

Chapter 1

Input-Output Formalism for Few-Photon Transport

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Abstract We extend the input-output formalism of quantum optics to analyze few-photon transport in waveguide quantum electrodynamics (QED) systems. We provide explicit analytical derivations for one- and two-photon scattering matrix elements based on the quantum causality relation. The computation scheme can be generalized to N -photon scattering systematically.

1.1 Introduction

The capability to create strong photon-photon interaction at a few-photon level in integrated photonic systems is of central importance for quantum information processing. To achieve such a capability, an important approach is to use the waveguide quantum electrodynamics (QED) system, which consists of a waveguide that is strongly coupled to a local quantum system. Experimentally, the waveguides that have been used for this purpose include optical fibers [1], metallic plasmonic nanowires [2], photonic crystal waveguides [3], and microwave transmission line [4]. The local quantum system typically incorporates a variety of quantum multi-level systems such as actual atoms [1], quantum dots [2, 3], or microwave qubits [4], where the strong nonlinearity of these multi-level systems forms the basis for strong photon-photon interactions. These multi-level systems moreover can be embedded in cavity structures to further control their nonlinear properties [5–10].

The rapid experimental developments, in turn, have motivated significant theoretical efforts. From a fundamental physics perspective, the photon-photon interaction is characterized by the multi-photon scattering matrix (S matrix). Therefore, a

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natural objective for theoretical works is to compute such multi-photon S matrix. Moreover, from an engineering perspective, the systems considered here are envisioned as devices that process quantum states. To describe these systems as a device one naturally have to specify its input-output relation. The S matrix, which relates the input and output states, therefore provides a natural basis for device engineering as well.

Motivated by both the physics and engineering considerations as discussed above, a large body of theoretical works have been therefore devoted to the computation the S matrix of various waveguide QED systems [11–37]. In this chapter, we extend the input-output formalism [38, 39] of quantum optics—a Heisenberg picture approach originally introduced to analyze the interaction between an atom in a cavity and a continuous set of electromagnetic states outside of the atom-cavity system—to analyze the transport of few-photon states in waveguide QED system [17, 20, 25, 32, 35–37].

The chapter is organized as follows. In Sect. 1.2 we introduce the Hamiltonian of the system and present the input-output formalism. In Sect. 1.3 we discuss the quantum causality condition and prove certain time-ordering relations, which are the key to compute the S matrix of waveguide photons. In Sect. 1.4 we build the link between the scattering theory and the input-output formalism and continue in Sect. 1.5 with the derivation of the one-photon transport properties. In Sect. 1.6 we show how to extend the calculations to the two-photon case. In Sect. 1.7 as an example of the application of this formalism, we calculate the exact single- and two-photon S matrix for a waveguide coupled a cavity containing a medium with Kerr nonlinearity. As a check, we calculate the same example in Sect. 1.8 in the wavefunction approach. We conclude in Sect. 1.9.

1.2 Hamiltonian and Input-Output Formalism

To illustrate the formalism, as a concrete example, we consider a cavity coupled to a single polarization, single-mode waveguide [40] and treat the transport properties of few-photon states in such a system (Fig. 1.1). The Hamiltonian $\tilde{H}$ is defined as ($\hbar = 1$)

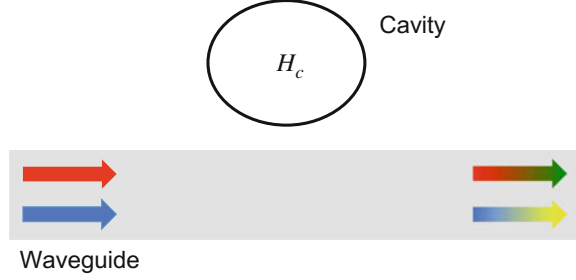
$$\tilde{H} = \tilde{H}_0 + \tilde{H}_1.$$

Here, $\tilde{H}_0$ describes a chiral (i.e. one-way) waveguide where photons propagate in only one direction:

$$\tilde{H}_0 = \int_0^\infty d\beta \tilde{\omega}(\beta) \tilde{c}_\beta^\dagger \tilde{c}_\beta,$$

where $\tilde{c}_\beta$ and $\tilde{c}_\beta^\dagger$ are the respective annihilation and creation operators for the photons with wave vector β that obey the commutation relation $[\tilde{c}_\beta, \tilde{c}_{\beta'}^\dagger] = \delta(\beta - \beta')$. $\tilde{H}_1$ describes the cavity as well as the waveguide-cavity interaction:

Fig. 1.1 Schematic representation of two photons in a waveguide moving to the right toward a side-coupled cavity



$$\tilde{H}_1 = \tilde{H}_c + V \int_0^\infty d\beta \left(\tilde{c}_\beta^\dagger a + a^\dagger \tilde{c}_\beta \right).$$

$\tilde{H}_c$ is the cavity Hamiltonian and a ($a^\dagger$) is its annihilation (creation) operator satisfying the commutation relation $[a, a^\dagger] = 1$. V denotes the coupling strength between the cavity modes and waveguide modes.

We assume that the cavity system, in the absence of the waveguide, conserves the total number of excitations inside the cavity, i.e. there exists a conserved excitation number operator N_c for the total number of excitations, satisfying

$$[N_c, \tilde{H}_c] = 0.$$

The operator N_c takes non-negative integer as its eigenvalues. Removing a cavity photon should reduce the total number of excitations in the cavity system by unity, and hence $[N_c, a] = -a$. A natural form of the number operator N_c is therefore

$$N_c = a^\dagger a + O, \quad (1.1)$$

where O consists of other degrees of freedom in the cavity with $[a, O] = 0$. In our form of the Hamiltonian $\tilde{H}_1$, only the cavity operator a couples to the waveguide, whereas these other degrees of freedom do not couple with the waveguide directly.

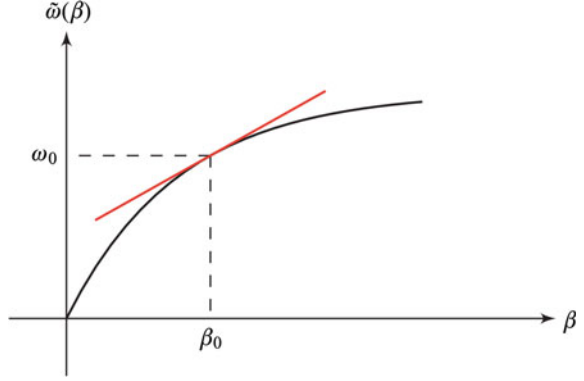
It will be useful to label the waveguide photon operators in terms of the frequencies rather than their wave vectors; therefore, we linearize the waveguide dispersion around (β_0, ω_0) as $\tilde{\omega}(\beta) = \omega_0 + v_g(\beta - \beta_0)$ (see Fig. 1.2). Notice that the total excitation operator of the whole system

$$N_E = \int_0^\infty d\beta \tilde{c}_\beta^\dagger \tilde{c}_\beta + N_c$$

commutes with $\tilde{H}$ (i.e. $[\tilde{H}, N_E] = 0$). We could thus equivalently solve a system described by

$$H = \tilde{H} - \omega_0 N_E = H_0 + H_1, \quad (1.2)$$

Fig. 1.2 Linearization of a surface-plasmon-like waveguide dispersion relation $\tilde{\omega}(\beta)$ around a wave vector β_0 . The *slope* of the line is equal to the group velocity v_g . The photon states in the text are assumed to have frequencies in the vicinity of ω_0 so that the linearization is justified



where

$$H_0 = \int_{-\infty}^{+\infty} d\beta v_g (\beta - \beta_0) \tilde{c}_\beta^\dagger \tilde{c}_\beta,$$

$$H_1 = H_c + V \int_{-\infty}^{\infty} d\beta \left(\tilde{c}_\beta^\dagger a + a^\dagger \tilde{c}_\beta \right).$$

Here $H_c = \tilde{H}_c - \omega_0 N_c$, and we also extended the lower limit of integration to $-\infty$ so that we can define the Fourier transform of operators later in this Chapter. Since we will be dealing with states with wave vectors around β_0 , the extension of the integration limit is well justified. With these transformations, we can now label the waveguide photon operators in terms of frequency $\omega \equiv v_g \beta$ with the definition $c_\omega \equiv \tilde{c}_{\beta+\beta_0} / \sqrt{v_g}$, which satisfies the commutation relation $[c_\omega, c_{\omega'}^\dagger] = \delta(\omega - \omega')$. From now on, besides ω , the labels for photon degrees of freedom, for example k and p , also refer to photon frequency. As a result of all these changes, we have

$$H_0 = \int dk k c_k^\dagger c_k, \quad (1.3)$$

$$H_1 = H_c + \frac{V}{\sqrt{v_g}} \int dk \left(c_k^\dagger a + a^\dagger c_k \right). \quad (1.4)$$

Following [17, 38], we now define the input and output operators as

$$c_{\text{in}}(t) \equiv \int \frac{dk}{\sqrt{2\pi}} c_k(t_0) e^{-ik(t-t_0)}, \quad (1.5)$$

$$c_{\text{out}}(t) \equiv \int \frac{dk}{\sqrt{2\pi}} c_k(t_1) e^{-ik(t-t_1)}, \quad (1.6)$$

with $t_0 \rightarrow -\infty$ and $t_1 \rightarrow +\infty$. We note that $c_{\text{in}}(t)$ and $c_{\text{out}}(t)$ consist of Heisenberg operators of waveguide photons at time $-\infty$ and $+\infty$, respectively. They satisfy the commutation relations

$$\begin{aligned} [c_{\text{in}}(t), c_{\text{in}}(t')] &= [c_{\text{out}}(t), c_{\text{out}}(t')] = 0, \\ [c_{\text{in}}(t), c_{\text{in}}^\dagger(t')] &= [c_{\text{out}}(t), c_{\text{out}}^\dagger(t')] = \delta(t - t'). \end{aligned} \quad (1.7)$$

As shown in the Appendix, for the system described by the Hamiltonian (1.2)–(1.4), one can develop the standard input-output formalism [38] that relates $c_{\text{in}}(t)$, $c_{\text{out}}(t)$ and a as:

$$c_{\text{out}}(t) = c_{\text{in}}(t) - i\sqrt{\gamma} a(t), \quad (1.8)$$

$$\frac{da}{dt} = -i [a, H_c] - \frac{\gamma}{2} a - i\sqrt{\gamma} c_{\text{in}} \quad (1.9)$$

$$= -i [a, H_c] + \frac{\gamma}{2} a - i\sqrt{\gamma} c_{\text{out}}, \quad (1.10)$$

where $\gamma \equiv 2\pi V^2/\nu_g$, and $a(t) \equiv e^{iHt}a(0)e^{-iHt}$ is the cavity photon operator in the Heisenberg picture.

In the standard quantum optics literature, the input-output formalism have been applied widely on computing properties related to an input state that is a coherent state, a thermal state, or a squeezed state. Here we will extend it to computations for Fock state input, since in general the transport property of Fock states is qualitatively different from that of the coherent state.

1.3 Quantum Causality Relation

Integrating (1.9) and (1.10) from $t = -\infty$ and $t = \infty$, respectively, result in:

$$a(t) = a(-\infty) - i \int_{-\infty}^t d\tau [a, H_c] - \frac{\gamma}{2} \int_{-\infty}^t d\tau a - i\sqrt{\gamma} \int_{-\infty}^t d\tau c_{\text{in}}, \quad (1.11)$$

$$a(t) = a(+\infty) - i \int_{+\infty}^t d\tau [a, H_c] + \frac{\gamma}{2} \int_{+\infty}^t d\tau a - i\sqrt{\gamma} \int_{+\infty}^t d\tau c_{\text{out}}, \quad (1.12)$$

where the integrands are operators at time τ . Equations (1.11) and (1.12) can be used to prove a quantum causality relation. When using (1.11) to evaluate $a(t)$ or $a^\dagger(t)$, the integral should result in an expression that involves only $c_{\text{in}}(\tau)$ and $c_{\text{in}}^\dagger(\tau)$ with $\tau < t$. Therefore, by the commutation relation (1.7), one concludes from (1.11) that for $t < t'$,

$$[a(t), I(t')] = [a(-\infty), I(t')], \quad [a^\dagger(t), I(t')] = [a^\dagger(-\infty), I(t')],$$

where $I(t')$ is a shorthand notation for the input operators that represent either $c_{\text{in}}(t')$ or $c_{\text{in}}^\dagger(t')$. On the other hand, the operator I is really a Heisenberg operator at time $-\infty$ for the waveguide photon as can be seen in (1.5) above, and hence commute with the cavity operator $a(-\infty)$ and $a^\dagger(-\infty)$. Therefore, we have

$$[a(t), I(t')] = [a^\dagger(t), I(t')] = 0, \quad \text{for } t < t'. \quad (1.13)$$

Similarly, one can prove

$$[a(t), O(t')] = [a^\dagger(t), O(t')] = 0, \quad \text{for } t > t', \quad (1.14)$$

where $O(t')$ is a shorthand notation for the output operators that represent either $c_{\text{out}}(t')$ or $c_{\text{out}}^\dagger(t')$, by utilizing (1.12) and the fact that the output operators are really Heisenberg operators for waveguide photons at time $+\infty$. Following [38], we refer to (1.13) and (1.14) as the *quantum causality condition*. The operator $a(t)$, which characterizes the physical field in the local system, depends only on the input field $c_{\text{in}}(\tau)$ with $\tau \leq t$, and generate only output field $c_{\text{out}}(\tau)$ with $\tau \geq t$.

With quantum causality condition, the commutator $[a(t), c_{\text{in}}^\dagger(t')]$ for $t > t'$ can then be computed as:

$$[a(t), c_{\text{in}}^\dagger(t')] = [a(t), c_{\text{out}}^\dagger(t') - i\sqrt{\gamma} a^\dagger(t')] = -i\sqrt{\gamma} [a(t), a^\dagger(t')],$$

which, in combination with (1.13), leads to the relation

$$[a(t), c_{\text{in}}^\dagger(t')] = -i\sqrt{\gamma} [a(t), a^\dagger(t')] \theta(t - t'), \quad (1.15)$$

where

$$\theta(t) \equiv \begin{cases} 1 & t > 0 \\ 1/2 & t = 0 \\ 0 & t < 0 \end{cases}$$

is the Heaviside step function. Similarly, we can derive

$$[a(t), c_{\text{out}}^\dagger(t')] = i\sqrt{\gamma} [a(t), a^\dagger(t')] \theta(t' - t). \quad (1.16)$$

To study the few-photon transport, we will need to consider some properties of a time-ordered product involving a and the input or output operators. Here, we define the time-ordered product of operators $A(t)$ and $B(t')$ as

$$\mathcal{T}A(t)B(t') \equiv \begin{cases} A(t)B(t') & t > t' \\ \frac{1}{2} [A(t)B(t') + B(t')A(t)] & t = t' \\ B(t')A(t) & t < t' \end{cases}.$$

With the proved commutation relations (1.15) and (1.16), we can prove that

$$\mathcal{T}a(t)c_{\text{in}}^\dagger(t') = a(t)c_{\text{in}}^\dagger(t') + \frac{i}{4}\sqrt{\gamma}\delta_{t,t'}, \quad (1.17)$$

$$\mathcal{T}a(t)c_{\text{out}}^\dagger(t') = c_{\text{out}}^\dagger(t')a(t) + \frac{i}{4}\sqrt{\gamma}\delta_{t,t'}, \quad (1.18)$$

where $\delta_{t,t'} = 1$ for $t = t'$ and 0 when $t \neq t'$. We emphasize that $\delta_{t,t'}$ is not the Dirac δ -function $\delta(t - t')$. Take (1.17) as an example. By definition, $\mathcal{T}a(t)c_{\text{in}}^\dagger(t') = a(t)c_{\text{in}}^\dagger(t')$ for $t > t'$; When $t < t'$, by the commutation relation (1.15), $\mathcal{T}a(t)c_{\text{in}}^\dagger(t') = c_{\text{in}}^\dagger(t')a(t) = a(t)c_{\text{in}}^\dagger(t')$; When $t = t'$, $\mathcal{T}a(t)c_{\text{in}}^\dagger(t) = \frac{1}{2}a(t)c_{\text{in}}^\dagger(t) + \frac{1}{2}c_{\text{in}}^\dagger(t)a(t) = a(t)c_{\text{in}}^\dagger(t) - \frac{1}{2}[a(t), c_{\text{in}}^\dagger(t)] = a(t)c_{\text{in}}^\dagger(t) + \frac{i}{4}\sqrt{\gamma}$, completing the proof. Equation (1.18) can be proved similarly.

In this chapter, our objective is to compute the few-photon scattering matrix in the frequency domain. For this purpose, we will perform Fourier transformations to the time-ordered products such as those in (1.17) and (1.18). Since the $\delta_{t,t'}$ term vanishes upon Fourier transformation, for our purpose, it can be safely ignored. With this consideration in mind, we rewrite the relations (1.17) and (1.18) as

$$\mathcal{T}a(t)I(t') = a(t)I(t'), \quad (1.19)$$

$$\mathcal{T}a(t)O(t') = O(t')a(t). \quad (1.20)$$

More generally, from (1.19) and (1.20), we have the following relation regarding the time-ordered product:

$$\mathcal{T} \prod_{i,j} a(t_i)I(t'_j) = \left[\mathcal{T} \prod_i a(t_i) \right] \cdot \left[\mathcal{T} \prod_j I(t'_j) \right], \quad (1.21)$$

$$\mathcal{T} \prod_{i,j} a(t_i)O(t'_j) = \left[\mathcal{T} \prod_j O(t'_j) \right] \cdot \left[\mathcal{T} \prod_i a(t_i) \right], \quad (1.22)$$

where bracket is used to indicate the range over which the time-ordering is being applied. Again, in (1.21) and (1.22), the equality is to be understood in the frequency domain, i.e., the equality holds after Fourier transformations to all the time variables are performed.

Equations (1.21) and (1.22) can be proved in a similar way. Here we show only the proof of (1.21). The proof of (1.21) can be constructed from induction with respect to the number of operators. The base case is already proved in (1.19). Now suppose (1.21) holds for all cases involving a total number of N operators of a and I . Consider

a time-ordered product involving $N + 1$ operators, if the operator with the largest time label is $a(t_{\max})$,

$$\begin{aligned} \mathcal{T} \prod_{I,j} a(t_I) I(t'_j) &= a(t_{\max}) \left[\mathcal{T} \prod_{i,j} a(t_i) I(t'_j) \right] = a(t_{\max}) \left[\mathcal{T} \prod_i a(t_i) \right] \cdot \left[\mathcal{T} \prod_j I(t'_j) \right] \\ &= \left[\mathcal{T} \prod_i a(t_i) \right] \cdot \left[\mathcal{T} \prod_j I(t'_j) \right], \end{aligned}$$

where the definition of time-ordered product is used in the first and last steps, and the induction hypothesis is used in the second step. On the other hand, if the operator with the largest time label is $I(t_{\max})$, we have

$$\begin{aligned} \mathcal{T} \prod_{i,j} a(t_i) I(t'_j) &= I(t_{\max}) \left[\mathcal{T} \prod_{i,j} a(t_i) I(t'_j) \right] = I(t_{\max}) \left[\mathcal{T} \prod_i a(t_i) \right] \cdot \left[\mathcal{T} \prod_j I(t'_j) \right] \\ &= \left[\mathcal{T} \prod_i a(t_i) \right] \cdot I(t_{\max}) \left[\mathcal{T} \prod_j I(t'_j) \right] = \left[\mathcal{T} \prod_i a(t_i) \right] \cdot \left[\mathcal{T} \prod_j I(t'_j) \right], \end{aligned}$$

where we use the induction hypothesis in the second step and the commutation relation (1.13) in the third step. Therefore, (1.21) holds for $N + 1$ operators, completing the proof.

1.4 Connection to Scattering Theory

In a typical scattering experiment, various input states are prepared and sent toward a scattering region. After the scattering takes place, the outgoing states of the experiment are observed, and information about the interaction is deduced. Here as an example we consider two-particle scattering. This process is commonly described using the scattering matrix with elements of the form

$$S_{p_1 p_2 k_1 k_2} = \langle p_1 p_2 | S | k_1 k_2 \rangle,$$

where $|k_1 k_2\rangle$ denotes an input state—here given as a two-particle state with frequencies k_1 and k_2 , and $|p_1 p_2\rangle$ denotes an outgoing state. The S operator is equal to the evolution operator U_I in the interaction picture from time $-\infty$ to $+\infty$:

$$S = \lim_{\substack{t_0 \rightarrow -\infty \\ t_1 \rightarrow +\infty}} U_I(t_1, t_0) = \lim_{\substack{t_0 \rightarrow -\infty \\ t_1 \rightarrow +\infty}} e^{i H_0 t_1} e^{-i H(t_1 - t_0)} e^{-i H_0 t_0},$$

where H_0 is the noninteracting part of the Hamiltonian, and $H = H_0 + H_I$ is the total Hamiltonian. In order to have a more compact notation, in this section whenever we use t_0 or t_1 , we imply a limiting process of $t_0 \rightarrow -\infty$ and $t_1 \rightarrow +\infty$, respectively, and we drop the limit notation.

An equivalent way to describe the scattering is in terms of the scattering eigenstates $|k_1 k_2^+\rangle$ and $|k_1 k_2^-\rangle$ defined as

$$\begin{aligned} |k_1 k_2^+\rangle &\equiv U_I(0, t_0) |k_1 k_2\rangle = e^{iHt_0} e^{-iH_0 t_0} |k_1 k_2\rangle, \\ |k_1 k_2^-\rangle &\equiv U_I(0, t_1) |k_1 k_2\rangle = e^{iHt_1} e^{-iH_0 t_1} |k_1 k_2\rangle. \end{aligned}$$

We can then write the scattering matrix elements as

$$\langle p_1 p_2 | S | k_1 k_2 \rangle = \langle p_1 p_2^- | k_1 k_2^+ \rangle.$$

It is possible to denote the scattering matrix elements by an appropriate definition of input and output operators such that

$$\langle p_1 p_2^- | k_1 k_2^+ \rangle = \langle 0 | c_{\text{out}}(p_1) c_{\text{out}}(p_2) c_{\text{in}}^\dagger(k_1) c_{\text{in}}^\dagger(k_2) | 0 \rangle, \quad (1.23)$$

where

$$c_{\text{in}}^\dagger(k) \equiv e^{iHt_0} e^{-iH_0 t_0} c_k^\dagger e^{iH_0 t_0} e^{-iHt_0}, \quad (1.24)$$

$$c_{\text{out}}^\dagger(k) \equiv e^{iHt_1} e^{-iH_0 t_1} c_k^\dagger e^{iH_0 t_1} e^{-iHt_1} \quad (1.25)$$

create input and output scattering eigenstates from vacuum, i.e.,

$$\begin{aligned} c_{\text{in}}^\dagger(k) | 0 \rangle &= | k^+ \rangle, \\ c_{\text{out}}^\dagger(p) | 0 \rangle &= | p^- \rangle, \end{aligned}$$

and satisfy the commutation relations

$$\left[c_{\text{in}}(k), c_{\text{in}}^\dagger(p) \right] = \left[c_{\text{out}}(k), c_{\text{out}}^\dagger(p) \right] = \delta(k - p).$$

We now relate the scattering theory, as briefly sketched above, to the input-output formalism [38, 39] of quantum optics. To do so, we start from the definition of the input field operator $c_{\text{in}}(t)$ (1.5), in which $c_k(t_0) \equiv e^{iHt_0} c_k e^{-iHt_0}$. The relationship between $c_{\text{in}}(t)$ —which is defined in the input-output formalism—and $c_{\text{in}}(k)$ —which is defined above in (1.24) as a part of the scattering theory—can then be determined by noting that

$$\begin{aligned}
c_{\text{in}}(t) &= \frac{1}{\sqrt{2\pi}} \int dk e^{iHt_0} c_k e^{-iHt_0} e^{-ik(t-t_0)} \\
&= \frac{1}{\sqrt{2\pi}} \int dk e^{iHt_0} e^{-iH_0 t_0} c_k e^{iH_0 t_0} e^{-iHt_0} e^{-ikt} \\
&= \frac{1}{\sqrt{2\pi}} \int dk c_{\text{in}}(k) e^{-ikt},
\end{aligned} \tag{1.26}$$

where in the second line we used the fact that $[H_0, c_k] = -k c_k$ to convert the $c_k e^{ikt_0}$ term into $e^{-iH_0 t_0} c_k e^{iH_0 t_0}$. As a result, $c_{\text{in}}(k)$ provides the spectral representation of $c_{\text{in}}(t)$. Similarly, the output field operator (1.6) in the input-output formalism is related to $c_{\text{out}}(k)$ in the scattering theory through

$$c_{\text{out}}(t) = \frac{1}{\sqrt{2\pi}} \int dk c_{\text{out}}(k) e^{-ikt}. \tag{1.27}$$

We have thus established a direct connection between the input-output formalism and the scattering theory.

1.5 Single-Photon Transport

Having established the relationship between the input-output formalism and the scattering theory, we now calculate the S matrix elements $\langle p|S|k \rangle$ between two single-photon states $|k \rangle$ and $|p \rangle$. The single-photon S matrix is related to the input and output operators by

$$S_{pk} = \langle p|S|k \rangle = \langle 0|c_{\text{out}}(p)c_{\text{in}}^\dagger(k)|0 \rangle = \int \frac{dt'}{\sqrt{2\pi}} e^{ipt'} \int \frac{dt}{\sqrt{2\pi}} e^{-ikt} \langle 0|c_{\text{out}}(t')c_{\text{in}}^\dagger(t)|0 \rangle,$$

where we used (1.26) and (1.27) to write $c_{\text{in}}^\dagger(k)$, $c_{\text{out}}(p)$ in terms of $c_{\text{in}}^\dagger(t)$, $c_{\text{out}}(t')$, respectively. It is therefore sufficient to first calculate $\langle 0|c_{\text{out}}(t')c_{\text{in}}^\dagger(t)|0 \rangle$ and then perform Fourier transformation to determine the single-photon S matrix. As the starting point, we use the input-output formalism (1.8) to obtain

$$\langle 0|c_{\text{out}}(t')c_{\text{in}}^\dagger(t)|0 \rangle = \langle 0|c_{\text{in}}(t')c_{\text{in}}^\dagger(t)|0 \rangle - i\sqrt{\gamma} \langle 0|a(t')c_{\text{in}}^\dagger(t)|0 \rangle.$$

The first term is simply $\delta(t' - t)$ following the commutation relation (1.7). The second term can be computed as

$$\begin{aligned}
\langle 0|a(t')c_{\text{in}}^\dagger(t)|0\rangle &= \langle 0|\mathcal{T}a(t')c_{\text{in}}^\dagger(t)|0\rangle - \frac{i}{4}\sqrt{\gamma}\delta_{t,t'} \\
&= \langle 0|\mathcal{T}a(t')c_{\text{out}}^\dagger(t)|0\rangle - i\sqrt{\gamma}\langle 0|\mathcal{T}a(t')a^\dagger(t)|0\rangle - \frac{i}{4}\sqrt{\gamma}\delta_{t,t'} \\
&= \langle 0|c_{\text{out}}^\dagger(t)a(t')|0\rangle - i\sqrt{\gamma}\langle 0|\mathcal{T}a(t')a^\dagger(t)|0\rangle \\
&= -i\sqrt{\gamma}\langle 0|\mathcal{T}a(t')a^\dagger(t)|0\rangle,
\end{aligned} \tag{1.28}$$

where we first utilized the time-ordered relation (1.17) to introduce the time-ordered operation, then inserted the input-output formalism (1.8) in the second line to transform $c_{\text{in}}^\dagger$ to $c_{\text{out}}^\dagger$, and finally utilized the time-ordered relation (1.18) to move $c_{\text{out}}^\dagger$ to the leftmost. We note that as indicated above in the discussions associated with (1.17) and (1.18), the $\delta_{t,t'}$ terms in (1.19) and (1.20) do not contribute after Fourier transformation and can be safely dropped in the calculation. Therefore, for the rest of the chapter, we will directly use (1.21) and (1.22).

We define the two-point Green function of the cavity as

$$G(t'; t) \equiv -\gamma \langle 0|\mathcal{T}a(t')a^\dagger(t)|0\rangle. \tag{1.29}$$

and relate single-photon S matrix to the cavity's two-point Green function as

$$S(t'; t) \equiv \langle 0|c_{\text{out}}(t')c_{\text{in}}^\dagger(t)|0\rangle = \delta(t' - t) + G(t'; t), \tag{1.30}$$

or

$$S_{pk} = \delta(p - k) + G(p; k), \tag{1.31}$$

where $G(p; k)$ is the Fourier transformation of (1.29) in the frequency domain. As shown in the Appendix, the two-point Green function (1.29) can be computed using an effective Hamiltonian

$$H_{\text{eff}} = H_c - i\frac{\gamma}{2}a^\dagger a \tag{1.32}$$

without involving the waveguide degrees of freedoms. As a result, we only need to solve a cavity system which has a finite, and typically small, number of degrees of freedom.

For cavities with total excitation number as defined in (1.1), we have $[H_{\text{eff}}, N_c] = 0$ because of $[H_c, N_c] = 0$ and $[a, O] = 0$. As a result, H_{eff} can be block-diagonalized as

$$H_{\text{eff}}|\mathcal{E}_n\rangle = \mathcal{E}_n|\mathcal{E}_n\rangle, \quad N_c|\mathcal{E}_n\rangle = n|\mathcal{E}_n\rangle,$$

where $|\mathcal{E}_n\rangle$ is a right eigenstate of H_{eff} with eigenvalue $\mathcal{E}_n$. Especially, $|\mathcal{E}_0\rangle$ is the ground state $|0\rangle$ and $\mathcal{E}_0 = 0$. Since H_{eff} is not Hermitian, $\mathcal{E}_n$ is in general complex. By inserting a complete set of biorthogonal basis states and noting that only the single excitation state contributes to the summation, we compute the two-point Green function (1.29) as

$$\begin{aligned}
G(t'; t) &= -\gamma \langle 0|a(t')a^\dagger(t)|0\rangle\theta(t' - t) = -\gamma \langle 0|a e^{-iH_{\text{eff}}(t'-t)}a^\dagger|0\rangle\theta(t' - t) \\
&= -\gamma \sum_{\mathcal{E}_1} \langle 0|a|\mathcal{E}_1\rangle \langle \bar{\mathcal{E}}_1|e^{-iH_{\text{eff}}(t'-t)}a^\dagger|0\rangle\theta(t' - t) \\
&= -\gamma \sum_{\mathcal{E}_1} \langle 0|a|\mathcal{E}_1\rangle \langle \bar{\mathcal{E}}_1|a^\dagger|0\rangle e^{-i\mathcal{E}_1(t'-t)}\theta(t' - t).
\end{aligned}$$

and thus

$$G(p; k) = -i\gamma \sum_{\mathcal{E}_1} \frac{\langle 0|a|\mathcal{E}_1\rangle \langle \bar{\mathcal{E}}_1|a^\dagger|0\rangle}{k - \mathcal{E}_1} \delta(p - k).$$

The single-photon S matrix is then

$$S_{pk} = \left[1 - i\gamma \sum_{\mathcal{E}_1} \frac{\langle 0|a|\mathcal{E}_1\rangle \langle \bar{\mathcal{E}}_1|a^\dagger|0\rangle}{k - \mathcal{E}_1} \right] \delta(p - k). \quad (1.33)$$

1.6 Two-Photon Transport

Our aim in this section is to calculate the two-photon S matrix based on the quantum causality condition, building upon the results we obtained for the single-photon case. The two-photon S matrix element (1.23) is related to the input and output operators by

$$S_{p_1 p_2 k_1 k_2} = \left(\prod_{l=1,2} \int \frac{dt'_l}{\sqrt{2\pi}} e^{ip_l t'_l} \int \frac{dt_l}{\sqrt{2\pi}} e^{-ik_l t_l} \right) \langle 0|c_{\text{out}}(t'_1)c_{\text{out}}(t'_2)c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle.$$

We begin by computing the two-photon S matrix element in the time domain. We first insert the input-output formalism (1.8) as

$$\begin{aligned}
S(t'_1 t'_2; t_1 t_2) &\equiv \langle 0|c_{\text{out}}(t'_1)c_{\text{out}}(t'_2)c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&= \langle 0| [\mathcal{T} c_{\text{out}}(t'_1)c_{\text{out}}(t'_2)] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&= \langle 0| [\mathcal{T} (c_{\text{in}}(t'_1) - i\sqrt{\gamma}a(t'_1)) (c_{\text{in}}(t'_2) - i\sqrt{\gamma}a(t'_2))] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&= \langle 0| [\mathcal{T} c_{\text{in}}(t'_1)c_{\text{in}}(t'_2)] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&\quad - i\sqrt{\gamma} \langle 0| [\mathcal{T} c_{\text{in}}(t'_1)a(t'_2)] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&\quad - i\sqrt{\gamma} \langle 0| [\mathcal{T} a(t'_1)c_{\text{in}}(t'_2)] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle \\
&\quad - \gamma \langle 0| [\mathcal{T} a(t'_1)a(t'_2)] c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle.
\end{aligned}$$

The first term in the final equality above is simply $\langle 0|c_{\text{in}}(t'_1)c_{\text{in}}(t'_2)c_{\text{in}}^\dagger(t_1)c_{\text{in}}^\dagger(t_2)|0\rangle = \delta(t'_1 - t_1)\delta(t'_2 - t_2) + \delta(t'_1 - t_2)\delta(t'_2 - t_1)$. By the time-ordered relation (1.19) and

the result in the single-photon case (1.28), the second term can be computed as

$$\begin{aligned}
 \langle 0 | [\mathcal{T} c_{\text{in}}(t'_1) a(t'_2)] c_{\text{in}}^\dagger(t_1) c_{\text{in}}^\dagger(t_2) | 0 \rangle &= \langle 0 | a(t'_2) c_{\text{in}}(t'_1) c_{\text{in}}^\dagger(t_1) c_{\text{in}}^\dagger(t_2) | 0 \rangle \\
 &= \langle 0 | a(t'_2) c_{\text{in}}^\dagger(t_2) | 0 \rangle \delta(t'_1 - t_1) + \langle 0 | a(t'_2) c_{\text{in}}^\dagger(t_1) | 0 \rangle \delta(t'_1 - t_2) \\
 &= -i\sqrt{\gamma} \langle 0 | \mathcal{T} a(t'_2) a^\dagger(t_2) | 0 \rangle \delta(t'_1 - t_1) - i\sqrt{\gamma} \langle 0 | \mathcal{T} a(t'_2) a^\dagger(t_1) | 0 \rangle \delta(t'_1 - t_2).
 \end{aligned}$$

Similarly, the evaluation of the third term gives $-i\sqrt{\gamma} \langle 0 | \mathcal{T} a(t'_1) a^\dagger(t_2) | 0 \rangle \delta(t'_2 - t_1) - i\sqrt{\gamma} \langle 0 | \mathcal{T} a(t'_1) a^\dagger(t_1) | 0 \rangle \delta(t'_2 - t_2)$. For the last term, we have

$$\begin{aligned}
 \langle 0 | [\mathcal{T} a(t'_1) a(t'_2)] c_{\text{in}}^\dagger(t_1) c_{\text{in}}^\dagger(t_2) | 0 \rangle &= \langle 0 | [\mathcal{T} a(t'_1) a(t'_2)] [\mathcal{T} c_{\text{in}}^\dagger(t_1) c_{\text{in}}^\dagger(t_2)] | 0 \rangle \\
 &= \langle 0 | \mathcal{T} a(t'_1) a(t'_2) c_{\text{in}}^\dagger(t_1) c_{\text{in}}^\dagger(t_2) | 0 \rangle \\
 &= \langle 0 | \mathcal{T} a(t'_1) a(t'_2) \left(c_{\text{out}}^\dagger(t_1) - i\sqrt{\gamma} a^\dagger(t_1) \right) \left(c_{\text{out}}^\dagger(t_2) - i\sqrt{\gamma} a^\dagger(t_2) \right) | 0 \rangle \\
 &= -\gamma \langle 0 | \mathcal{T} a(t'_1) a(t'_2) a^\dagger(t_1) a^\dagger(t_2) | 0 \rangle + \langle 0 | c_{\text{out}}^\dagger(t_1) c_{\text{out}}^\dagger(t_2) a(t'_1) a(t'_2) | 0 \rangle \\
 &\quad - i\sqrt{\gamma} \langle 0 | c_{\text{out}}^\dagger(t_1) [\mathcal{T} a(t'_1) a(t'_2) a^\dagger(t_2)] | 0 \rangle - i\sqrt{\gamma} \langle 0 | c_{\text{out}}^\dagger(t_2) [\mathcal{T} a(t'_1) a(t'_2) a^\dagger(t_1)] | 0 \rangle \\
 &= -\gamma \langle 0 | \mathcal{T} a(t'_1) a(t'_2) a^\dagger(t_1) a^\dagger(t_2) | 0 \rangle.
 \end{aligned}$$

where we utilized time-ordered relation (1.21) in the second line and inserted the input-output formalism (1.8) in the third line. In the fourth line, we applied the time-ordered relation (1.22) to move the output operators to the leftmost to annihilate the $|0\rangle$ state.

Combing all the computations leads to the result of two-photon S matrix in the time domain. To make further simplification, we define the four-point Green function of the cavity system as

$$G(t'_1, t'_2; t_1, t_2) \equiv \gamma^2 \langle 0 | \mathcal{T} a(t'_1) a(t'_2) a^\dagger(t_1) a^\dagger(t_2) | 0 \rangle. \quad (1.34)$$

In general, its Fourier component $G(p_1, p_2; k_1, k_2)$ can be expressed as a sum of various terms containing products of several δ -functions [41]. Among all these terms, we define the term that contains only $\delta(p_1 + p_2 - k_1 - k_2)$ and no other δ functions as the *connected* Green function, $G_C(p_1, p_2; k_1, k_2)$. We thus have the decomposition

$$G(p_1, p_2; k_1, k_2) = G(p_1; k_1)G(p_2; k_2) + G(p_1; k_2)G(p_2; k_1) + G_C(p_1, p_2; k_1, k_2),$$

or in the time domain,

$$G(t'_1, t'_2; t_1, t_2) = G(t'_1; t_1)G(t'_2; t_2) + G(t'_1; t_2)G(t'_2; t_1) + G_C(t'_1, t'_2; t_1, t_2).$$

Consequently, the two-photon S matrix can be written in a compact form [35]

$$S(t'_1, t'_2; t_1, t_2) = S(t'_1, t_1)S(t'_2, t_2) + S(t'_2, t_1)S(t'_1, t_2) + G_C(t'_1, t'_2; t_1, t_2)$$

with single-photon S matrix (1.30) and the connected four-point Green function. Or in the frequency domain, we have

$$S_{p_1 p_2 k_1 k_2} = S_{p_1 k_1} S_{p_2 k_2} + S_{p_2 k_1} S_{p_1 k_2} + G_C(p_1, p_2; k_1, k_2), \quad (1.35)$$

where S_{pk} is computed in (1.31) or (1.33). The form of this decomposition satisfies the cluster decomposition principle [28, 42, 43] in quantum field theory. From the computational perspective, the result here reduces the computation of the two-photon S matrix to the evaluation of the connected four-point Green function of the cavity system, which can again be computed using the effective Hamiltonian (1.32).

In general, for N -photon S matrix, similar decompositions hold and our computational scheme based on the input-output formalism and quantum causality condition can be generalized systematically [35].

1.7 Example: A Waveguide Coupled to a Kerr-Nonlinear Cavity

As an example of the application of the formalism developed above, we compute the S matrix of two-photon transport in a single-mode waveguide that is side-coupled to a ring resonator incorporating Kerr nonlinear media. The full Hamiltonian has the same form as (1.2) with the specific form of H_c :

$$H_c = \omega_c a^\dagger a + \frac{\chi}{2} a^\dagger a^\dagger a a.$$

Let $\alpha \equiv \omega_c - i\frac{\gamma}{2}$, the effective Hamiltonian (1.32) in this case is

$$H_{\text{eff}} = \alpha a^\dagger a + \frac{\chi}{2} a^\dagger a^\dagger a a,$$

and can be diagonalized as

$$H_{\text{eff}}|n\rangle = \left[\alpha n + \frac{\chi}{2} n(n-1) \right] |n\rangle, \quad (1.36)$$

with the eigenvalues $\mathcal{E}_n \equiv \alpha n + \frac{\chi}{2} n(n-1)$ and the eigenstates $|\mathcal{E}_n\rangle \equiv |n\rangle$.

The single-photon S matrix can be computed directly by (1.33) as

$$\begin{aligned} S_{pk} &= \left[1 - i\gamma \frac{\langle 0|a|1\rangle\langle 1|a^\dagger|0\rangle}{k - \alpha} \right] \delta(p - k) = \left[1 - i\gamma \frac{1}{k - \omega_c + i\gamma/2} \right] \delta(p - k) \\ &= \frac{k - \omega_c - i\gamma/2}{k - \omega_c + i\gamma/2} \delta(p - k) = [1 + s_k] \delta(p - k), \end{aligned} \quad (1.37)$$

where, for later convenience, we defined

$$s_k \equiv -\gamma \frac{i}{k - \alpha}.$$

For two-photon S matrix, from (1.35), we only need to compute the connected four-point Green function. We start by computing the four-point Green function $G(t'_1, t'_2; t_1, t_2)$. Depending on the values of the four time labels, the time ordering operation would give rise non-zero terms that can be classified into two types: $\langle aa^\dagger aa^\dagger \rangle$ and $\langle a aa^\dagger a^\dagger \rangle$, i.e.

$$G(t'_1, t'_2; t_1, t_2) \equiv \sum_{j=1}^2 G^{(j)}(t'_1, t'_2; t_1, t_2),$$

with

$$\begin{aligned} G^{(1)}(t'_1, t'_2; t_1, t_2) &= (-\gamma)^2 \sum_{P,Q} \langle 0 | a(t'_{Q_1}) a^\dagger(t_{P_1}) a(t'_{Q_2}) a^\dagger(t_{P_2}) | 0 \rangle \theta(t'_{Q_1} - t_{P_1}) \theta(t_{P_1} - t'_{Q_2}) \theta(t'_{Q_2} - t_{P_2}), \\ G^{(2)}(t'_1, t'_2; t_1, t_2) &= (-\gamma)^2 \sum_{P,Q} \langle 0 | a(t'_{Q_1}) a(t'_{Q_2}) a^\dagger(t_{P_1}) a^\dagger(t_{P_2}) | 0 \rangle \theta(t'_{Q_1} - t'_{Q_2}) \theta(t'_{Q_2} - t_{P_1}) \theta(t_{P_1} - t_{P_2}), \end{aligned}$$

where both P and Q are permutations over indices $\{1, 2\}$. We calculate each term by inserting the complete sets of eigenstates, which results in:

$$\begin{aligned} \langle 0 | a(t'_1) a^\dagger(t_1) a(t'_2) a^\dagger(t_2) | 0 \rangle &= \sum_{m,n,l} \langle 0 | a(t'_1) | m \rangle \langle m | a^\dagger(t_1) | n \rangle \langle n | a(t'_2) | l \rangle \langle l | a^\dagger(t_2) | 0 \rangle \\ &= \langle 0 | a(t'_1) | 1 \rangle \langle 1 | a^\dagger(t_1) | 0 \rangle \langle 0 | a(t'_2) | 1 \rangle \langle 1 | a^\dagger(t_2) | 0 \rangle \\ &= e^{-ia(t'_1 - t_1)} e^{-ia(t'_2 - t_2)}, \end{aligned}$$

and

$$\begin{aligned} \langle 0 | a(t'_1) a(t'_2) a^\dagger(t_1) a^\dagger(t_2) | 0 \rangle &= \langle 0 | a(t'_1) | 1 \rangle \langle 1 | a(t'_2) | 2 \rangle \langle 2 | a^\dagger(t_1) | 1 \rangle \langle 1 | a^\dagger(t_2) | 0 \rangle \\ &= 2e^{-ia(t'_1 - t_2)} e^{-i(\alpha + \chi)(t'_2 - t_1)}. \end{aligned}$$

Their Fourier transformations are

$$\begin{aligned} G^{(1)}(p_1, p_2; k_1, k_2) &= -\frac{i}{2\pi} \sum_{P,Q} s_{p_{Q_1}} s_{k_{P_2}} \frac{1}{p_{Q_2} - k_{P_2} - i\epsilon} \delta(p_1 + p_2 - k_1 - k_2), \\ G^{(2)}(p_1, p_2; k_1, k_2) &= \frac{i}{\pi} \sum_{P,Q} s_{p_{Q_1}} s_{k_{P_2}} \frac{1}{k_1 + k_2 - 2\alpha - \chi} \delta(p_1 + p_2 - k_1 - k_2), \end{aligned}$$

where an infinitesimal imaginary part in the denominator arises due to the Fourier transform of the θ function. Moreover, we note that

$$\frac{1}{p-k-i\epsilon} = \frac{\mathcal{P}}{p-k} + i\pi\delta(p-k).$$

On the other hand, since the connected four-point Green function contains only a single δ function, only the principal part contributes to $G_C(p_1, p_2; k_1, k_2)$. Therefore, we have

$$G_C(p_1, p_2; k_1, k_2) = \sum_{j=1}^2 i\mathcal{M}_{p_1 p_2; k_1 k_2}^{(j)} \delta(p_1 + p_2 - k_1 - k_2),$$

with

$$\begin{aligned} i\mathcal{M}_{p_1 p_2; k_1 k_2}^{(1)} &= -\frac{i}{2\pi} \sum_{P,Q} s_{p_{Q_1}} s_{k_{P_2}} \frac{\mathcal{P}}{p_{Q_2} - k_{P_2}}, \\ i\mathcal{M}_{p_1 p_2; k_1 k_2}^{(2)} &= \frac{i}{\pi} \sum_{P,Q} s_{p_{Q_1}} s_{k_{P_2}} \frac{1}{k_1 + k_2 - 2\alpha - \chi}. \end{aligned}$$

Finally, we can sum over all the permutation terms and obtain a compact form:

$$G_C(p_1, p_2; k_1, k_2) = -\frac{\chi}{\pi\gamma} s_{k_1} s_{k_2} (s_{p_1} + s_{p_2}) \frac{1}{k_1 + k_2 - 2\alpha - \chi} \delta(p_1 + p_2 - k_1 - k_2). \quad (1.38)$$

The summation of all principal parts vanishes. The final result (1.38) indeed has the exact analytical structure constrained by the cluster decomposition principle [28]. The only singularities are isolated poles corresponding to one and two-photon excitations in the cavity.

1.8 Wavefunction Approach

As a check on the input-output formalism, we recalculate the example problem in the last section using the wavefunction approach [12, 13, 15, 16, 19, 22, 23, 26, 29, 31, 33]. We start by rewriting the system's Hamiltonian in $H = H_0 + H_{\text{int}}$ in the coordinate space

$$\begin{aligned} H_0 &= \int dx c^\dagger(x) \left(-i \frac{d}{dx} \right) c(x) + \omega_c a^\dagger a + \frac{\chi}{2} a^\dagger a^\dagger a a, \\ H_{\text{int}} &= +\sqrt{\gamma} \int dx \delta(x) [c^\dagger(x) a + a^\dagger c(x)], \end{aligned}$$

where $c^\dagger(x)$ is the creation operator for a right-going photon at position x satisfying the commutation relation $[c(x), c^\dagger(x')] = \delta(x - x')$. For an input state of one-photon Fock state, the most general time-independent interacting eigenstate for this Hamiltonian is

$$|k^+\rangle = \int dx \phi_k(x) c^\dagger(x) |0\rangle + e_a a^\dagger |0\rangle.$$

The time-independent Schrodinger equation $H|k^+\rangle = k|k^+\rangle$ yields the following equations of motion:

$$-i \frac{d}{dx} \phi_k(x) + \sqrt{\gamma} e_a \delta(x) = k \phi_k(x), \quad (1.39)$$

$$\omega_c e_a + \sqrt{\gamma} \phi(0) = k e_a. \quad (1.40)$$

Our aim is to solve the transmission amplitude for an incident photon. For this purpose, we take

$$\phi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}} [\theta(-x) + t_k \theta(x)],$$

where t_k is the transmission amplitude. Submitting the above ansatz into the equations of motion (1.39) and (1.40) gives the solution

$$e_a = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{\gamma}}{k - \omega_c + i\gamma/2}, \quad t_k = \frac{k - \omega_c - i\gamma/2}{k - \omega_c + i\gamma/2}. \quad (1.41)$$

For two-photon transport, consider the two-excitation eigenstate

$$|E_2\rangle = \int dx_1 dx_2 g(x_1, x_2) c^\dagger(x_1) c^\dagger(x_2) |0\rangle + f_a \frac{1}{\sqrt{2}} a^\dagger a^\dagger |0\rangle + \int dx h(x) c^\dagger(x) a^\dagger |0\rangle.$$

From $H|E_2\rangle = E_2|E_2\rangle$, by equating the coefficients of the terms $c^\dagger c^\dagger |0\rangle$, $c^\dagger a^\dagger |0\rangle$, $a^\dagger a^\dagger |0\rangle$, respectively, we obtain the equations of motion

$$\begin{aligned} \left(-i \frac{\partial}{\partial x_1} - i \frac{\partial}{\partial x_2} - E_2 \right) g(x_1, x_2) + \frac{\sqrt{\gamma}}{2} [\delta(x_1) h(x_2) + h(x_1) \delta(x_2)] &= 0, \\ \left(-i \frac{d}{dx} + \omega_c - E_2 \right) h(x) + \sqrt{\gamma} [g(x, 0) + g(0, x)] + \sqrt{2\gamma} f_a \delta(x) &= 0, \\ (2\omega_c + \chi - E_2) f_a + \sqrt{2\gamma} h(0) &= 0, \end{aligned}$$

where $g(x, 0) \equiv [g(x, 0^+) + g(x, 0^-)]/2 = g(0, x) \equiv [g(0^+, x) + g(0^-, x)]/2$ and $h(0) \equiv [h(0^+) + h(0^-)]/2$. We eliminate $h(x)$ and f_a from the preceding equations and obtain equations on $g(x_1, x_2)$:

$$\left(-i\frac{\partial}{\partial x_1} - i\frac{\partial}{\partial x_2} - E_2\right)g(x_1, x_2) = 0, \quad (1.42)$$

$$\left(-i\frac{d}{dx} - E_2 + \omega_c - i\frac{\gamma}{2}\right)g(0^+, x) = \left(-i\frac{d}{dx} - E_2 + \omega_c + i\frac{\gamma}{2}\right)g(0^-, x), \quad (1.43)$$

$$\frac{g(0^+, 0^+) - g(0^-, 0^+)}{g(0^+, 0^-) - g(0^-, 0^-)} = \frac{E - 2\omega_c - \chi - i\gamma}{E - 2\omega_c - \chi + i\gamma}. \quad (1.44)$$

From (1.42), the general solution of $g(x_1, x_2)$ thus has the form of

$$g(x_1, x_2) = \tilde{g}(x_1 - x_2)e^{iE_2x_2}. \quad (1.45)$$

Because of the exchange symmetry of $g(x_1, x_2)$, we can restrict to the half space $x_1 \leq x_2$. Following [13, 16], we divide this half space into three regions (a) $x_1 \leq x_2 < 0$, (b) $x_1 < 0 < x_2$, (c) $0 < x_1 \leq x_2$ and denote $g^{(a)}(x_1, x_2)$, $g^{(b)}(x_1, x_2)$, $g^{(c)}(x_1, x_2)$ as the function $g(x_1, x_2)$ in each respective region. Using (1.43) and (1.44), we have

$$\left(-i\frac{d}{dx} - E_2 + \omega_c - i\frac{\gamma}{2}\right)g^{(b)}(x, 0^+) = \left(-i\frac{d}{dx} - E_2 + \omega_c + i\frac{\gamma}{2}\right)g^{(a)}(x, 0^-), \quad (1.46)$$

$$\left(-i\frac{d}{dx} - E_2 + \omega_c - i\frac{\gamma}{2}\right)g^{(c)}(0^+, x) = \left(-i\frac{d}{dx} - E_2 + \omega_c + i\frac{\gamma}{2}\right)g^{(b)}(0^-, x), \quad (1.47)$$

$$\frac{g^{(c)}(0^+, 0^+) - g^{(b)}(0^-, 0^+)}{g^{(b)}(0^-, 0^+) - g^{(a)}(0^-, 0^-)} = \frac{E_2 - 2\omega_c - \chi - i\gamma}{E_2 - 2\omega_c - \chi + i\gamma}. \quad (1.48)$$

In order to construct the S matrix, one interprets $g(x_1, x_2)$ in the third quadrant ($x_1, x_2 < 0$) as the in-state, and in the first quadrant ($x_1, x_2 > 0$) as the out-state. We consider an incident two-photon planewave state comprised of two photons with frequencies k_1 and k_2 , i.e.,

$$g^{(a)}(x_1, x_2) = \frac{1}{2\sqrt{2\pi}} \left(e^{ik_1x_1} e^{ik_2x_2} + e^{ik_1x_2} e^{ik_2x_1} \right), \quad \text{for } x_1, x_2 < 0,$$

which gives $E_2 = k_1 + k_2$ and $g^{(a)}(x, 0^-) = \frac{1}{2\sqrt{2\pi}} (e^{ik_1x} + e^{ik_2x})$ directly. We can then obtain $g^{(b)}(x, 0^+)$ by solving (1.46) as

$$g^{(b)}(x, 0^+) = \frac{1}{2\sqrt{2\pi}} \left(t_{k_2} e^{ik_1x} + t_{k_1} e^{ik_2x} \right) + A e^{i(k_1+k_2-\omega_c+i\frac{\gamma}{2})x},$$

where t_k is the single-photon transmission amplitude solved in (1.41) and A is a constant to be determined. Using (1.45), we can determine $g^{(b)}(x_1, x_2)$ from $g^{(b)}(x_1, 0^+)$ as

$$g^{(b)}(x_1, x_2) = \frac{1}{2\sqrt{2\pi}} \left[t_{k_2} e^{i(k_1x_1+k_2x_2)} + t_{k_1} e^{i(k_1x_2+k_2x_1)} \right] + A e^{i(\omega_c-i\frac{\gamma}{2})(x_2-x_1)} e^{i(k_1+k_2)x_1}.$$

To avoid the divergence when $x_2 - x_1 \rightarrow +\infty$, we have to set $A = 0$. As a result, the final solution of $g^{(b)}(x_1, x_2)$ is

$$g^{(b)}(x_1, x_2) = \frac{1}{2\sqrt{2}\pi} \left[t_{k_2} e^{i(k_1 x_1 + k_2 x_2)} + t_{k_1} e^{i(k_1 x_2 + k_2 x_1)} \right].$$

Similarly, with $g^{(b)}(0^-, x_2)$, we can solve $g^{(c)}(0^+, x_2)$ from (1.47) and then determine $g^{(c)}(x_1, x_2)$ as

$$g^{(c)}(x_1, x_2) = \frac{1}{2\sqrt{2}\pi} t_{k_1} t_{k_2} \left[e^{i(k_1 x_1 + k_2 x_2)} + e^{i(k_1 x_2 + k_2 x_1)} \right] + B e^{-i\left(\omega_c - i\frac{\gamma}{2}\right)(x_2 - x_1)} e^{i(k_1 + k_2)x_2}.$$

The constant B can be determined by (1.48) as

$$B = -\frac{\chi}{\sqrt{2}\pi} \frac{\gamma^2}{\left(k_1 - \omega_c + i\frac{\gamma}{2}\right) \left(k_2 - \omega_c + i\frac{\gamma}{2}\right) (k_1 + k_2 - 2\omega_c - \chi + i\gamma)}.$$

Finally, to solve the two-photon S matrix, we compute the initial and final wave-functions, $\psi_i(x_1, x_2)$ and $\psi_f(x_1, x_2)$, respectively, by the Lippmann-Schwinger equations [13]. That is,

$$\begin{aligned} \psi_i(x_1, x_2) &= \langle x_1, x_2 | E_2 \rangle - \langle x_1, x_2 | \frac{1}{k_1 + k_2 - H_0 + i0^+} H_{\text{int}} | E_2 \rangle \\ &= g^{(a)}(x_1, x_2) \theta(x_2 - x_1) + g^{(a)}(x_2, x_1) \theta(x_1 - x_2), \\ \psi_f(x_1, x_2) &= \langle x_1, x_2 | E_2 \rangle - \langle x_1, x_2 | \frac{1}{k_1 + k_2 - H_0 - i0^+} H_{\text{int}} | E_2 \rangle \\ &= g^{(c)}(x_1, x_2) \theta(x_2 - x_1) + g^{(c)}(x_2, x_1) \theta(x_1 - x_2). \end{aligned}$$

$\psi_i(x_1, x_2)$ is the plane wave consisting of two photons with frequencies k_1 and k_2 , and forms a complete basis for the two-photon Hilbert space. Therefore, the two-photon S matrix can be computed by

$$S_{p_1 p_2 k_1 k_2} = \int dx_1 dx_2 \frac{1}{2\sqrt{2}\pi} \left[e^{-i(p_1 x_1 + p_2 x_2)} + e^{-i(p_1 x_2 + p_2 x_1)} \right] \psi_f(x_1, x_2),$$

which leads to the exactly the same result as (1.35) and (1.38).

1.9 Conclusion

In this chapter, we extend the input-output formalism of quantum optics to analyze few-photon scattering in waveguide QED systems. We develop the relationship between the input-output operators and the scattering theory, which in turn enables

us to analytically calculate the photon scattering matrix elements. With the quantum causality condition, We relate the S matrix to the cavity's Green function without the need of knowing the specific details of the cavity Hamiltonian. The approach is therefore generally applicable for a large number of waveguide QED systems with different local quantum systems. Finally, the computation is systematic and can be generalized to N -photon scattering case.

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Appendix

Derivation of Input-Output Formalism

The Heisenberg equations associated with the Hamiltonian (1.2)–(1.4) are

$$\frac{d}{dt}c_k = -ik c_k - i \frac{V}{\sqrt{V_g}} a, \quad (1.49)$$

$$\frac{d}{dt}a = -i [a, H_c] - i \frac{V}{\sqrt{V_g}} \int dk c_k. \quad (1.50)$$

We let

$$\Phi(t) \equiv \int \frac{dk}{\sqrt{2\pi}} c_k(t),$$

and define the input and output operators

$$c_{\text{in}}(t) = \int \frac{dk}{\sqrt{2\pi}} c_k(t_0) e^{-ik(t-t_0)},$$

$$c_{\text{out}}(t) = \int \frac{dk}{\sqrt{2\pi}} c_k(t_1) e^{-ik(t-t_1)},$$

with $t_0 \rightarrow -\infty, t_1 \rightarrow +\infty$.

After multiplying (1.49) by the factor $\exp(ikt)$, we integrate it from an initial time t_0 to get

$$c_k(t) = c_k(t_0) e^{-ik(t-t_0)} - i \frac{V}{\sqrt{V_g}} \int_{t_0}^t d\tau a(\tau) e^{-ik(t-\tau)},$$

and then integrate it with respect to k to get

$$\Phi(t) = c_{\text{in}}(t) - i \frac{V}{\sqrt{V_g}} \frac{1}{2} \sqrt{2\pi} a(t) = c_{\text{in}}(t) - i \frac{\sqrt{\gamma}}{2} a(t). \quad (1.51)$$

Here, notice that we integrate over half the delta function, which results in a factor of $1/2$ and γ is defined as $\gamma \equiv 2\pi V^2/v_g$.

Furthermore, plugging (1.51) into (1.50) results in

$$\frac{d}{dt}a = -i [a, H_c] - \frac{\gamma}{2}a - i\sqrt{\gamma}c_{\text{in}}(t).$$

Similarly, we integrate (1.49) up to a final time $t_1 > t$ and obtain

$$\Phi(t) = c_{\text{out}}(t) + i\frac{\sqrt{\gamma}}{2}a(t). \quad (1.52)$$

Combining (1.51) and (1.52), we finally obtain

$$c_{\text{out}}(t) = c_{\text{in}}(t) - i\sqrt{\gamma}a(t). \quad (1.53)$$

Derivation of Effective Hamiltonian

We first prove that the propagator of the cavity can be computed using the effective Hamiltonian (1.32). That is, when $H_c = H_c^{(0)} \equiv \omega_c a^\dagger a$,

$$G^{(0)}(t', t) = \tilde{G}^{(0)}(t', t),$$

where

$$\begin{aligned} G^{(0)}(t', t) &\equiv \langle 0 | \mathcal{T} a(t') a^\dagger(t) | 0 \rangle, \\ \tilde{G}^{(0)}(t', t) &\equiv \langle 0 | \mathcal{T} \tilde{a}(t') \tilde{a}^\dagger(t) | 0 \rangle. \end{aligned}$$

$a(t)$ and $a^\dagger(t)$ are Heisenberg operators in the input-output formalism (1.8)–(1.10). $\tilde{a}(t)$ and $\tilde{a}^\dagger(t)$ are defined as

$$\tilde{a}(t) = e^{iH_{\text{eff}}t} a e^{-iH_{\text{eff}}t}, \quad \tilde{a}^\dagger(t) = e^{iH_{\text{eff}}t} a^\dagger e^{-iH_{\text{eff}}t}, \quad (1.54)$$

whose evolution is controlled by the effective Hamiltonian (1.32).

The proof is as follows. When $t' > t$,

$$\begin{aligned} \frac{\partial}{\partial t'} G^{(0)}(t', t) &= \langle 0 | \frac{da(t')}{dt'} a^\dagger(t) | 0 \rangle \\ &= -i \left(\omega_c - i\frac{\gamma}{2} \right) \langle 0 | a(t') a^\dagger(t) | 0 \rangle - i\sqrt{\gamma} \langle 0 | c_{\text{in}}(t') a^\dagger(t) | 0 \rangle \\ &= -i \left(\omega_c - i\frac{\gamma}{2} \right) G^{(0)}(t', t), \end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial t} G^{(0)}(t', t) &= \langle 0 | a(t') \frac{da^\dagger(t)}{dt} | 0 \rangle \\
&= i \left(\omega_c - i \frac{\gamma}{2} \right) \langle 0 | a(t') a^\dagger(t) | 0 \rangle + i \sqrt{\gamma} \langle 0 | a(t') c_{\text{out}}^\dagger(t) | 0 \rangle \\
&= i \left(\omega_c - i \frac{\gamma}{2} \right) G^{(0)}(t', t),
\end{aligned}$$

where we plug in the input-output formalism (1.9) and (1.10) and use the respective quantum causality (1.15) and (1.16) so that $\langle 0 | c_{\text{in}}(t') a^\dagger(t) | 0 \rangle = \langle 0 | a^\dagger(t) c_{\text{in}}(t') | 0 \rangle = 0$ and $\langle 0 | a(t') c_{\text{out}}^\dagger(t) | 0 \rangle = \langle 0 | c_{\text{out}}^\dagger(t) a(t') | 0 \rangle = 0$ when $t' > t$. On the other hand, by (1.54), one can compute

$$\begin{aligned}
\frac{\partial}{\partial t'} \tilde{G}^{(0)}(t', t) &= \langle 0 | \frac{d\tilde{a}(t')}{dt'} \tilde{a}^\dagger(t) | 0 \rangle = -i \langle 0 | [\tilde{a}, H_{\text{eff}}](t') \tilde{a}^\dagger(t) | 0 \rangle \\
&= -i \left(\omega_c - i \frac{\gamma}{2} \right) \langle 0 | \tilde{a}(t') \tilde{a}^\dagger(t) | 0 \rangle = -i \left(\omega_c - i \frac{\gamma}{2} \right) \tilde{G}^{(0)}(t', t), \\
\frac{\partial}{\partial t} \tilde{G}^{(0)}(t', t) &= \langle 0 | \tilde{a}(t') \frac{d\tilde{a}^\dagger(t)}{dt} | 0 \rangle = -i \langle 0 | \tilde{a}(t') [\tilde{a}^\dagger, H_{\text{eff}}](t) | 0 \rangle \\
&= i \left(\omega_c - i \frac{\gamma}{2} \right) \langle 0 | \tilde{a}(t') \tilde{a}^\dagger(t) | 0 \rangle = i \left(\omega_c - i \frac{\gamma}{2} \right) \tilde{G}^{(0)}(t', t).
\end{aligned}$$

So $G^{(0)}(t', t)$ and $\tilde{G}^{(0)}(t', t)$ satisfy exactly the same differential equations when $t' > t$. They also have the same initial values at $t' = t$. Therefore, by the uniqueness theorem for differential equations, we can conclude that $G^{(0)}(t', t) = \tilde{G}^{(0)}(t', t)$.

Now for a general Hamiltonian $H_c = H_c^{(0)} + V$, according to the perturbation theory in quantum field theory, all Green functions in principle are completely determined by the propagator $G^{(0)}$ and the interaction vertices. The vertices only rely on the form of the interaction term V and is independent of the waveguide photons. As a result, all Green functions, including higher-order ones, can be computed by the effective Hamiltonian (1.32).

In [18, 35], the effective Hamiltonian is obtained in the path integral formalism by integrating out the waveguide degrees of freedom in the full Hamiltonian. The derivation here only relies on the input-output formalism (1.8)–(1.10) and the resulting quantum causality (1.15) and (1.16).

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