflection component and superbunching in the transmission one (see panels (b) and (d)). This structure was already found in the RWA [60]. For long distances, the fluorescence F vanishes (see panels (e) and (f)). In these cases, the output state is clearly uncorrelated: in position space it is formed by two well-defined wave packets and $\phi_{p_1,p_2}(t_+)$ goes to zero if $|p_1| \neq \bar{k}$ or $|p_2| \neq \bar{k}$. All this is a consequence of the cluster decomposition, see equation (22) and theorem 4 in appendix C.

4.2. Inelastic scattering and linear dispersion relation: the cluster decomposition revisited

We set $\omega_k = c|k|$ in H_0. The scatterer and interaction are described by

$$H_{\mathrm{sc}} = \sum_{\nu=0}^{M-1} E_\nu |\Omega_\nu\rangle \langle \Omega_\nu| + \sum_{J=0}^{M'-1} \tilde{E}_J |J\rangle \langle J|, \tag{27}$$

$$H_{\mathrm{int}} = \sum_{J=0}^{M'-1} \sum_{\nu=0}^{M-1} g_{J,\nu} (|J\rangle \langle \Omega_\nu| \, a_0 + \mathrm{H.c.}), \tag{28}$$

where $\{|\Omega_\nu\rangle\}$ and $\{|J\rangle\}$ are the ground and decaying states of the scatterer, respectively, $\{E_\nu\}$ and $\{\tilde{E}_J\}$ are their energies, M and M' is the number of ground and excited states, respectively, and $g_{J,\nu}$ is the coupling strength corresponding to the transition $|\Omega_\nu\rangle \leftrightarrow |J\rangle$ (see figure 4). This is a prototypical situation in waveguide QED. E.g., if there are two ground states, $M = 2$, and the decaying state is unique, $M' = 1$, the scatterer is a Λ atom. From now on, we work in units such that $c = 1$. We further assume chiral waveguides: the scatterer only couples to $k > 0$, which simplifies the final expressions, so we can start from equation (24). Before writing down the two-photon S^0-matrix in momentum space, we need the one-photon scattering matrix. Imposing energy conservation, it has to be

$$(S_{pk})_{\mu\nu} = t_{\mu\nu}(k) \delta(p + E_\mu - k - E_\nu), \tag{29}$$

with k and p the incident and outgoing momenta, respectively, and $|\Omega_\nu\rangle$ and $|\Omega_\mu\rangle$ the initial and final ground states. The factor $t_{\mu\nu}(k)$ is the so-called transmission amplitude. The Dirac delta guarantees energy conservation. Then, the two-photon S^0-matrix, equation (24) in momentum space is

$$\begin{aligned}(S^0_{\mathbf{pk}})_{\mu\nu} &= \frac{1}{(2\pi)^2} \iint (S^0_{\mathbf{yx}})_{\mu\nu} \mathrm{e}^{-\mathrm{i}\mathbf{p}^T\mathbf{y} + \mathrm{i}\mathbf{x}^T\mathbf{k}} \mathrm{d}^2\mathbf{y}\mathrm{d}^2\mathbf{x} \\ &= \frac{\mathrm{i}}{2\pi} \sum_{n,m=1}^{2} \sum_{\lambda=0}^{M-1} \frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_m + E_\mu - k_n - E_\lambda + \mathrm{i}0^+} \delta(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu).\end{aligned} \tag{30}$$

Here, $n' \neq n$, e.g., $n' = 2$ if $n = 1$. The computation is detailed in appendix F. This structure has recently been found by Xu and Fan for a Λ atom ($M = 2$, $M' = 1$) within the RWA and Markovian approximations [38]. At first sight (30) may look striking. The matrix S^0 is not the product of two Dirac-delta functions conserving the single-photon energy, as discussed in section 3.2. The mathematical origin of the structure can be traced back to its form in position space, equation (24). The Heaviside functions set the order in which the different wave packets impinge on the scatterer. The product of Dirac-delta functions is recovered if $M = 1$ (see appendix F). Besides, equation (30) is also remarkable because presents the generalization of the cluster decomposition for the S-matrix (see equations (16) and (17)) when inelastic processes occur in the scattering.

A consequence of (30) is that S^0 contributes to the fluorescence F, equation (26). This seems to contradict our previous arguments, since S^0 is built from causally disconnected one-photon events (they do not overlap in the scatterer). To solve the apparent paradox we recall that (30) is a matrix element in momentum space (delocalized photons). For wave packets (5), the scattering amplitude is the integral of these wave packets with (30). In doing so we find that the fluorescence decays to zero as the separation grows, thus solving the puzzle.

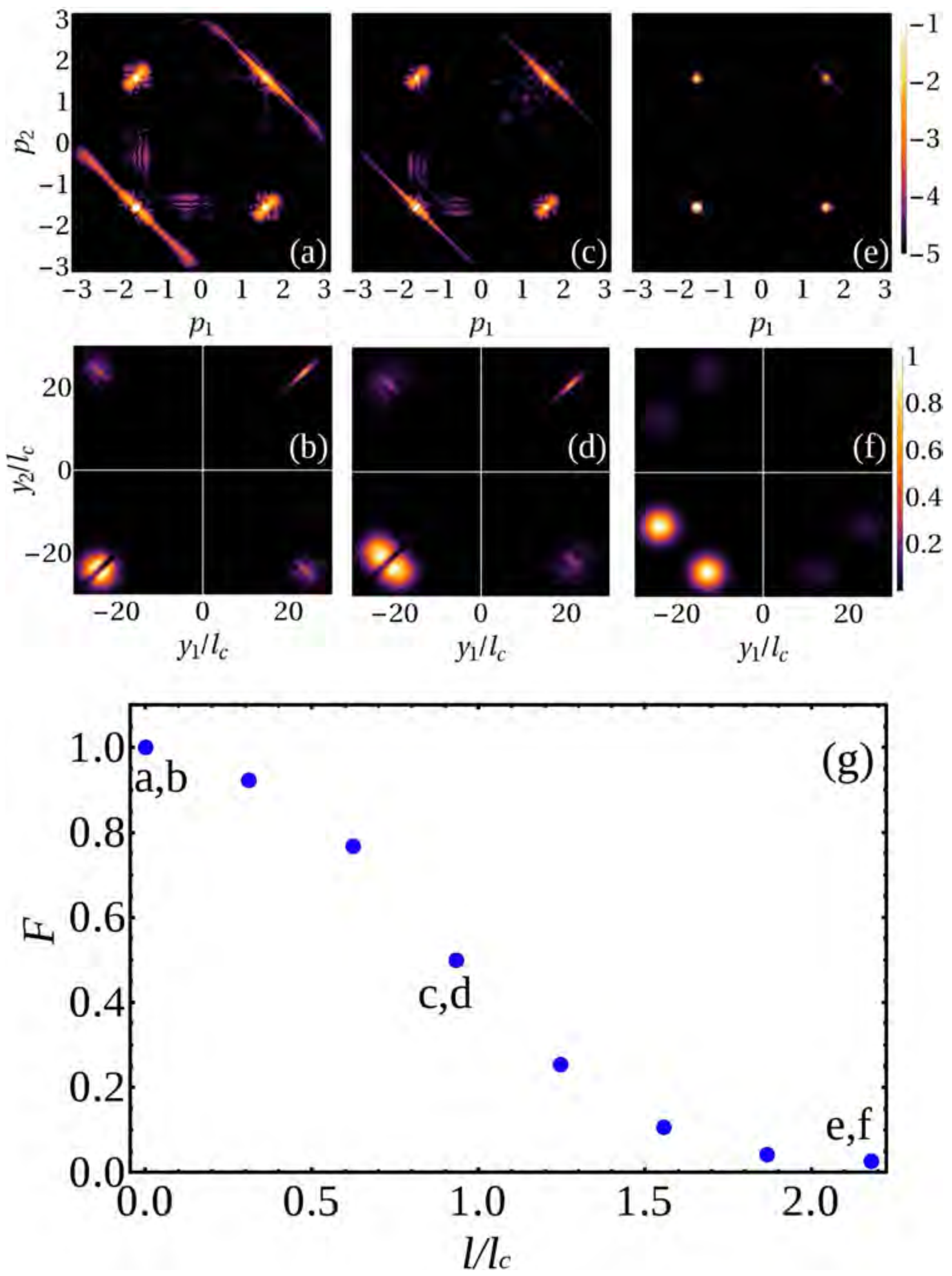

Figure 3. Output wave function in momentum/position space, (a)/(b), (c)/(d), and (e)/(f) for several values of the distance between the input photons and (g) fluorescence F for the two-photon output state as a function of the distance l between the two input wave packets. The values of the distances of the panels (a)–(f) are indicated in the panel (g). We choose $g = 0.3$. The values for the other parameters coincide with those of figure 2. Both incoming photons are on resonance with the qubit, $\omega_k = \Delta$. The distance l is in units of $l_c \simeq 1.719\sigma$, with l_c such that we can resolve the incident packets if and only if $l > l_c$.

In what follows the fluorescence decay is discussed within the *full* S-matrix, i.e. we consider the contributions to F from S^0 and T (see equation (16)). Energy conservation imposes that $(T_{p_1p_2k_1k_2})_{\mu\nu} = (C_{p_1p_2k_1k_2})_{\mu\nu}\, \delta(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu)$. Since the contribution of T vanishes as the photon–photon separation increases, C must be sufficiently smooth, at least smoother than a Dirac delta [1]. Then, we assume that $(C_{p_1p_2k_1k_2})_{\mu\nu}$ has simple poles with imaginary parts $\{\gamma_n^C\}$. Similarly, we expect that divergences of $t_{\mu\nu}(k)$ come from simple poles with imaginary parts $\{\gamma_n^t\}$. As far as we know, this structure has been found for all S-matrices in waveguide QED [27, 38, 61, 62].

Let us write down the input state in momentum space

$$|\Psi_{\rm in}\rangle = \int \mathrm{d}k_1 \mathrm{d}k_2\ \phi_1(k_1)\phi_2(k_2)\mathrm{e}^{\mathrm{i}k_2 l} a_{k_1}^\dagger a_{k_2}^\dagger |\Omega_\nu\rangle. \tag{31}$$

The functions $\phi_1(k)$ and $\phi_2(k)$ are localized far away the scattering region in position space. The exponential factor $\mathrm{e}^{\mathrm{i}k_2 l}$ ensures the separation between both wave packets is l. The output state reads

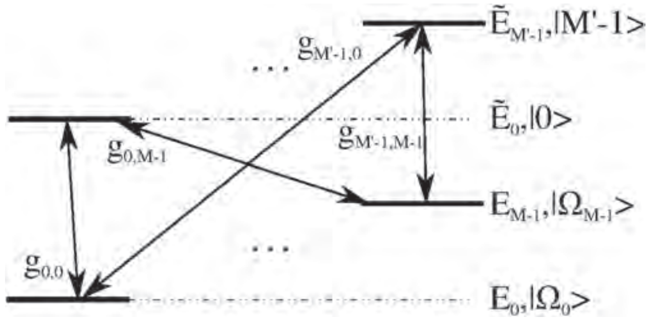

Figure 4. Level structure of the scatterer described by the Hamiltonian (27), interacting with a waveguide via (28). The photons induce transitions between the set of states $\{|J\rangle\}$ and the ground states $\{|\Omega_\nu\rangle\}$ with coupling strengths $g_{J,\nu}$.

$$|\Psi_{\rm out}\rangle = S|\Psi_{\rm in}\rangle = \sum_\mu \int {\rm d}p_1 {\rm d}p_2\ \phi_\mu^{\rm out}(p_1, p_2) a_{p_1}^\dagger a_{p_2}^\dagger |\Omega_\mu\rangle \tag{32}$$

with the two-photon wave function $\phi_\mu^{\rm out}(p_1, p_2)$

$$\phi_\mu^{\rm out}(p_1, p_2) \propto \sum_{n=1}^{2}\sum_{m=1}^{2} \int {\rm d}k_n \left(\frac{\rm i}{2\pi}\sum_\lambda \frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(p_1+p_2+E_\mu-k_n-E_\nu)}{p_m+E_\mu-k_n-E_\lambda+{\rm i}0^+} + {\rm i}(\tilde{C}_{p_1p_2k_n})_{\mu\nu}\right)$$
$$\times\ (\phi_1(k_n){\rm e}^{{\rm i}(p_1+p_2+E_\mu-k_n-E_\nu)l}\phi_2(p_1+p_2+E_\mu-k_n-E_\nu) + \phi_1(p_1+p_2+E_\mu-k_n-E_\nu){\rm e}^{{\rm i}k_n l}\phi_2(k_n)), \tag{33}$$

being $(\tilde{C}_{p_1p_2k_n})_{\mu\nu} = \int {\rm d}k_{\bar n}(C_{p_1p_2k_nk_{\bar n}})_{\mu\nu}\delta(p_1+p_2+E_\mu-k_n-k_{\bar n}-E_\nu)$, with $\bar n \neq n$. Even though this expression is cumbersome, we can clearly identify the contribution of S^0 and T. We solve this integral by means of the residue theorem. Each pole γ_n^t and γ_n^C, together with the exponentials ${\rm e}^{{\rm i}k_n l}$ and ${\rm e}^{{\rm i}(p_1+p_2+E_\mu-k_n-E_\lambda)l}$, gives an exponentially decaying term, ${\rm e}^{-|\gamma_n^t|l}$ or ${\rm e}^{-|\gamma_n^C|l}$. We choose Lorentzian envelopes for the wave packets. They have a pole at $\bar{k} - {\rm i}\sigma$ (see equation (7)). In consequence, the wave packets will give a term proportional to ${\rm e}^{-\sigma l}$. Lastly, the imaginary part of the pole of the first term vanishes, $\sim{\rm i}0^+$, so it gives a nondecaying term, ${\rm e}^{-0^+l} = 1$. The real part of this denominator imposes the single-photon-energy conservation. Thus, it results in the amplitude for the single-photon events, $\sum_\lambda A_{1,\nu\to\lambda}A_{2,\lambda\to\mu}$. Therefore, nor S^0 neither T contains fluorescent terms as the separation between the wave packets grows. The technical details are in appendix G.

As a final application, one can find experimentally the poles of the one- and two-photon scattering matrices $\{\gamma_n^t\}$ and $\{\gamma_n^C\}$ by measuring the decay of F with the distance.

5. Final comments

Our work represents a significant evolution over the field-theoretical methods [13] that have been so successfully adapted to the study of waveguide QED. Developing an extensive set of theorems shown in the appendices, we have completed a program that derives the properties of the N-photon S-matrix from the emergent causal structure of a nonrelativistic photonic system. This, together with the fact that the ground states of the Hamiltonian are trivial far away from the scatterer and the asymptotic independence of input and output wave packets, allows us to build a consistent scattering theory. Among the consequences of this framework, we have explained how the existence of Raman (inelastic) processes modifies the usual form of the cluster decomposition to produce a structure that includes the particular example developed in [38].

Our formal results also provide insight in the outcome of simulations for problems where no analytical derivation is possible, such as a qubit ultrastrongly coupled to a waveguide [35, 37]. As a second example, we have considered a non-dispersive media $\omega_k = c|k|$, where we found the general form for the scattering matrix in momentum space (independent of the scatterer and the coupling to the waveguide), which has been recently calculated for a Λ atom [38] as a particular case. On top of that, we have clarified how fluorescence decays in a general scattering experiment.

Throughout the previous discussion we have focused our attention to scattering processes which involve the same number of flying photons both at the input and the output (see section 2.4), but this is just a convenient restriction that can be lifted. One may incorporate more scattering channels for the photons using extra indices to keep track of the photon-annihilation and creation processes, which results in a slightly more involved version of theorem 4. In particular, we can incorporate photon-creation events (see e.g. [59]). Finally, our program can be extended to treat other systems, deriving a cluster decomposition for the scattering of spin waves in quantum-magnetism models or for fermionic excitations in many-body systems.

Acknowledgments

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Appendix A. The ground state of the light–matter interaction

In this appendix we demonstrate that the ground state converges to the trivial vacuum far away from the scatterer, equation (13). The next lemma is neccessary to proof the main theorem.

Lemma 1. *Given the waveguide-QED model (2), we have the following bounds for the expectation values on its minimum-energy state* $|\Omega_0\rangle$,

$$|\langle\Omega_0|a_k^\dagger a_p|\Omega_0\rangle| \leqslant \sqrt{\left|\frac{g_k g_p}{\omega_k\omega_p}\right|}\langle\Omega_0|GG^\dagger|\Omega_0\rangle. \tag{A1}$$

Proof. Let us assume that $|\Omega_0\rangle$ is the minimum-energy state of H as given by equation (2), and thus $(H - E_0)|\Omega_0\rangle = 0$. The energy of the unnormalized state

$$|\chi\rangle = O|\Omega_0\rangle, \tag{A2}$$

created by any operator O must be larger or equal to that of the ground state, $\langle\chi|(H - E_0)|\chi\rangle \geqslant 0$. Using (A2)

$$\langle\chi|(H - E_0)|\chi\rangle = \langle\Omega_0|O^\dagger HO - O^\dagger OH|\Omega_0\rangle \tag{A3}$$

we conclude with the useful relation

$$\langle\chi|H - E_0|\chi\rangle = \langle\Omega_0|O^\dagger[H, O]|\Omega_0\rangle \geqslant 0. \tag{A4}$$

Let us take $O = a_k$. The previous statement leads to

$$\langle\Omega_0|a_k^\dagger(-\omega_k a_k - g_k G)|\Omega_0\rangle \geqslant 0, \tag{A5}$$

or equivalently

$$0 \leqslant \langle\Omega_0|a_k^\dagger a_k|\Omega_0\rangle \leqslant -\frac{g_k}{\omega_k}\langle\Omega_0|Ga_k^\dagger|\Omega_0\rangle. \tag{A6}$$

Using Cauchy–Schwatz, this translates into the upper bound

$$\langle\Omega_0|a_k^\dagger a_k|\Omega_0\rangle \leqslant \frac{|g_k|}{\omega_k}\sqrt{\langle\Omega_0|GG^\dagger|\Omega_0\rangle\langle\Omega_0|a_k^\dagger a_k|\Omega_0\rangle}. \tag{A7}$$

Once the diagonal elements of the correlation matrix are bounded the nondiagonal can also be bounded. The correlation matrix is positive $C \geqslant 0$ with $C_{kp} = \langle\Omega_0|a_k^\dagger a_p|\Omega_0\rangle$. A property of positive matrices is [63]

$$|C_{kp}| \leqslant \sqrt{|C_{kk}||C_{pp}|} \tag{A8}$$

which implies (A1).

With this lemma at hand we state:

Theorem 1. *Let us define* $\psi_{\bar{k}\bar{x}x}^\dagger$ *as the operator (5) removing the time-dependent part, where* $\phi_{\bar{k}}(k)$ *is infinitely differentiable with a finite support K centered around* $\bar{k}$. *Then, the expected value of* $\psi_{\bar{k}\bar{x}}^\dagger\psi_{\bar{k}\bar{x}}$ *in the minimum-energy state fulfills*

$$\langle\Omega_0|\psi_{\bar{k}\bar{x}}^\dagger\psi_{\bar{k}\bar{x}}|\Omega_0\rangle \to 0, \quad |\bar{x}| \to \infty, \tag{A9}$$

where we choose $x_{\rm sc} = 0$. *Moreover, if we can assume that* $\langle a_k^\dagger a_p\rangle$ *is an n-times differentiable function of k and p, the bound will be improved*

$$\langle\Omega_0|\psi_{\bar{k}\bar{x}}^\dagger\psi_{\bar{k}\bar{x}}|\Omega_0\rangle \leqslant \mathcal{O}(|\bar{x}|^{-n}), \quad |\bar{x}| \to \infty. \tag{A10}$$

Proof. Let us compute the expectation value of the number operator for a wave packet $N := \langle\Omega_0|\psi_{\bar{k}\bar{x}}^\dagger\psi_{\bar{k}\bar{x}}|\Omega_0\rangle$,

$$N = \iint \langle\Omega_0|a_k^\dagger a_p|\Omega_0\rangle\, \mathrm{e}^{\mathrm{i}(k-p)\bar{x}}\phi_{\bar{k}}(k)^*\phi_{\bar{k}}(p)\mathrm{d}k\mathrm{d}p. \tag{A11}$$

We can rewrite N as the Fourier transform of another function $N = \int \mathrm{e}^{\mathrm{i}u\bar{x}} F(u)\,\mathrm{d}u$, where

$$F(u) := \frac{1}{2}\int \phi_{\bar{k}}((u+v)/2)^* \phi_{\bar{k}}((u-v)\Big/2)\langle a^\dagger_{(u+v)/2} a_{(u-v)/2}\rangle \mathrm{d}v. \tag{A12}$$

We are now going to assume that $\phi_{\bar{k}}(k)$ is a test function with compact support K of size $|K|$ centered around $\bar{k}$, and infinitely differentiable. We will also assume that within its support $|g_k/\omega_k|^2\langle GG^\dagger\rangle \leqslant C_\phi$ for some constant C_ϕ. Then we can bound

$$\int |F(u)|\mathrm{d}u \leqslant |K|^2 C_\phi. \tag{A13}$$

Assuming that $\langle\Omega_0|a_k^\dagger a_p|\Omega_0\rangle$ is n-times differentiable and using the Riemann–Lebesgue theorem, we have then that

$$\left|\int \mathrm{e}^{\mathrm{i}u\bar{x}} F(u)\mathrm{d}u\right| \leqslant \mathcal{O}(|\bar{x}|^{-n}) \tag{A14}$$

at long distances.

Appendix B. Approximate causality

B.1. Free-field causality

We first prove causal relations in a free theory. In order to do so, we work with localized wave packets $\psi_{\bar{k}\bar{x}}(t)$, equation (5). Actual calculations are done with Gaussian wave packets, equation (6). The following two lemmas are used in the demonstration of the theorem.

Lemma 2. *Let the dispersion relation* ω_k *have an upper bounded group velocity* $v_k = \partial_k\omega_k$:

$$|v_k| \leqslant c. \tag{B1}$$

Then, the function $f(k) = kx - \omega_k t$ *only has stationary points if the distance to the light cone is nonnegative. In other words*

$$d_c(x, t) = |x| - c|t| > 0 \Leftrightarrow |f'(k)| > 0, \forall k. \tag{B2}$$

Proof. Solving the equation $f'(k) = x - \partial_k\omega_k t = 0$ leads to the condition $\frac{x}{t} = v_k$ or $|x/t| = |v_k| \leqslant c$. Then, provided $f'(k) = 0$, it follows $|x| \leqslant c|t| \Rightarrow d_c(x, t) \leqslant 0$, which shows (B2). □

Lemma 3. *Assume that* ω_k *is* n*-times differentiable and that every derivative* $|\omega_k^{(r\leqslant n)}|$ *is upper bounded by an* m*th order polynomial in* $|k|$*. Then the following integral bound applies*

$$\left|\int \mathrm{e}^{\mathrm{i}kx - \frac{1}{\sigma^2}(k-k_0)^2 - \mathrm{i}\omega_k t} p(k)\mathrm{d}k\right| = \max(\sigma^{m+n+r}, 1)\max(t^n, 1)\mathcal{O}\left(\frac{1}{|x|^n}\right),$$

where $p(k)$ *is a polynomial of degree* r.

Proof. Result 5.1 from [64] states that the integral $I(x) = \int_a^b \mathrm{e}^{\mathrm{i}kx} q(k)\mathrm{d}k$ may be integrated by parts n times, obtaining

$$I(x) = \sum_{s=0}^{n-1}\left(\frac{\mathrm{i}}{x}\right)^{s+1}[\mathrm{e}^{\mathrm{i}ax} q^{(s)}(a) - \mathrm{e}^{\mathrm{i}bx} q^{(s)}(b)] + \epsilon_n(x), \tag{B3}$$

where the error term satisfies

$$\epsilon_n(x) = \left(\frac{\mathrm{i}}{x}\right)^n \int \mathrm{e}^{\mathrm{i}kx} q^{(n)}(k)\mathrm{d}k = o(x^{-n}) \tag{B4}$$

provided that $q(k)$ is n-times differentiable and that $q^{(n)} \in L^1$. Based on the conditions of the lemma, this is satisfied since $q(k) = \mathrm{e}^{-\frac{1}{\sigma^2}(k-k_0)^2 - \mathrm{i}\omega_k t} p(k)$. The limits of the integral may be easily extended to $\pm\infty$, as explained in result 5.2 from [64]. Since $x^{-s} q^{(s)}(a) \to 0$ when $a \to \pm\infty$, $\forall x$, we obtain

$$I(x) = \int \mathrm{e}^{\mathrm{i}kx} q(k)\,\mathrm{d}k = \left(\frac{\mathrm{i}}{x}\right)^n \int \mathrm{e}^{\mathrm{i}kx} q^{(n)}(k)\mathrm{d}k. \tag{B5}$$

Moreover, $q^{(n)}$, resulting from a product of derivatives of $\omega_k t$, $-k^2/\sigma^2$ and the polynomial $p(k)$ of degree r, is bounded by a polynomial of at most $(m+n+r)$th order in $|k|$. Such a polynomial is integrable together with the Gaussian wave packet giving a constant prefactor. In estimating this factor, we can take the worst-case scenario for the terms in t, which appears at most n times together with $(\partial_k\omega_k)^n$, and the monomials in $|k|$, which produce another prefactor σ^{m+n+r}.

Note that it would suffice to consider $q(k)$ as a test function or even a Schwartz function since in this case all the differentiability requisities are fullfilled and $x^{-s}q^{(s)}(a) \to 0 \to 0$ when $a \to \pm\infty$, $\forall\, x$ still holds, because these functions and their derivatives are rapidly decreasing.

With these lemmas at hand we can prove:

Theorem 2. *Let the Hamiltonian be given just by the photonic part,* $H_0 = \int \mathrm{d}k\ \omega_k a_k^\dagger a_k$. *Let* $\psi_{\bar{k}\bar{x}}(t)$ *and* $\psi_{\bar{p}\bar{y}}(t')$ *denote two localized wave packets of the form (6). We will assume that: (i) the absolute value for the group velocity of these wave packets is upper bounded by a constant c within the domain of the wave packets* ($|v_k| = |\partial_k\omega_k| \leqslant c$) *and (ii) the dispersion relation is n-times differentiable and that each derivative is upper bounded by a polynomial of at most order m:*

$$|\partial_k^{(r\leqslant n)}\omega_k| \leqslant a_r + (|k|/b_r)^m,\ \ 0 < a_r,\, b_r < +\infty. \tag{B6}$$

The commutator between these wave packets is small whenever they are outside of their respective light cones, that is, whenever $d = |\bar{y} - \bar{x}| - c|t' - t| \gg 0$,

$$\|[\psi_{\bar{k}\bar{x}}(t),\, \psi_{\bar{p}\bar{y}}(t')^\dagger]\| = \mathcal{O}\left(\frac{1}{|d|^n}\right),\ \ d \to \infty. \tag{B7}$$

Proof. Let us assume that the model evolves freely according to the free Hamiltonian $H_0 = \int \mathrm{d}k\ \omega_k a_k^\dagger a_k$. In this case, our wave packet operators have the simple form

$$\psi_{\bar{k}\bar{x}}(t) = \int \mathrm{e}^{\mathrm{i}k\bar{x} - \mathrm{i}\omega_k t}\phi_{\bar{k}}(k)^* a_k(0)\,\mathrm{d}k, \tag{B8}$$

and analogously for $\psi_{\bar{p}\bar{y}}(t')$. The commutator between operators reads

$$I := [\psi_{\bar{k}\bar{x}}(t),\, \psi_{\bar{p}\bar{y}}(t')^\dagger] = \int \mathrm{e}^{\mathrm{i}k(\bar{x}-\bar{y}) - \mathrm{i}\omega_k(t-t')}\phi_{\bar{k}}(k)\phi_{\bar{p}}(k)^*\mathrm{d}k. \tag{B9}$$

Let $d = d_c(\bar{x} - \bar{y},\, t - t') = |\bar{x} - \bar{y}| - c|t - t'| > 0$, using lemma 2 we know that the exponent has no stationary point. Assuming w.l.o.g. $\bar{x} > \bar{y}$, $t > t'$ (other combinations are analogous) and writing $\tilde{\omega}_k = \omega_k - ck$, we obtain

$$I = \int \mathrm{e}^{\mathrm{i}k(\bar{x}-\bar{y}) - \mathrm{i}\omega_k(t-t')}\phi_{\bar{k}}(k)^*\phi_{\bar{p}}(k)\,\mathrm{d}k = \int \mathrm{e}^{\mathrm{i}k\ d_c(\bar{x}-\bar{y}, t-t') - \mathrm{i}\tilde{\omega}_k(t-t')}\phi_{\bar{k}}(k)^*\phi_{\bar{p}}(k)\,\mathrm{d}k.$$

The exponent $\tilde{\omega}_k = \omega_k - ck$ is n-times differentiable and is upper bounded in modulus by a polynomial of degree $m \geqslant 1$. Lemma 3 therefore allows us to bound the commutator by a term $\mathcal{O}(d^{-n})$. □

Note that for a linear dispersion, $\omega_k = c|k|$, we can rewrite this integral as a function of the distance between world lines from equation (B2), $d = (\bar{x} - \bar{y}) - c(t - t')$. Introducing $k_\pm = (\bar{k} \pm \bar{p})/2$ and using our Gaussian wave packets (6), we obtain

$$|I| = \exp\left[-\frac{k_-^2}{\sigma^2} - \frac{d^2\sigma^2}{4}\right]. \tag{B10}$$

This bound is better than the one we have found but it is compatible with lemma 3 and theorem 2.

B.2. Full model causality

Causal relation (B7) can be extended to the full model (2).

Theorem 3. *Let H be the light–matter Hamiltonian given by equation (2). We assume the conditions of theorem 2: differentiable, polynomially bounded functions* ω_k *and* g_k, *with degrees* $n \geqslant 2$. *Then, all wave packets outside the light cone of the scatterer evolve approximately with the free Hamiltonian,* H_0. *More precisely, if* $(\bar{x},\, t_1)$ *and* $(\bar{x},\, t_0)$ *are two points outside the light cone*

$$\psi_{\bar{k}\bar{x}}(t_1) = U_0(t_1,\, t_0)^\dagger\psi_{\bar{k}\bar{x}}(t_0)U_0(t_1,\, t_0) + \mathcal{O}\left(\frac{1}{|d_{\min}|^{n-1}}\right), \tag{B11}$$

where $d_{\min} = \min\{d(\bar{x},\, t_1),\, d(\bar{x},\, t_0)\} \gg 0$ *and*

$$U_0(t,\, t_0) = \exp(-\mathrm{i}(t - t_0)H_0) \tag{B12}$$

is the free-evolution operator for the photons at time t_0.

Proof. We start by building the Heisenberg equations for the operators

$$\partial_t a_k(t) = -\mathrm{i}\omega_k a_k(t) - \mathrm{i}g_k G(t). \tag{B13}$$

Making the change of variables $a_k(t) = \mathrm{e}^{-\mathrm{i}\omega_k t} b_k(t)$, we have

$$\partial_t b_k(t) = -\mathrm{i}g_k G(t)\mathrm{e}^{\mathrm{i}\omega_k t}, \tag{B14}$$

so that the wave packet operators evolved from some initial time t_s are

$$\psi_{\bar{k}\bar{x}}(t) = \int \mathrm{e}^{\mathrm{i}k\bar{x}-\mathrm{i}\omega_k t}\left[b_k(t_s) - \mathrm{i}\int_{t_s}^{t} g_k G(\tau)\mathrm{e}^{+\mathrm{i}\omega_k\tau}\mathrm{d}\tau\right]\phi_{\bar{k}}(k)\mathrm{d}k \tag{B15}$$

$$= U_0(t,\, t_s)\psi_{\bar{k}\bar{x}}(t_s)U_0(t,\, t_s)^{\dagger} - \mathrm{i}\int_{t_s}^{t}\left[\int \mathrm{e}^{\mathrm{i}k\bar{x}-\mathrm{i}c(t-\tau)}g_k\phi_{\bar{k}}(k)\mathrm{d}k\right]G(\tau)\mathrm{d}\tau \tag{B16}$$

$$= U_0(t,\, t_s)\psi_{\bar{k}\bar{x}}(t_s)U_0(t,\, t_s)^{\dagger} - \mathrm{i}\int_{0}^{t-t_s}\left[\int \mathrm{e}^{\mathrm{i}k\bar{x}-\mathrm{i}c\tau'}g_k\phi_{\bar{k}}(k)\mathrm{d}k\right]G(\tau)\mathrm{d}\tau'. \tag{B17}$$

The first part corresponds to free evolution, while the second part is an error term $\varepsilon(t)$, which can be bounded. We will assume without loss of generality $\|G\| = 1$, with $\|\cdot\|$ the Hilbert–Schmidt norm, and $|t_1| > |t_0|$. We have to choose the integration limits t and t_s so that $\mathrm{sign}(\tau') = \mathrm{sign}(x)$. If $x > 0$ then $t_1 > t_0 > 0$ and $(t,\, t_s) = (t_1,\, t_0)$ is a good choice. If $x < 0$ then $0 > t_0 > t_1$ and again $(t,\, t_s) = (t_1,\, t_0)$ is also a valid choice $(\tau' < 0)$. This means we can introduce $\tau'' = \mathrm{sign}(x)\tau' \geqslant 0$ and bound

$$|\varepsilon(t_1)| \leqslant \int_0^{|t_1-t_0|}\left|\int \mathrm{e}^{\mathrm{i}\,\mathrm{sign}(\bar{x})kd_c(|\bar{x}|,\tau'')}q(k)\mathrm{d}k\right|\mathrm{d}\tau'' \leqslant \int_0^{|t_1-t_0|}\mathcal{O}\left(\frac{1}{d_c(|\bar{x}|,\, \tau'')^n}\right)\mathrm{d}\tau'' \tag{B18}$$

$$\leqslant \mathcal{O}\left(\frac{1}{c(n-1)}\frac{1}{(|\bar{x}| - c\tau)^{n-1}}\Bigg|_{\tau=0}^{\tau=|t_1-t_0|}\right) \leqslant \mathcal{O}\left(\frac{1}{d_c(|\bar{x}|,\, |t_1 - t_0|)^{n-1}}\right). \tag{B19}$$

Here we have taken into account that $d_c(|\bar{x}|,\, \tau'') \geqslant d_c(|\bar{x}|,\, |t_1 - t_0|) > 0$ in the domain of integration. We can now use the fact that $d_c(|\bar{x}|,\, |t_1 - t_0|) \geqslant d_c(|\bar{x}|,\, |t_1|) \geqslant \min\{d_c(\bar{x},\, t_1),\, d_c(\bar{x},\, t_0)\}$, obtaining the expression in the theorem. □

B.3. Asymptotic condition

One important limitation of theorem 3 is that it is focused on the operators, not on the states themselves. This is a key point. For having a well defined scattering theory, the asymptotic condition must holds (see section 2.3 and equation (9)). However, using theorems 1 and 3 we have that, given a state $|\Psi\rangle \equiv \psi_{\bar{k},\bar{x}}(t_0)^{\dagger}|\Omega_\nu\rangle$, then

$$\begin{aligned} U(t_\pm)|\Psi\rangle &= U(t_\pm)\psi_{\bar{k},\bar{x}}(t_0)U(t_\pm)^{\dagger}|\Omega_\nu\rangle \\ &= U_0(t_\pm)\psi_{\bar{k},\bar{x}}(t_0)U_0(t_\pm)^{\dagger}|\Omega_\nu\rangle \equiv U_0(t_\pm)|\Psi_{\mathrm{in}}\rangle. \end{aligned} \tag{B20}$$

The first equality is up to a global phase. In the second line, we have used theorem 3. In the last line, we can introduce input (output) states since the wave packets are well separated ($t_\pm \to \pm\infty$) from the scatterer and, by means of theorem 1 and the conditions presented in 2.4 they are well defined free particle states.

This last result warrants that, under rather general conditions, the light–matter Hamiltonian (2) gives a physical scattering theory.

Appendix C. Scattering amplitude decomposition

Theorem 4. *Let us suppose the input state is*

$$|\Psi_{\mathrm{in}}\rangle = \psi_{\mathrm{in}}^{\dagger}|\Omega_\nu\rangle = \left(\prod_{n=1}^{N}\psi_{\bar{k}_n\bar{x}_n}^{\mathrm{in}\,\dagger}\right)|\Omega_\nu\rangle, \tag{C1}$$

with $|\bar{x}_n - \bar{x}_m| \to \infty\ \forall\, n \neq m$. Thus, the scattering amplitude of going to

$$|\Psi_{\mathrm{out}}\rangle = \psi_{\mathrm{out}}^{\dagger}|\Omega_\mu\rangle = \left(\prod_{n=1}^{N}\psi_{\bar{p}_m\bar{y}_m}^{\mathrm{out}\,\dagger}\right)|\Omega_\mu\rangle, \tag{C2}$$

with $|\bar{y}_n - \bar{y}_m| \to \infty\ \forall\, n \neq m$, is reduced to a product of single-photon events:

$$A = \sum_{\lambda_1,\ldots,\lambda_{N-1}=0}^{M-1}\prod_{n=1}^{N}\langle\Omega_{\lambda_{n-1}}|\,\psi_{\bar{p}_n\bar{y}_n}^{\mathrm{out}}(t_+)\psi_{\bar{k}_n\bar{x}_n}^{\mathrm{in}}(t_-)^{\dagger}|\Omega_{\lambda_n}\rangle, \tag{C3}$$

being $\lambda_0 = \mu$ and $\lambda_N = \nu$, with the wave packet operators given in the Heisenberg picture for $t = t_\pm \to \pm\infty$.

The proof is based directly on causality. Therefore, we find convenient to discuss it here.

Proof. The proof is done for the two-photon scattering. The generalization for N photons is straightforward. The scattering operator S is nothing but the evolution operator in the interaction picture, see equation (11). This permits to write the scattering amplitudes as,

$$A = \langle \Psi_{\rm out}|S|\Psi_{\rm in}\rangle = \langle \Omega_\nu|\psi_{\rm out}\, U_I(t_+,\, t_-)\psi_{\rm in}^\dagger|\Omega_\mu\rangle = \langle \Omega_\nu|\psi_{\rm out}(t_+)\psi_{\rm in}(t_-)^\dagger|\Omega_\mu\rangle.$$

In the second equality we have dropped an irrelevant global phase. Here, $\psi_{\rm in}^\dagger$ and $\psi_{\rm out}^\dagger$ are operators creating wave packets localized far away from the scatterer. Because of theorem 1, they are well defined N-photon wave packets.

Using equations (C1) and (C2) the amplitude is given by

$$A = \langle \Omega_\mu|\prod_{m=1}^{2}\psi_{\bar p_m \bar y_m}^{\rm out}(t_+)\prod_{n=1}^{2}\psi_{\bar k_n \bar x_n}^{\rm in}(t_-)^\dagger|\Omega_\nu\rangle. \tag{C4}$$

As $|\bar x_1 - \bar x_2|$ can be arbitrarily large, we can always choose a time t_1 such that $\psi_{\bar p_1 \bar y_1}^{\rm out}(t)^\dagger|\Omega_\mu\rangle$ is well separated from the scatterer for $t > t_1$, so $\psi_{\bar p_1 \bar y_1}^{\rm out}(t) \cong U_0(t,\, t_1)^\dagger \psi_{\bar p_1 \bar y_1}^{\rm out}(t_1)U_0(t,\, t_1)$. Besides, t_1 is such that the second wave packet is still far away from the scatterer. Therefore $\psi_{\bar k_2 \bar x_2}^{\rm in}(t') \cong U_0(t',\, t_1)^\dagger \psi_{\bar k_2 \bar x_2}^{\rm in}(t)U_0(t',\, t_1)$, for $t' < t_1$. Using theorem 2, $[\psi_{\bar p_1 \bar y_1}^{\rm out}(t_+),\, \psi_{\bar k_2 \bar y_2}^{\rm in}(t_-)^\dagger] \to 0$ and equation (C4), the amplitude equals to

$$A = \langle \Omega_\mu|\, \psi_{\bar p_2 \bar y_2}^{\rm out}(t_+)\psi_{\bar k_2 \bar y_2}^{\rm in}(t_-)^\dagger \psi_{\bar p_1 \bar x_1}^{\rm out}(t_+)\psi_{\bar k_1 \bar x_1}^{\rm in}(t_-)^\dagger|\Omega_\nu\rangle. \tag{C5}$$

Finally, we insert the identity between the operators $\psi_{\bar k_2 \bar x_2}^{\rm in}(t_-)^\dagger$ and $\psi_{\bar p_1 \bar y_1}^{\rm out}(t_+)$. Assuming there is not particle creation and just the ground states $\{|\Omega_\lambda\rangle\}_{\lambda=0}^{M-1}$ will contribute to the identity, $\sum_{\lambda=0}^{M-1}|\Omega_\lambda\rangle\langle\Omega_\lambda|$, and we arrive to (C3).

This comes because $\psi_{\bar k_2 \bar x_2}^{\rm in}(t_-)^\dagger$ and $\psi_{\bar p_1 \bar y_1}^{\rm out}(t_+)$ asymptotically commute but not $\psi_{\bar k_1 \bar x_1}^{\rm in}(t_-)^\dagger$ and $\psi_{\bar p_2 \bar y_2}^{\rm out}(t_+)$. This is a clear signature of causality, saying which one is arriving first. Lastly, notice that if the ground state is unique, $|\Omega_{\lambda_n}\rangle = |\Omega_0\rangle$, this ordering is not important as the amplitude is simply the product of single-photon scattering amplitudes.

Appendix D. Scattering amplitude from equation (24)

In this appendix, we prove that (24) is consistent with the amplitude factorization from theorem 4, equation (C3). We do it in the two-photon subspace.

Before, we need the one-photon amplitude as an intermediate result.

D.1. One photon

We first need to compute the one photon amplitude. Let the one-photon input state be,

$$|\Psi_{\rm in}^1\rangle = \psi_{\bar k_1, \bar x_1}^{\rm in\,\dagger}|\Omega_\nu\rangle, \tag{D1}$$

with the creation operator $\psi_{\bar k_1, \bar x_1}^{\rm in\,\dagger}$ given by equation (5), removing the time dependence. For simplicity, we absorb the factor $e^{ik\bar x_1}$ into the wave packet: $\phi_{\bar k_1, \bar x_1}(k) = e^{ik\bar x_1}\phi_{\bar k_1}(k)$. In position space, the output state will read

$$|\Psi_{\rm out}^1\rangle = S|\Psi_{\rm in}^1\rangle = \sum_{\mu=1}^{M}\int {\rm d}y{\rm d}x\, (S_{yx})_{\mu\nu}\phi_{\bar k_1, \bar x_1}(x)|y,\, \Omega_\mu\rangle. \tag{D2}$$

Defining

$$\phi_{1,\mu\nu}(y) = \int {\rm d}x\, (S_{yx})_{\mu\nu}\phi_{\bar k_1, \bar x_1}(x) \tag{D3}$$

and

$$|\xi_{\rm out}^1\rangle_{1,\mu\nu} = \int {\rm d}y\, \phi_{1,\mu\nu}(y)|y;\, \Omega_\mu\rangle, \tag{D4}$$

being $|y;\, \Omega_\mu\rangle = a_y^\dagger|\Omega_\mu\rangle$ the state with a photon at y and the scatterer in the ground state $|\Omega_\mu\rangle$, the output state (D2) can be rewritten as

$$|\Psi_{\rm out}^1\rangle = \sum_{\mu=1}^{M}|\xi_{\rm out}^1\rangle_{1,\mu\nu}. \tag{D5}$$

The probability amplitude will read

$$A_{1,\nu\to\mu} = \langle \Omega_\mu|\psi_{\bar p_1, \bar y_1}^{\rm out}\, S\, \psi_{\bar k_1, \bar x_1}^{\rm in\,\dagger}|\Omega_\nu\rangle = \int {\rm d}y\, \phi_{\bar p_1, \bar y_1}(y)^*\phi_{1,\mu\nu}(y). \tag{D6}$$

If the wave packets are monochromatic with momenta k_1 and p_1, respectively, this amplitude is

$$A_{1,\nu\to\mu} = (S_{p_1 k_1})_{\mu\nu}. \tag{D7}$$

D.2. Two photons

The two-photon wave packet, as sketched in figure 1, is

$$|\Psi^2_{\rm in}\rangle = \psi^{\rm in\,\dagger}_{\bar{k}_1,\bar{x}_1}\psi^{\rm in\,\dagger}_{\bar{k}_2,\bar{x}_2}|\Omega_\nu\rangle. \tag{D8}$$

By definition, the output state is

$$|\Psi^2_{\rm out}\rangle = S|\Psi^2_{\rm in}\rangle. \tag{D9}$$

Here, we are interested in he limit of well separated incident photons. Thus, only the linear part of the scattering matrix S^0 is considered. We introduce the identity operator

$$|\Psi^2_{\rm out}\rangle = \mathbb{I}S\mathbb{I}|\Psi^2_{\rm in}\rangle, \tag{D10}$$

with

$$\mathbb{I} = \frac{1}{2}\sum_{\mu=1}^{M}\int {\rm d}x_1{\rm d}x_2\ |x_1x_2;\ \Omega_\nu\rangle\langle x_1x_2;\ \Omega_\nu|, \tag{D11}$$

being $|x_1x_2;\ \Omega_\nu\rangle = a^\dagger_{x_1}a^\dagger_{x_2}|\Omega_\mu\rangle$ the symmetrized state with two photons at x_1 at x_2 and the scatterer at $|\Omega_\nu\rangle$.

Introducing (D11) in (D10) and considering (D8) and (24) we get

$$|\Psi^2_{\rm out}\rangle = \frac{1}{4}\int {\rm d}y_1{\rm d}y_2{\rm d}x_1{\rm d}x_2\sum_{\mu,\lambda=1}^{M}\sum_{n,m=1}^{2}(S_{y_n x_m})_{\mu\lambda}(S_{y_{n'}x_{m'}})_{\lambda\nu}\theta(y_{n'}-y_n)(\phi_{\bar{k}_1,\bar{x}_1}(x_1)\phi_{\bar{k}_2,\bar{x}_2}(x_2)$$
$$+\ \phi_{\bar{k}_1,\bar{x}_1}(x_2)\phi_{\bar{k}_2,\bar{x}_2}(x_1))|y_1y_2;\ \Omega_\mu\rangle. \tag{D12}$$

with $n' \neq n$ and $m' \neq m$. Now, we have to compute integrals as

$$C = \int {\rm d}x_1{\rm d}x_2\sum_{n,m}(S_{y_n x_m})_{\mu\lambda}(S_{y_{n'}x_{m'}})_{\lambda\nu}\phi_{\bar{k}_i,\bar{x}_i}(x_1)\phi_{\bar{k}_j,\bar{x}_j}(x_2)\theta(y_{n'}-y_n). \tag{D13}$$

Using equation (D3)

$$C = \sum_{n=1}^{2}(\phi_{i,\mu\lambda}(y_n)\phi_{j,\lambda\nu}(y_{n'}) + \phi_{j,\mu\lambda}(y_n)\phi_{i,\lambda\nu}(y_{n'}))\theta(y_{n'}-y_n). \tag{D14}$$

Following the sketch drawn in figure 1, if $x_m < x_{m'}$, then $\phi_1(x_m)\phi_2(x_{m'})$ is zero, so $\phi_{1,\mu\nu}(y_n)\phi_{2,\mu\nu}(y_{n'})$ is zero if $y_n < y_{n'}$. Therefore, choosing $i = 1$ and $j = 2$, the integral C reads

$$C = \sum_{n=1}^{2}\phi_{2,\mu\lambda}(y_n)\phi_{1,\lambda\nu}(y_{n'}). \tag{D15}$$

One can easily show that the same expression holds if we take $i = 2$ and $j = 1$. The output state, equation (D12), then reads

$$|\Psi^2_{\rm out}\rangle = \frac{1}{2}\int {\rm d}y_1{\rm d}y_2\sum_{\mu,\lambda=1}^{M}(\phi_{2,\mu\lambda}(y_1)\phi_{1,\lambda\nu}(y_2) + \phi_{2,\mu\lambda}(y_2)\phi_{1,\lambda\nu}(y_1))|y_1y_2;\ \Omega_\mu\rangle. \tag{D16}$$

Finally, the probability amplitude of going to the output state $\psi^{\rm out\,\dagger}_{\bar{p}_1,\bar{y}_1}\psi^{\rm out\,\dagger}_{\bar{p}_2,\bar{y}_2}|\Omega_\mu\rangle$ will be the overlap between this state and (D16). Using (D6)

$$A_{\rm in\to out} = \langle\Omega_\mu|\psi^{\rm out}_{\bar{p}_1,\bar{y}_1}\psi^{\rm out}_{\bar{p}_2,\bar{y}_2}S\psi^{\rm in\,\dagger}_{\bar{k}_1,\bar{x}_1}\psi^{\rm out\,\dagger}_{\bar{k}_2,\bar{x}_2}|\Omega_\nu\rangle = \sum_{\lambda=0}^{M-1}A_{1,\nu\to\lambda}A_{2,\lambda\to\mu}, \tag{D17}$$

as expected. In the calculations, we have set $\langle\Omega_\mu|\psi^{\rm out}_{\bar{p}_i,\bar{y}_i}\ S\ \psi^{\rm in\,\dagger}_{\bar{k}_j\bar{x}_j}|\Omega_\nu\rangle = 0$ for $i \neq j$, since we assume that both incident wave packets are far away.

A final comment is in order. Without the step functions in (24), the unphysical amplitude $A_{2,\nu\to\lambda}A_{1,\lambda\to\mu}$ would appear in the final probability amplitude.

Appendix E. S^0 for nonchiral waveguides

In this appendix, we generalize the expression for S^0 (24) to nonchiral media. As introduced in [27], in this case we can define two sets of bosonic operators: one for right-moving photons and one for left-moving ones. That is, we have to add a new index to the operators: $a_{x,s}$, where $s = \pm$ for right/left-moving modes. Therefore, the matrix elements of the scattering operator S has indices corresponding to the direction of those photons:

$(S_{\mathbf{ys'xs}})_{\mu\nu}$. Considering the scatterer is placed at $x = 0$, the expression of the free part of S for the chiral waveguide (equation (24)) is easily generalized

$$(S^0_{\mathbf{ys'xs}})_{\mu\nu} = \sum_{\lambda_1 \ldots \lambda_{N-1}=0}^{M-1} \prod_{n=1}^{N} (S_{y_n s'_n x_n s_n})_{\lambda_{N+1-n}\lambda_{N-n}} \prod_{m=1}^{N-1} \theta(|y_{m+1}| - |y_m|)$$
$$+ \text{ permutations}[x_n, s_n \leftrightarrow x_m, s_m; y_n, s'_n \leftrightarrow y_m, s'_m]. \tag{E1}$$

For a chiral waveguide, the Heavisides ensure that the coordinate of an output photon y_{m+1} is larger than the output coordinate y_m of a photon which interacted with the scatterer later. Now, this condition is slightly modified: the absolute value of the coordinate $|y_{m+1}|$ is the quantity necessarily larger than $|y_m|$ if the $m + 1$th photon interacted with the scatterer before the mth photon.

Notice that the structure is essentially identical to that of the chiral case (equation (24)). Therefore, the conclusions of the manuscript also hold for the nonchiral case.

Appendix F. S^0 in momentum space

Here, we show S^0 in momentum space follows equation (30). After that, we prove the Dirac-delta structure is recovered if the ground state is unique.

Let us write $(S^0_{p_1 p_2 k_1 k_2})_{\mu\nu}$ as the Fourier transform of $(S^0_{y_1 y_2 x_1 x_2})_{\mu\nu}$

$$(S^0_{p_1 p_2 k_1 k_2})_{\mu\nu} = \frac{1}{(2\pi)^2} \int \mathrm{d}y_1 \mathrm{d}y_2 \mathrm{d}x_1 \mathrm{d}x_2 \, (S^0_{y_1 y_2 x_1 x_2})_{\mu\nu} \mathrm{e}^{-\mathrm{i}(p_1 y_1 + p_2 y_2)} \mathrm{e}^{\mathrm{i}(k_1 x_1 + k_2 x_2)}. \tag{F1}$$

Due to the form of $(S^0_{y_1 y_2 x_1 x_2})_{\mu\nu}$, (24), we have to compute integrals as

$$I = \int \mathrm{d}x \, \mathrm{e}^{\mathrm{i}kx} (S_{yx})_{\mu\nu}. \tag{F2}$$

Notice that $(S_{yx})_{\mu\nu}$ is the Fourier transform of $(S_{pk})_{\mu\nu}$, equation (29). Therefore,

$$I = \mathrm{e}^{\mathrm{i}(k + E_\nu - E_\mu)y} t_{\mu\nu}(k). \tag{F3}$$

Considering this in (F1), we get

$$(S^0_{p_1 p_2 k_1 k_2})_{\mu\nu} = \frac{1}{(2\pi)^2} \int \mathrm{d}y_1 \mathrm{d}y_2 \, \mathrm{e}^{-\mathrm{i}(p_1 y_1 + p_2 y_2)}$$
$$\times \sum_{n,m=1}^{2} \sum_{\lambda=0}^{M-1} \mathrm{e}^{\mathrm{i}(k_n y_1 + k_{n'} y_2)} \mathrm{e}^{\mathrm{i}[(E_\lambda - E_\mu) y_m + (E_\nu - E_\lambda) y_{m'}]} t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'}) \theta(y_{m'} - y_m), \tag{F4}$$

with $n' \neq n$ and $m' \neq m$. The Fourier transform of the step function is

$$\frac{1}{\sqrt{2\pi}} \int \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}qy} \theta(\mp(y - y_0)) = \pm \frac{\mathrm{i}}{\sqrt{2\pi}} \frac{\mathrm{e}^{-\mathrm{i}qy_0}}{q \pm \mathrm{i}0^+}. \tag{F5}$$

Therefore, integrating equation (F4) first in y_1 and later in y_2, we get

$$\begin{aligned}
(S^0_{p_1 p_2 k_1 k_2})_{\mu\nu} &= \frac{\mathrm{i}}{(2\pi)^2} \int \mathrm{d}y_2 \, \mathrm{e}^{-\mathrm{i}(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu) y_2} \sum_{n=1}^{2} \left(\frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_1 + E_\mu - k_n - E_\lambda + \mathrm{i}0^+} \right. \\
&\quad \left. - \frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_1 + E_\lambda - k_n - E_\nu - \mathrm{i}0^+} \right) \\
&= \frac{\mathrm{i}}{2\pi} \delta(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu) \sum_{n=1}^{2} \sum_{\lambda=0}^{M-1} \left(\frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_1 + E_\mu - k_n - E_\lambda + \mathrm{i}0^+} \right. \\
&\quad \left. - \frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_1 + E_\lambda - k_n - E_\nu - \mathrm{i}0^+} \right) \\
&= \frac{\mathrm{i}}{2\pi} \sum_{n,m=1}^{2} \sum_{\lambda=0}^{M-1} \frac{t_{\mu\lambda}(k_n) t_{\lambda\nu}(k_{n'})}{p_m + E_\mu - k_n - E_\lambda + \mathrm{i}0^+} \delta(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu),
\end{aligned} \tag{F6}$$

which is the expression given in the main text, equation (30). This result has been recently reported for a Λ atom by Xu and Fan in [38]. Here, we show this is completely general due to our ansatz (equation (24)).

Lastly, we prove that equation (30) is formed by two Dirac-delta functions if $M = 1$. To do so, we use the following identity

$$\frac{1}{k + \mathrm{i}0^+} = -\mathrm{i}\pi\delta(k) + \mathcal{P}\left(\frac{1}{k}\right), \tag{F7}$$

with $\mathcal{P}$ the principal value. Applying this identity to equation (30) we get,

$$(S^0_{p_1p_2k_1k_2})_{\mu\nu} = \frac{\mathrm{i}}{2\pi}\sum_{n,m=1}^{2} t(k_n)t(k_{n'})\left(-\mathrm{i}\pi\delta(p_m - k_n) + \mathcal{P}\left(\frac{1}{p_m - k_n}\right)\right)\delta(p_1 + p_2 - k_1 - k_2). \tag{F8}$$

Now, we sum over n and m

$$\begin{aligned}(S^0_{p_1p_2k_1k_2})_{\mu\nu} &= \frac{1}{2}t(k_1)t(k_2)\delta(p_1 + p_2 - k_1 - k_2)(\delta(p_1 - k_1) + \delta(p_1 - k_2) + \delta(p_2 - k_1) + \delta(p_2 - k_2) \\ &\quad + \mathcal{P}\left(\frac{1}{p_1 - k_1}\right) + \mathcal{P}\left(\frac{1}{p_1 - k_2}\right) + \mathcal{P}\left(\frac{1}{p_2 - k_1}\right) + \mathcal{P}\left(\frac{1}{p_2 - k_2}\right)\Bigg).\end{aligned} \tag{F9}$$

Applying the constraint imposed by the global Dirac delta to p_2 to the second row, it is straightforward to see that they cancel each other, arriving to

$$\begin{aligned}(S^0_{p_1p_2k_1k_2})_{\mu\nu} &= \frac{1}{2}t(k_1)t(k_2)\delta(p_1 + p_2 - k_1 - k_2)(\delta(p_1 - k_1) + \delta(p_1 - k_2) + \delta(p_2 - k_1) + \delta(p_2 - k_2)) \\ &= \frac{1}{2}t(k_1)t(k_2)(\delta(p_2 - k_2)\delta(p_1 - k_1) + \delta(p_2 - k_1)\delta(p_1 - k_2) + \delta(p_1 - k_2)\delta(p_2 - k_1) \\ &\quad + \delta(p_1 - k_1)\delta(p_2 - k_2)) = t(k_1)t(k_2)(\delta(p_1 - k_1)\delta(p_2 - k_2) + \delta(p_1 - k_2)\delta(p_2 - k_1)),\end{aligned} \tag{F10}$$

which is the usual expression in translational invariant (momentum conserving) QFT for the cluster decomposition, which also holds in waveguide QED if the ground state is unique.

Appendix G. Fluorescence decay

In this appendix, we calculate how the correlations and thus the fluorescence decay as the distance l between the packets grows (see figures 1 and 3).

The input state (C1) in momentum space is given by,

$$|\Psi_{\mathrm{in}}\rangle = \int \mathrm{d}k_1\mathrm{d}k_2\ \phi^{\mathrm{in}}(k_1, k_2)a^\dagger_{k_1}a^\dagger_{k_2}|\Omega_\nu\rangle, \tag{G1}$$

with

$$\phi^{\mathrm{in}}(k_1, k_2) = \phi_{\bar{k}_1}(k_1)\mathrm{e}^{\mathrm{i}k_2 l}\phi_{\bar{k}_2}(k_2). \tag{G2}$$

In these expressions, the wave packets $\phi_{\bar{k}_n}(k)$ are Lorentzian functions (see equation (7)). The out state is computed by means of equation (10)

$$|\Psi_{\mathrm{out}}\rangle = S|\Psi_{\mathrm{in}}\rangle = \mathbb{I}S\mathbb{I}|\Psi_{\mathrm{in}}\rangle. \tag{G3}$$

With $\mathbb{I}$ the identity operator in the two-photon sector: $\mathbb{I} = 1/2\int \mathrm{d}p_1\mathrm{d}p_2\sum_\mu a^\dagger_{p_1}a^\dagger_{p_2}|\Omega_\mu\rangle\langle\Omega_\mu|\ a_{p_1}a_{p_2}$. The scattering matrix S in momentum space is $(S_{p_1p_2k_1k_2})_{\mu\nu} = (S^0_{p_1p_2k_1k_2})_{\mu\nu} + \mathrm{i}(T_{p_1p_2k_1k_2})_{\mu\nu}$, with $(S^0_{p_1p_2k_1k_2})_{\mu\nu}$ given by equation (30) and $(T_{p_1p_2k_1k_2})_{\mu\nu} = (C_{p_1p_2k_1k_2})_{\mu\nu}\delta(p_1 + p_2 + E_\mu - k_1 - k_2 - E_\nu)$ yielding

$$|\Psi_{\mathrm{out}}\rangle = \int \mathrm{d}p_1\mathrm{d}p_2\sum_\mu \phi^{\mathrm{out}}_\mu(p_1, p_2)a^\dagger_{p_1}a^\dagger_{p_2}|\Omega_\mu\rangle, \tag{G4}$$

with

$$\begin{aligned}\phi^{\mathrm{out}}_\mu(p_1, p_2) \propto \sum_{n=1}^{2}\sum_{m=1}^{2}\int \mathrm{d}k_n\left(\frac{\mathrm{i}}{2\pi}\sum_\lambda \frac{t_{\mu\lambda}(k_n)t_{\lambda\nu}(p_1 + p_2 + E_\mu - k_n - E_\nu)}{p_m + E_\mu - k_n - E_\lambda + \mathrm{i}0^+} + \mathrm{i}(\tilde{C}_{p_1p_2k_n})_{\mu\nu}\right) \\ \times (\phi_{\bar{k}_1}(k_n)\mathrm{e}^{\mathrm{i}(p_1+p_2+E_\mu-k_n-E_\nu)l}\phi_{\bar{k}_2}(p_1 + p_2 + E_\mu - k_n - E_\nu) + \phi_{\bar{k}_1}(p_1 + p_2 + E_\mu - k_n - E_\nu)\mathrm{e}^{\mathrm{i}k_n l}\phi_{\bar{k}_2}(k_n)).\end{aligned}$$

Which is nothing but equation (33) that we have rewritten here for the discussion. As said in section 4.2, we assume that $t_{\mu\nu}(k)$ and $(C_{p_1p_2k_nk_{\bar{n}}})_{\mu\nu}$ have simple poles with imaginary parts $\{\gamma^t_n\}$ and $\{\gamma^C_n\}$ respectively. Then, this integral is solved by taking complex contours and applying the residue theorem. In order to integrate the term proportional to $\mathrm{e}^{\mathrm{i}(p_1+p_2+E_\mu-k_n-E_\lambda)l}$, we take the contour shown in figure G1(a) so that the exponential factor does not diverge. For the same reason, for that proportional to $\mathrm{e}^{\mathrm{i}k_n l}$ we take the contour of figure G1(b). As t and C have first-order poles, when integrating each pole, we just have to evaluate the rest of the function at the pole. Then, t and C give terms proportional to $\mathrm{e}^{-|\gamma^t_n|l}$ and $\mathrm{e}^{-|\gamma^C_n|l}$, respectively.

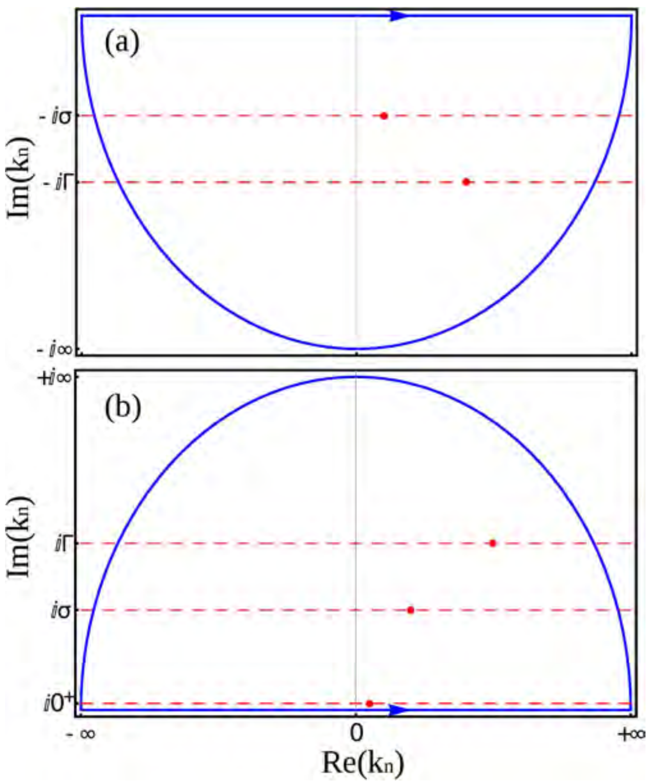

Figure G1. (a) Lower and (b) upper contour for integrating equation (33). We show the poles coming from the Lorentzian, $\pm i\sigma$, those coming from one of the transmission amplitudes or from C, $\pm i\Gamma$, and those with vanishing imaginary part. The real parts are arbitrary.

Now we consider the contribution to the integral of the wave packets, $\phi_{\bar{k}_n}(k)$. We choose Lorentzian functions, with a simple pole at $k = \bar{k}_n - i\sigma$ (see equation (7)). In consequence, we have a term proportional to $e^{-\sigma l}$. Lastly, the denominator in the first term has a pole with zero imaginary part. Therefore, its contribution does not decay with l. Importantly enough, this pole enforces single-photon energy conservation giving single-photon amplitudes, $\sum_\lambda A_{1,\nu\to\lambda} A_{2,\lambda\to\mu}$.

Finally, let us mention that we do not need to impose that that $t_{\mu\nu}(k)$ and $(C_{p_1p_2k_nk_{\bar{n}}})_{\mu\nu}$ have simple poles. Higher order poles, by virtue of the Cauchy Integral formula for the derivatives, also would yield exponential decay.

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