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Perturbative and iterative methods for photon transport in one-dimensional waveguides

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ABSTRACT

The problems of photon transport in one-dimensional waveguides have recently attracted great attentions. We consider the case of single photons scattering off a Λ-type three-level quantum emitter, and discuss the perturbative treatments of the scattering processes in terms of Born approximation for the Lippmann–Schwinger formalism. We show that the iterative Born series of the scattering amplitudes converge to the exact results obtained by other approaches. The generalization of our work provides a foundational basis for efficient computational schemes for photon scattering problems in one-dimensional waveguides.

Recently the transport problems of photons scattering off a quantum emitter in a one-dimensional continuum such as an optical waveguide have attracted considerable attentions [1–8]. Such transport problems are directly related to cavity quantum electrodynamics (cavity QED), and several simple models have been shown to permit exact solutions. All of which were obtained by postulating the functional forms of the scattering states, i.e., ansatz. As the complexities of the system increases (e.g., more complicated energy levels or more cavities), it becomes more challenging to postulate the ansatz, and to justify the solutions for specified input states. It is thus of great interest to seek a systematic and computationally efficient procedure for obtaining the scattering states for more complicated cases, either eliminating the use of any ansatz, or serving as an independent check. On a separate front, scattering phenomena are common in many fields of physics, ranging from, for example, particle scattering [9], spectroscopy, surface characterization [10], to imaging and sensing. As the dynamics of the scattering processes in general cannot be solved exactly, many approximate computational schemes have been developed for scattering problems. Among these approximate schemes, the Born series expansion is perhaps the most commonly used technique. Despite its simplicity, the Born series is known to diverge near a resonance (where non-trivial scattering processes typically occur) [11], and one often questions the validity of the Born series when approaching a resonance. The summation of the Born series to yield a closed form is also not possible in general. Here we consider the case of single photons scattering off a Λ-type three-level quantum emitter. We show that, for any input states, the Born series expansion of the scattering amplitudes can be summed to arbitrary order; and in the off-resonance regime, the series converges to the exact solutions given by the Lippmann–Schwinger equations and other methods. The generalization of the perturbative treatments for the case of multiple photons could provide a foundational basis for efficient computational schemes for photon scattering problems in one-dimensional waveguides.

We begin with a time-dependent formulation of the scattering processes [9]. Consider the case when the Hamiltonian of the system has the form $\hat{H} = \hat{H}_0 + \hat{V}$,where $\hat{H}_0$ is the Hamiltonian describing the free constituents;$\hat{V}$ describes the interaction between the constituents and has a finite range. Both $\hat{H}$ and $\hat{H}_0$ exhibit continuous energy spectra. Let $|\psi\rangle$ be the interacting scattering state of the system at $t=0$ (which can be a linear superposition of different energy eigen states),the state of the system at any time

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thus is $|\Psi(t)\rangle = \hat{U}(t)|\psi\rangle \equiv e^{-i\hat{H}t/\hbar}|\psi\rangle$,which satisfies the Schrödinger equation $i\hbar\partial/\partial t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$. When followed back in time well before the scattering, $|\Psi(t)\rangle$ represents constituents that are localized far away from each other and, therefore, behaves like *free* constituents and is experimentally indistinguishable from the freely evolving state $|\Phi(t)\rangle = \hat{U}^0(t)|\phi_i\rangle \equiv e^{-i\hat{H}_0 t/\hbar}|\phi_i\rangle$, for some free state $|\phi_i\rangle$. Consequently the two states satisfy the causality condition:

$$\hat{U}(t)|\psi\rangle \longrightarrow \hat{U}^0(t)|\phi_i\rangle \quad \text{when } t \to -\infty. \tag{1}$$

From the adiabatic switching of the interaction $\hat{V}$ [9,12,13], it follows from Eq. (1) that

$$|\psi\rangle = |\phi_i\rangle + i\lim_{\epsilon\to 0^+}\int_0^{-\infty} d\tau e^{+\epsilon\tau}\hat{U}(\tau)^\dagger\hat{V}\hat{U}^0(\tau)|\phi_i\rangle. \tag{2}$$

When $|\psi\rangle$ and $|\phi_i\rangle$ are stationary states (i.e., $\hat{H}|\psi\rangle = E|\psi\rangle$ and $\hat{H}_0|\phi_i\rangle = E|\phi_i\rangle$), Eq. (2) can be shown to become

$$\begin{aligned}|\psi\rangle_E &= |\phi_i\rangle_E + \lim_{\epsilon\to 0^+}\frac{1}{E-\hat{H}+i\epsilon}\hat{V}|\phi_i\rangle_E \\ &= |\phi_i\rangle_E + \lim_{\epsilon\to 0^+}\frac{1}{E-\hat{H}_0+i\epsilon}\hat{V}|\psi\rangle_E,\end{aligned} \tag{3}$$

where the $+i\epsilon$ in the denominator of each Green's function specifies the causality condition in Eq. (1). A subscript E is used to explicitly denote that these states are stationary states (energy eigen states) of energy E. Similarly, there exists a free state $|\phi_f\rangle$ such that $\hat{U}(t)|\psi\rangle \longrightarrow \hat{U}^0(t)|\phi_f\rangle$ when $t \to +\infty$; when both $|\psi\rangle$ and $|\phi_f\rangle$ are stationary states (i.e., $\hat{H}|\psi\rangle = E|\psi\rangle$ and $\hat{H}_0|\phi_f\rangle = E|\phi_f\rangle$), the two states satisfy

$$\begin{aligned}|\psi\rangle_E &= |\phi_f\rangle_E + \lim_{\epsilon\to 0^+}\frac{1}{E-\hat{H}-i\epsilon}\hat{V}|\phi_f\rangle_E \\ &= |\phi_f\rangle_E + \lim_{\epsilon\to 0^+}\frac{1}{E-\hat{H}_0-i\epsilon}\hat{V}|\psi\rangle_E,\end{aligned} \tag{4}$$

where the $-i\epsilon$ specifies the causality.

Eqs. (3) and (4) are called the Lippmann–Schwinger equations. In practical computations, one often uses the latter expression in Eqs. (3) and (4), respectively, as it involves only the free Hamiltonian $\hat{H}_0$. The physical interpretation is that if $|\phi_i(t)\rangle \equiv \int dE g(E)e^{-i(E/\hbar)t}|\phi_i\rangle_E$ at $t=-\infty$ is the prepared free input state (a wave packet, where $g(E)$ is the amplitude of the distribution), then $|\psi(t)\rangle \equiv \int dE g(E)e^{-i(E/\hbar)t}|\psi\rangle_E$ is the interacting scattering state (also a wave packet), and $|\phi_f(t)\rangle \equiv \int dE g(E)e^{-i(E/\hbar)t}|\phi_f\rangle_E$ at $t=+\infty$ is the free outgoing state (yet another wave packet). As long as the time-dependent interpretation is clearly understood, it is harmless and convenient to speak of $|\psi\rangle_E$ (an extended state) as the actual state at $t=0$ that has evolved from the initial input state $|\phi_i\rangle_E$ (also an extended state), and that $|\phi\rangle_E$ would eventually evolve into the final state $|\phi_f\rangle_E$ (yet another extended state) [9]. These three states are said to be *causally related*. When any one of the three states $|\phi_i\rangle_E$, $|\psi\rangle_E$, or $|\phi_f\rangle_E$, is specified, Eqs. (3) and (4) provide a scheme to systematically compute the other two states. Note that in Eq. (3) of the Lippmann–Schwinger equations, the state $|\phi_i\rangle_E$ is incorporated as a *boundary condition*, while in the time-dependent description, $|\phi_i\rangle_E$ serves as an *initial condition*. More importantly, in the stationary state calculation (i.e., $|\Psi(t)\rangle = e^{-iEt/\hbar}|\psi\rangle_E$ and $|\Phi(t)\rangle = e^{-iEt/\hbar}|\phi_i\rangle_E$) using the Schrödinger equation, the eigen-equation $\hat{H}|\psi\rangle_E = E|\psi\rangle_E$ generally permits more than one solutions; only one of the solutions is causally related to $|\phi_i\rangle_E$. For complicated scattering processes, it is not always straightforward to find the causally related scattering states by directly using the Schrödinger equation.

We now discuss how to solve the Lippmann–Schwinger equations. For brevity, we will drop the subscript E in each state hereafter. Because the unknown state $|\psi\rangle$ appears on both sides of the Lippmann–Schwinger equations, Eqs. (3) and (4) are difficult to solve. Nonetheless, an iterative approximation can be straightforwardly developed: when the input state $|\phi_i\rangle$ is specified, the first-order Born approximation $|\psi\rangle_1$ is obtained by replacing the unknown state $|\psi\rangle$ at the right hand side of the LS equation (Eq. (3)) by $|\phi_i\rangle$:

$$|\psi\rangle \simeq |\psi_i\rangle_1 \equiv |\phi\rangle + \frac{1}{E-\hat{H}_0+i0^+}\hat{V}|\phi_i\rangle, \tag{5}$$

where we have used 0^+ to represent the limit. Higher-order Born state is obtained by iteratively repeating the procedure:

$$|\psi\rangle_n \equiv |\phi_i\rangle + \frac{1}{E-\hat{H}_0+i0^+}\hat{V}|\psi\rangle_{n-1} = \sum_{j=0}^{n}\left(\frac{1}{E-\hat{H}_0+i0^+}\hat{V}\right)^j|\phi_i\rangle, \tag{6}$$

where $|\psi\rangle_0 \equiv |\phi_i\rangle$ is the input state. A well-known example of the first-order Born approximation is the three-dimensional scattering of a plane wave off a scatterer [14]: $\psi(\mathbf{r}) \simeq e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}', \mathbf{k})e^{ikr}/r$ when $r = |\mathbf{r}|$ is large. $f(\mathbf{k}', \mathbf{k})$ is the scattering amplitude that the momentum of the incoming wave is $\mathbf{k}$ while the momentum of the outgoing wave is $\mathbf{k}' \equiv k\hat{\mathbf{r}}$. For a given potential, e.g., the Coulomb potential, the n-th order Born approximation of the wave function can be formally written down but the series cannot be summed to yield a closed form.

With these considerations, here we investigate the following scattering processes in quantum optics: a single photon scatters off a Λ-type (Lambda-type) three-level quantum emitter. The photon propagates in an optical waveguide to which the quantum emitter is coupled (Fig. 1 inset). The Hamiltonian $\hat{H}_0 = \hat{H}_p + \hat{H}_q$, where $\hat{H}_p$ describes the free photons and $\hat{H}_p$ the quantum emitter. $\hat{H}_p$ has the following form [15]:

$$\hat{H}_p = \hbar\int dx\left\{c_R^\dagger(x)(\omega_0 - iv_g\partial_x)c_R(x) + c_L^\dagger(x)(\omega_0 + iv_g\partial_x)c_L(x)\right\}, \tag{7}$$

where $c_R^\dagger(x)$ and $c_R(x)$ are creation and annihilation operators for a right-moving photon at position x, and $c_L^\dagger(x)$ and $c_L(x)$ are creation and annihilation operators for a left-moving photon at position x. v_g is the group velocity of the photon, and ω_0 is a reference frequency. The dispersion relation between the wave vector $k(\omega)$ and the frequency of the photon $\omega$is given by $\omega - \omega_0 = v_g k(\omega)$. $\hat{H}_q$ is given by

$$\hat{H}_q = \hbar\left(\Omega_1 a_1^\dagger a_1 + \Omega_2 a_2^\dagger a_2 + \Omega_3 a_3^\dagger a_3\right), \tag{8}$$

where $a_i^\dagger$ and a_i creation and annihilation operators for the atomic $|i\rangle$ state. The interaction term describes the scattering between photons and the emitter and is given by

$$\begin{aligned}\hat{V} = \int dx\hbar\delta(x)\{&V_1[(c_R^\dagger(x) + c_L^\dagger(x))\sigma_{13} + (c_R(x) + c_L(x))\sigma_{31}] \\ &+ V_2[(c_R^\dagger(x) + c_L^\dagger(x))\sigma_{23} + (c_R(x) + c_L(x))\sigma_{32}]\},\end{aligned} \tag{9}$$

where $\sigma_{ij} = a_i^\dagger a_j$ is the transition operator from atomic state $|j\rangle$ to atomic state $|i\rangle$; V_1 and V_2 describe the coupling strengths for the corresponding transitions; the emitter is located at $x=0$ (for an emitter at $x = x_q$, $\delta(x)$ must be replaced by $\delta(x - x_q)$). $\hat{V}$ describes all absorption and emission processes of photons by the quantum emitter. For example, the term proportional to $(c_R^\dagger(x) + c_L^\dagger(x))\sigma_{13}$