Single-photon scattering by two separated atoms in a supercavity*

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(Received 15 September 2015; revised manuscript received 19 January 2016; published online 20 April 2016)

We study the single-photon scattering along a one-dimensional cavity array with two distant two-level atoms in a supercavity, which aims to simulate a recent x-ray experiment [*Nature* **482**, 199 (2012)]. Without introducing dissipation, we find that when one atom is exactly located at a node of a mode of the supercavity and the other is at the antinode of that mode, no splitting of the reflectivity peak can appear. Nevertheless, the atom at the node significantly changes the positions of the reflectivity valleys. On the other hand, when the atom is shifted a little from the exact node, then the splitting can appear. We also explain these results with an analysis based on the general formal scattering theory. Our result implies the importance of non-resonant modes of the supercavity in our problem.

Keywords: cavity array, single-photon scattering, x-ray quantum optics

PACS: 42.50.Pq, 42.50.Nn, 32.70.Jz, 32.80.Qk **DOI:** 10.1088/1674-1056/25/6/064203

1. Introduction

Recently, some important experimental progress in x-ray quantum optics was made by Röhlsberger *et al.* in the group of Deutsches–Elektronen–Synchrotron.[1,2] In their experiments, the high-energy photons from an x-ray synchrotron radiation were injected into an effective cavity formed by two layers of Pt atoms. In this effective cavity there are one or two layers of ^{57}Fe atoms. In the system with one layer of ^{57}Fe atoms, the reflectivity of a single x-ray photon, as a function of the energy of this photon, has a single peak. The collective Lamb shift of the ^{57}Fe can be detected from the position of this peak. Nevertheless, when there are two layers of ^{57}Fe atoms, the following two interesting effects can appear.

(i) The peak of the single-photon reflectivity can split, as observed in the experiment of electromagnetically-induced-transparency effect.

(ii) The splitting of the peak of reflectivity depends on the position of the ^{57}Fe atoms. In particular, when the first layer of the ^{57}Fe atoms are at an antinode of an eigen-mode of the effective cavity, and the second layer is at a node of that mode, the splitting disappears and the reflectivity has only a single peak.

The purpose of our research is to understand the physics of the above effects with some simple models, rather than the complicated analysis provided by Röhlsberger *et al.*[1,2] In their papers, the transmission matrix method with many external parameters is applied to obtain the reflected magnitude, which is compared with that from a three level EIT to get the physical explanation. However, the microscopic mechanism to explain the phenomena is not clear in their work, which motivates us to build a microscopic model without any external parameter to understand the basic physics in their settings.

In our previous works[3,4] we have used the atom-array and cavity-array models to study the collective behaviors of the Fe atoms, as well as the effect of the cavity in the single-photon scattering on a single layer of ^{57}Fe atom. In this paper, we use a one-dimensional (1D) cavity array model to study the physics of the single-photon scattering on an effective cavity with two layers of atoms. In our model the photon propagates in the 1D array of cavities. We further assume that there is one supercavity in that array, and two two-level atoms are coupled to the photon in this supercavity. Here we use the photon in the cavity array to simulate the x-ray photon in the experiment,[2] use the supercavity to simulate the effective cavity formed by the Pt atoms, and use each two-level atom to simulate one layer of Fe atoms.

We exactly calculate the single-photon reflectivity in this toy model. Our result shows that, when one atom is exactly at the node of an eigen-mode of the supercavity, there is almost no splitting of the peak of the reflectivity, i.e., the effect (i) cannot appear. Nevertheless, the atom at the node can change the positions of the reflectivity valleys. On the other hand, when the atom is shifted a little from the exact node, the effect (i) can appear, and effect (ii) can still not appear. We further explained these behaviors with an analysis with formal scattering theory. Our results show that, to completely explain the effects (i) and (ii) in the experiments, it is necessary to take into account the

*Project supported by the National Natural Science Foundation of China (Grant Nos. 11222430, 11434011, 11475254, and 11175247) and the National Key Basic Research Program of China (Grant Nos. 2012CB922104 and 2014CB921202).

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spontaneous emission of the atoms in the excited state, and the non-resonant modes of the supercavity in our problem.

The remaining part of this paper is organized in the following way. In Section 2 we introduce our model and calculate the single-photon reflectivity with exact numerical calculation. In Section 3 we explain our results with formal scattering theory. We draw our conclusions in Section 4. We show some details of our calculations in Appendix A.

2. Single-photon reflectivity

2.1. System and calculation

We consider a one-dimensional (1D) single-mode cavity array with infinite length, which is shown in Fig. 1. Here we assume the frequency of the cavity mode is ω_c, the single-photon hopping intensity between the l-th and $(l+1)$-th cavity is ξ for $l \neq 0, N$, and $\eta\xi$ for $l = 0$ or $l = N$, with $0 < \eta \ll 1$. As a result, the cavities between 1 and N can form a supercavity. We further assume that two two-level atoms $1, 2$ are coupled to the photon in the n_1-th and n_2-th cavity, respectively. The energy gap between the excited state $|e\rangle_j$ and the ground state $|g\rangle_j$ of atom j ($j = 1, 2$) takes a j-independent value ω_a. For simplicity, here we take $2 < n_1 < n_2 - 2$ and $n_2 < N - 1$.

In the rotated frame, the Hamiltonian of our system is given by

$$H = H_0 + V_{\rm bg} + H_{\rm I}. \tag{1}$$

Here H_0 is the free Hamiltonian for the cavity array and atoms and can be expressed as ($\hbar = 1$)

$$H_0 = -\xi \sum_l \left(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l \right) + \Delta \sum_{j=1,2} |e\rangle_j\langle e|, \tag{2}$$

with a_l the annihilation operator of the photon in the l-th cavity, and $\Delta = \omega_a - \omega_c$ the atom–photon detuning. In Eq. (1), $V_{\rm bg}$ is defined as

$$V_{\rm bg} = -(\eta - 1)\xi \sum_{l=0,N} \left(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l \right). \tag{3}$$

It describes the interaction between the "walls" of the supercavity and the photon. The atom–photon interaction is described by the term H_I which is defined as

$$H_{\rm I} = \sum_{j=1,2} \Omega_j |e\rangle_j\langle g| a_{n_j} + \text{h.c.}, \tag{4}$$

where $|g\rangle_j$ is the ground state of atom j and Ω_j coupling intensity between the atom j and the photon in the cavity n_j.

In the absence of the supercavity and the atom–photon coupling (i.e., $\eta = 1$ and $\Omega_1 = \Omega_2 = 0$), the eigen-state of a single photon with momentum k is

$$|\psi_k^{(0)}\rangle = \frac{1}{\sqrt{2\pi}} \sum_{l=-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}kl} |l\rangle, \tag{5}$$

with the state $|l\rangle$ defined as

$$|l\rangle = a_l^\dagger |\text{vac}\rangle |g\rangle_1 |g\rangle_2, \tag{6}$$

where $|\text{vac}\rangle$ is the vacuum state of all the cavities. It is clear that in this simple case $|\psi_k^{(0)}\rangle$ is the eigen-state of the Hamiltonian H with eigen-energy

$$E_k = -2\xi \cos k. \tag{7}$$

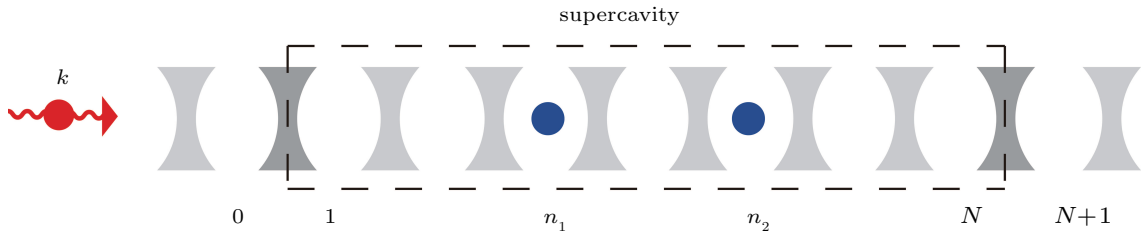


Fig. 1. (color online) Schematic configuration of the single-photon scattering problem in a single-mode cavity array. A single photon (filled red circle) with the wave vector k injects from the left side of the super cavity composed of N cavities, which is formed by a relatively small coupling strength $\eta\xi$ with the outside cavities. Two two-level atoms (filled blue circle) are each in the n_1-th and n_2-th cavity.

When $\eta \ll 1$ and $\Omega_{1,2} \neq 0$, the photon will be scattered by the supercavity and the two atoms. In this paper we consider this single-photon scattering problem. The scattering state of a photon with incident momentum k can be expressed as follows:[4,5]

$$|\psi_k^{(+)}\rangle = \sum_l C_l |l\rangle + \alpha_1 |e_1\rangle + \alpha_2 |e_2\rangle, \tag{8}$$

where the states $|e_{1,2}\rangle$ are defined as

$$|e_1\rangle = |\text{vac}\rangle |e\rangle_1 |g\rangle_2, \tag{9}$$

$$|e_2\rangle = |\text{vac}\rangle |g\rangle_1 |e\rangle_2. \tag{10}$$

Here the coefficient C_l can be expressed as

$$C_l = \begin{cases} \dfrac{1}{\sqrt{2\pi}} \left(\mathrm{e}^{\mathrm{i}kl} + r\,\mathrm{e}^{-\mathrm{i}kl} \right), & l \leq 0 \\ c_1 \mathrm{e}^{\mathrm{i}kl} + d_1 \mathrm{e}^{-\mathrm{i}kl}, & 0 < l < n_1 \\ C_{n_1}, & l = n_1 \\ c_2 \mathrm{e}^{\mathrm{i}kl} + d_2 \mathrm{e}^{-\mathrm{i}kl}, & n_1 < l < n_2; \\ C_{n_2}, & l = n_2 \\ c_3 \mathrm{e}^{\mathrm{i}kl} + d_3 \mathrm{e}^{-\mathrm{i}kl}, & n_2 < l \leq N \\ \dfrac{t}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}kl}, & l > N \end{cases} \tag{11}$$

Here the parameters t and r are the single-photon transmission and reflection amplitudes, respectively. According to the scattering theory,[6] the scattering state $|\psi_k^{(+)}\rangle$ is an eigen-state of the Hamiltonian H with eigen-energy E_k, i.e., we have

$$H|\psi_k^{(+)}\rangle = E_k|\psi_k^{(+)}\rangle. \tag{12}$$

Therefore, we can derive the algebraic equations for the parameters $r, t, c_{1,2,3}, d_{1,2,3}, C_{n_{1,2}}$, and $\alpha_{1,2}$ by submitting the expression (8) into Eq. (12) (In particular, by comparing the coefficients of the states $|n_1 \pm 1\rangle$ and $|n_2 \pm 1\rangle$ in the two sides of Eq. (12), we can obtain the results $C_{n_1} = c_1 e^{ikn_1} + d_1 e^{-ikn_1} = c_2 e^{ikn_1} + d_2 e^{-ikn_1}$ and $C_{n_2} = c_2 e^{ikn_2} + d_2 e^{-ikn_2} = c_3 e^{ikn_2} + d_3 e^{-ikn_2}$. Namely, the single-photon wave function is "continuous" at the cavities $n_{1,2}$.). Numerically solving these equations, we obtain the value of the reflection amplitude r. The single-photon reflectivity R can be calculated as

$$R = |r|^2. \tag{13}$$

2.2. Results

We numerically solve Eq. (11) and obtain the reflectivity R for various cases. In Fig. 2 we show our result for the system where there is only one atom in the supercavity. It is clear that in this system the reflectivity, as a function of the detuning Δ, has a single-peak behavior (see Fig. 2, the peak appears in the region of two red dashed vertical lines, i.e., the region where $-2.404 \times 10^{-2}\xi \lesssim \Delta \lesssim +2.342 \times 10^{-2}\xi$). That is qualitatively similar as the behavior of the single-photon reflectivity in the experiment with one layer of ^{57}Fe atoms.[2] Furthermore, our numerical calculation reveals the existence of a small Lamb shift about $10^{-9}\xi$.

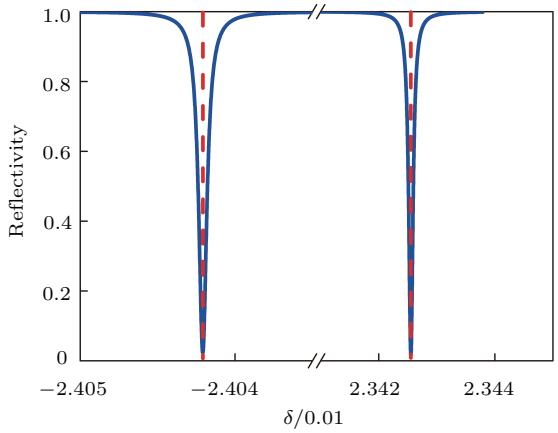


Fig. 2. (color online) The single-photon reflectivity in the system with one atom in the supercavity. The part between two red dashed vertical lines is the reflectivity peak. Here we choose the parameters as $N = 31$, $\Omega = 0.1$, $n_1 = 12$ (antinode), $\xi = 1$, $\eta = 0.01$ while the atom is resonant with the 4-th eigen-mode of the supercavity with $\Delta = -2\cos(4\pi/N+1)$. In our calculation we fix the value of Δ and calculate the single-photon reflectivity R as a function of the momentum k of the incident photon. The horizontal label of the figure is $\delta/0.01$, with $\delta = \Delta - E_k$.

We also numerically investigate the system with two atoms in the supercavity. In Fig. 3 we show our results for the system where one atom is at the anti-node of an eigen-mode of the supercavity while the other atom is at the node of that eigen-mode. No splitting (sudden drop of reflectivity) appears, no matter if the first atom (in the n_1-th cavity) is at the anti-node or node. Therefore, with our model we cannot re-obtain the splitting effect in the experiment with two layers of ^{57}Fe atoms,[2] i.e., the effect (i) introduced in Section 1.

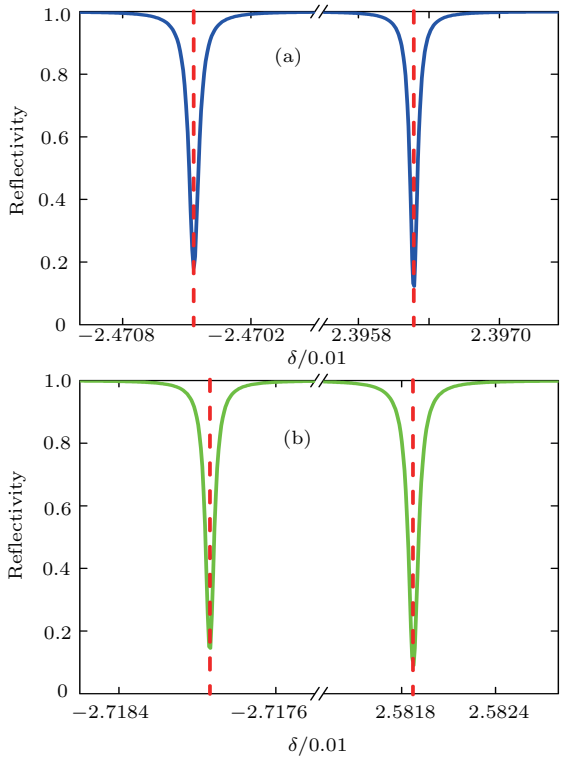


Fig. 3. (color online) The single-photon reflectivity in the system with two atoms in the supercavity. (a) With $n_1 = 8$ (node) and $n_2 = 12$ (antinode). (b)$n_1 = 12$ (antinode) and $n_2 = 16$ (node). The part between two red dashed vertical lines is the reflectivity peak. All the other parameters are the same as those in Fig. 2, and δ is also defined as $\delta = \Delta - E_k$.

However, in our system the two-level atom at the node of the resonant mode obviously changes the positions of the peaks. As shown in Fig. 2 and Fig. 3, for the parameter region of these two figures, this change is about 2% of the width of the peak for the case where the first atom is at the node of the supercavity, and about 10% of the width of the peak for the case where the second atom is at the node of the supercavity. This change implies that the non-resonant modes in the supercavity cannot be ignored in our analysis.

We also study the system where one atom is at the anti-node of the supercavity mode, and another atom is slightly shifted from the node. As shown in Fig. 4, in that case a drop of the reflectivity appears in the middle of the peak, i.e., in the region around $\Delta = 0$. Due to this drop, the single peak of the reflectivity quantitatively splits into two peaks. Namely, we can obtain the splitting effect of the single-photon reflectivity, i.e., the effect (i) observed in the experiments[1,2] (see Section 1). Nevertheless, as shown in Fig. 4, the reflectivity curve has the same behavior for the cases where the first or second atom is near the node. Thus, we still cannot obtain the effect (ii).

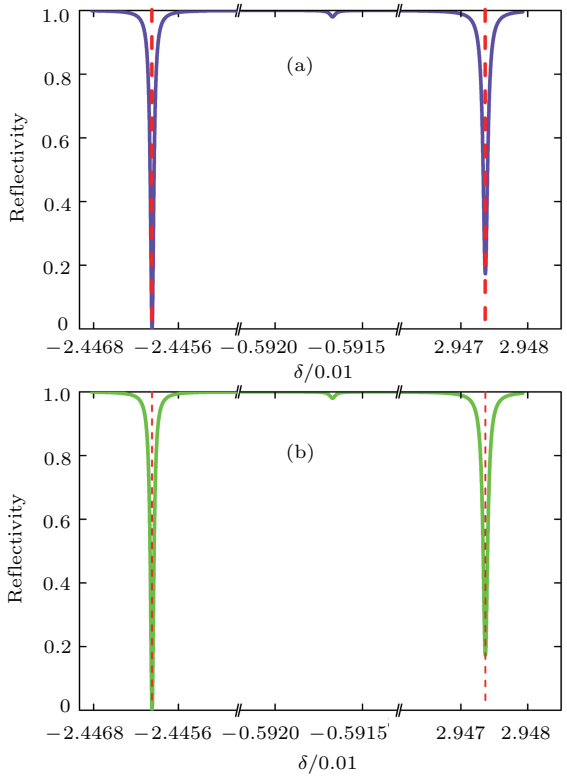


Fig. 4. (color online) The single-photon reflectivity in the system with two atoms in the supercavity. (a) With $n_1 = 9$ (near node) and $n_2 = 12$ (antinode). (b)$n_1 = 12$ (antinode) and $n_2 = 15$ (near node). All the other parameters are the same as those in Fig. 2. The part between the two red dashed vertical lines is the reflectivity peak. It is clear that a drop appears in the middle of that peak, i.e., in the region around $\Delta = 0$. Due to this drop, the single peak of the reflectivity quantitatively splits into two peaks, and δ is also defined as $\delta = \Delta - E_k$.

3. Energy shift and effective coupling of atoms

In this section we provide a physical explanation for the splitting of the single-photon reflectivity in the case where the photon is coupled to both of the two atoms. We will show that this splitting can be understood as a result of the atom–photon-coupling-induced energy shifts and effective coupling of the two atoms. Although the following analysis is done for our mode in Section 2, it can be directly generalized to the system in the experiment[2] of the x-ray photon scattering.

Before going into the detail of the calculations, here we first give a qualitative physical picture for shift and splitting of the single-photon reflectivity. We consider the scattering of a single photon on a single two-level atom. We first focus on the case in which there is no supercavity and the photon is just moving in a simple 1D cavity array (i.e., the case with $\eta = 1$ and $\Omega_2 = 0$). In this case, if the atom is far-off resonant to the incident photon, then the photon cannot be influenced by the atom, and just goes across it. Thus, the single-photon reflectivity is almost zero. Nevertheless, if the atom is near-resonant to the photon, the atom can absorb the photon and re-emit it. Furthermore, when the photon is re-emitted, it can go along either the same or the opposite direction of movement of the incident photon. In the latter case, the photon is reflected by the atom. Therefore, the single-photon reflectivity $|r_A(k)|^2$ has a peak when the atom is near-resonant to the photon, i.e., when $\omega_a = \omega_c + E_k$ or $\Delta = E_k$.

In the system with a supercavity, when the atom in the supercavity absorbs the photon and re-emits it, the photon can stay in the supercavity for a long time, and thus will not become far away from the atom immediately. During that time, the photon can be re-absorbed by the atom and re-emitted again. As a result of this process, the effective energy of the atom can be shifted. That shift effect is just like the AC Stark effect. Furthermore, the single-photon reflectivity $|r_A(k)|^2$ peaks when the single photon energy is resonant to the effective energy of the atom. Thus, when the effective energy of the atom is shifted, the peak of the single-photon reflectivity is also shifted.

Now let us consider the system with two atoms 1 and 2. By absorbing a single photon, these two atoms can jump from the two-atom ground state $|g\rangle_1|g\rangle_2$ to the two-atom excited states $|e\rangle_1|g\rangle_2$ or $|g\rangle_1|e\rangle_2$. Furthermore, when there is a supercavity, then the incident photon can be absorbed by the 1st atom, and be re-emitted by this atom, and then be absorbed and re-emitted by the 2nd atom, and then be absorbed and re-emitted by the 1st atom again, ... Since the photon can stay in the supercavity for a long time, these processes can occur for many cycles. During these processes, the states $|e\rangle_1|g\rangle_2$ or $|g\rangle_1|e\rangle_2$, whose bare energies are the same, can be effectively coupled. As a result of this coupling, the degeneracy of these two states is destroyed and thus the effective energies of these two states becomes different. In addition, the single-photon reflectivity peaks when the photon is near resonant to the transition from $|g\rangle_1|g\rangle_2$ to $|e\rangle_1|g\rangle_2$ or $|g\rangle_1|e\rangle_2$. Therefore, there will be two peaks corresponding to the effective energy gap between $|e\rangle_1|g\rangle_2$ and $|g\rangle_1|g\rangle_2$ and the one between $|g\rangle_1|e\rangle_2$ and $|g\rangle_1|g\rangle_2$.

Now we illustrate the above picture with analytical calculations.

According to Eq. (13), the reflectivity is given by the relation $R = |r|^2$. Furthermore, as shown in Appendix A, the reflection amplitude r, as a function of the incident wave vector k of the photon, can be re-written as

$$r(k) = r_{\rm bg}(k) + r_A(k). \tag{14}$$

Here $r_{\rm bg}(k)$ is the reflection amplitude of the supercavity itself, i.e., the reflection amplitude in the case where $\Omega_1 = \Omega_2 = 0$. When the incident photon is near resonant with a mode of the supercavity, $|r_{\rm bg}(k)|$ is very small. In Eq. (14) the contribution from the atoms to the reflection amplitude is described by the term $r_A(k)$. As shown in Appendix A, it is given by

$$\begin{aligned} r_A(k) &= -\frac{2\pi \mathrm{i}}{\xi \sin k}\langle \psi_k^{(\mathrm{bg}-)}|H_I|\psi_k^{(+)}\rangle \\ &= -\frac{2\pi \mathrm{i}}{\xi \sin k}\left(\Omega_1^*\langle \psi_{-k}^{(\mathrm{bg}-)}|n_1\rangle\alpha_1 + \Omega_2^*\langle \psi_{-k}^{(\mathrm{bg}-)}|n_2\rangle\alpha_2\right). \end{aligned} \tag{15}$$

Here the parameters $\alpha_{1,2}$ are defined in Eq. (8), and $|\psi_k^{(\mathrm{bg}-)}\rangle$ is the single-photon scattering state in the case where $\Omega_1 =$

$\Omega_2 = 0$, with incident wave vector k and the in-coming boundary condition (Appendix A).

3.1. Single-atom case

We first discuss the case where the photon is only coupled to atom 1, i.e., $\Omega_2 = 0$. In this case we have $\alpha_2 = 0$, and thus the reflection amplitude $r_A(k)$ contributed by the atom is determined by the parameter α_1. This parameter can be calculated as follows. As shown in Appendix A, the scattering state $|\psi_k^{(+)}\rangle$ satisfies the equation

$$|\psi_k^{(+)}\rangle = |\psi_k^{(\mathrm{bg}+)}\rangle + G_{\mathrm{bg}}^{(+)}(E_k) H_{\mathrm{I}} |\psi_k^{(+)}\rangle, \tag{16}$$

where $|\psi_k^{(\mathrm{bg}+)}\rangle$ is the single-photon scattering state in the system with $\Omega_1 = \Omega_2 = 0$, with incident wave vector k and the out-going boundary condition, and $G_{\mathrm{bg}}^{(+)}(E_k)$ is the Green's operator of that system. It is defined as

$$G_{\mathrm{bg}}^{(+)}(E_k) = \frac{1}{E_k + i0^+ - (H_0 + V_{\mathrm{bg}})}. \tag{17}$$

On the other hand, since $\Omega_2 = 0$, the scattering state $|\psi_k^{(+)}\rangle$ can be expressed as

$$|\psi_k^{(+)}\rangle = \sum_l C_l |l\rangle + \alpha_1 |e_1\rangle. \tag{18}$$

Substituting Eqs. (17) and (18) into Eq. (16), we obtain

$$\sum_l C_l |l\rangle = |\psi_k^{(\mathrm{bg}+)}\rangle + \alpha_1 \Omega_1^* G_{\mathrm{bg}}^{(+)}(E_k) |n_1\rangle, \tag{19}$$

$$\alpha_1 = \frac{\Omega_1}{E_k - \Delta} \langle n_1 | \left(\sum_l C_l |l\rangle \right). \tag{20}$$

Substituting Eq. (19) and the fact $\alpha_2 = 0$ into Eq. (20), we obtain the expression of the parameter α_1:

$$\alpha_1 = \frac{\Omega_1 \langle n_1 | \psi_k^{(\mathrm{bg}+)} \rangle}{E_k - \Delta - \Sigma^{(s)}(k)}. \tag{21}$$

Here the term $\Sigma^{(s)}$ is given by

$$\Sigma^{(s)}(k) = |\Omega_1|^2 \langle n_1 | G_{\mathrm{bg}}^{(+)}(E_k) | n_1 \rangle \tag{22}$$

and can be understood as a shift of the self-energy of atom 1 (Lamb shift). As shown above, this shift is induced by the coupling between the atom and the photon in the supercavity. Substituting Eq. (21) into Eq. (14), we obtain the reflection amplitude

$$r(k) = r_{\mathrm{bg}}(k) - \frac{2\pi \mathrm{i}}{\xi \sin k} |\Omega_1|^2 \frac{\langle \psi_{-k}^{(\mathrm{bg}-)} | n_1 \rangle \langle n_1 | \psi_k^{(\mathrm{bg}+)} \rangle}{E_k - \Delta - \Sigma^{(s)}(k)}. \tag{23}$$

This result shows that the single-photon reflectivity $R = |r(k)|^2$ peaks when the energy E_k satisfies the condition $E_k \approx \mathrm{Re}[\Delta + \Sigma^{(s)}(k)]$.

3.2. Two-atom case

Now we consider the case where the photon is coupled to both of the atoms. For simplicity, we assume $\Omega_1 = \Omega_2 = \Omega$ as shown in Eq. (15). In this case the reflection amplitude is determined by both of the parameters α_1 and α_2. We can calculate these two parameters with a similar method as above. In our system, the scattering state $|\psi_k^{(+)}\rangle$ has the expression (8). Notice that now both α_1 and α_2 are non-zero. Substituting Eq. (8) into Eq. (16), we obtain

$$\sum_l C_l |l\rangle = |\psi_k^{(\mathrm{bg}+)}\rangle + \Omega^* \sum_{j=1,2} \alpha_j G_{\mathrm{bg}}^{(+)}(E_k) |n_j\rangle, \tag{24}$$

where

$$\alpha_1 = \frac{\Omega}{E_k - \Delta} \langle n_1 | \left(\sum_l C_l |l\rangle \right), \tag{25}$$

$$\alpha_2 = \frac{\Omega}{E_k - \Delta} \langle n_2 | \left(\sum_l C_l |l\rangle \right). \tag{26}$$

Substituting Eq. (24) into Eqs. (25) and (26), we obtain the equation

$$\alpha_l = \frac{\Omega}{E_k - \Delta} \langle n_l | \psi_k^{(\mathrm{bg}+)} \rangle + \frac{|\Omega|^2}{E_k - \Delta} \sum_{j=1,2} \alpha_j \langle n_l | G_{\mathrm{bg}}^{(+)}(E_k) | n_j \rangle \tag{27}$$

for $l = 1, 2$. This equation yields

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \frac{\Omega}{E_k - \Delta - \Sigma^{(d)}(k)} \begin{pmatrix} \langle n_1 | \psi_k^{(\mathrm{bg}+)} \rangle \\ \langle n_2 | \psi_k^{(\mathrm{bg}+)} \rangle \end{pmatrix}. \tag{28}$$

Here $\Sigma^{(d)}(k)$ is the generalized Lamb shift of the self-energy of the two atoms. It is a 2×2 matrix

$$\Sigma^{(d)}(k) = \begin{pmatrix} \Sigma_{11}^{(d)}(k) & \Sigma_{12}^{(d)}(k) \\ \Sigma_{21}^{(d)}(k) & \Sigma_{22}^{(d)}(k) \end{pmatrix} \tag{29}$$

with matrix element

$$\Sigma_{lj}^{(d)}(k) = |\Omega|^2 \langle n_l | G_{\mathrm{bg}}^{(+)}(E_k) | n_j \rangle. \tag{30}$$

As shown above, the diagonal elements $\Sigma_{11}^{(d)}(k)$ and $\Sigma_{22}^{(d)}(k)$ can be understood as the energy shifts of atoms 1 and 2, respectively, and the non-diagonal element $\Sigma_{12}^{(d)}(k)$ can be understood as the effective coupling between the two atoms. Substituting Eq. (28) into Eq. (15), we eventually obtain the reflection amplitude

$$r(k) = r_{\mathrm{bg}}(k) - \frac{2\pi \mathrm{i}}{\xi \sin k} |\Omega|^2 \beta_-^\dagger(k) \frac{1}{E_k - \Delta - \Sigma^{(d)}(k)} \beta_+(k), \tag{31}$$

where the vector $\beta_\pm(k)$ is defined as

$$\beta_\pm(k) = \begin{pmatrix} \langle n_1 | \psi_{\pm k}^{(\mathrm{bg}\pm)} \rangle \\ \langle n_2 | \psi_{\pm k}^{(\mathrm{bg}\pm)} \rangle \end{pmatrix}. \tag{32}$$

Now we use Eq. (31) to explain our numerical results for the cases with two atoms. Since in our system the incident photon is near resonance to one eigen-mode of the super cavity, the probability amplitude $\langle n_j | \psi_{\pm k}^{(\mathrm{bg}\pm)} \rangle$ ($j = 1, 2$) is proportional to the photon wave function at the n_j-th cavity. We first consider the system where the n_1-th cavity is at the node of that eigen-node. In this case we have

$$\langle n_1 | \psi_{\pm k}^{(\mathrm{bg}\pm)} \rangle \approx 0. \tag{33}$$

Furthermore, the matrix element $\Sigma_{lj}^{(d)}(k)$ defined in Eq. (30) can be re-written as

$$\Sigma_{lj}^{(d)}(k) = |\Omega|^2 \int_{-\pi}^{\pi} \mathrm{d}k' \frac{\langle n_l | \psi_{k'}^{(\mathrm{bg}+)} \rangle \langle \psi_{k'}^{(\mathrm{bg}+)} | n_j \rangle}{E_k + i0^+ - E_{k'}}. \tag{34}$$

It is clear that the integration in the right-hand side of the above expression is mainly contributed by the terms in which

$E_{k'}$ is very close to E_k. According to our above analysis, for these terms $\langle n_l|\psi_{k'}^{(\mathrm{bg}+)}\rangle$ and $\langle\psi_{k'}^{(\mathrm{bg}+)}|n_j\rangle$ are also proportional to the photon wave function at the n_l-th and n_j-th cavity, respectively. Therefore, we have

$$\Sigma_{11}^{(d)}(k)\approx\Sigma_{12}^{(d)}(k)\approx\Sigma_{21}^{(d)}(k)\approx 0. \tag{35}$$

Substituting Eqs. (33) and (35) into Eqs. (31 and (32), we obtain

$$r(k)\approx r_{\mathrm{bg}}(k)-\frac{2\pi\mathrm{i}}{\xi\sin k}|\Omega|^2\frac{\langle\psi_{-k}^{(\mathrm{bg}-)}|n_1\rangle\langle n_1|\psi_k^{(\mathrm{bg}+)}\rangle}{E_k-\Delta-\Sigma_{22}^{(d)}(k)}, \tag{36}$$

which is quite similar as the result Eq. (23) for the case with only one atom in the supercavity. As shown in the above subsection, this result implies that the reflection rate R has only one peak.

On the other hand, when both of the atoms are not set at the node of the eigen-mode of the supercavity, all the elements of the matrix-type Lamb shift $\Sigma^{(d)}(k)$, as well as the components of the vectors $\beta_\pm(k)$, are non-zero. In that case, the condition of the peak of R becomes $E_k\approx\mathrm{Re}[\Delta+\lambda_a]$ or $E_k\approx\mathrm{Re}[\Delta+\lambda_b]$, where $\lambda_{a,b}$ are the two eigen-values of $\Sigma^{(d)}(k)$. In most of the cases we have $\lambda_a\neq\lambda_b$. Therefore, the reflectivity R, has two splitting peaks.

4. Conclusion

We present a supercavity model based on one dimensional cavity array to simulate a recent x-ray experiment in Ref. [2]. Without introducing the dissipation, we find that for the system with one atom exactly at a node of the supercavity, there is no splitting of the reflectivity peak. That peak can only appear when the atom is slightly shifted from the node. This result shows that it is very difficult to use our model to explain the splitting of the reflectivity peak appearing in the node–antinode arrangement of the two layers of ^{56}Fe atoms. However, we find that the appearance of the two-level atom at the node significantly changes the positions of the two reflectivity valleys, which implies that the non-resonant modes of the supercavity play an important role in the single photon scattering problem.

Appendix A: Proof of Eqs. (15) and (16)

In this appendix we prove Eqs. (15) and (16). We will first prove Eq. (16), and then prove Eq. (15).

A1. Eq. (16) and other related equations

According to the scattering theory,[7] the scattering state $|\psi_k^{(+)}\rangle$ satisfies the equation

$$|\psi_k^{(+)}\rangle=\lim_{\eta\to0^+}\frac{\mathrm{i}\eta}{E_k+\mathrm{i}\eta-H}|\psi_k^{(0)}\rangle. \tag{A1}$$

Similarly, the scattering states $|\psi_k^{(\mathrm{bg}\pm)}\rangle$ for the system with $\Omega_1=\Omega_2=0$ with out-going and in-coming boundary conditions satisfy

$$|\psi_k^{(\mathrm{bg}\pm)}\rangle=\lim_{\eta\to0^\pm}\frac{\mathrm{i}\eta}{E_k+\mathrm{i}\eta-(H_0+V_{\mathrm{bg}})}|\psi_k^{(0)}\rangle. \tag{A2}$$

Using the above two equations and the fact

$$\lim_{\eta\to0^+}\frac{\mathrm{i}\eta}{E_k+\mathrm{i}\eta-H}=\lim_{\eta\to0^+}\frac{\mathrm{i}\eta}{E_k+\mathrm{i}\eta-(H_0+V_{\mathrm{bg}})}+G_{\mathrm{bg}}^{(+)}(E_k)H_{\mathrm{I}}\left(\lim_{\eta\to0^+}\frac{\mathrm{i}\eta}{E_k+\mathrm{i}\eta-H}\right), \tag{A3}$$

we can directly obtain

$$|\psi_k^{(+)}\rangle=|\psi_k^{(\mathrm{bg}+)}\rangle+G_{\mathrm{bg}}^{(+)}(E_k)H_{\mathrm{I}}|\psi_k^{(+)}\rangle. \tag{A4}$$

with $G_{\mathrm{bg}}^{(+)}(E_k)$ defined in Eq. (17) in our main text. It is clear that equation (A4) is Eq. (16) in our main text.

With similar methods, we can also obtain the equations

$$|\psi_k^{(+)}\rangle=|\psi_k^{(0)}\rangle+G_0^{(+)}(E_k)V|\psi_k^{(+)}\rangle, \tag{A5}$$

and

$$|\psi_{-k}^{(\mathrm{bg}-)}\rangle=|\psi_{-k}^{(0)}\rangle+G_{\mathrm{bg}}^{(+)}(E_k)^\dagger V_{\mathrm{bg}}|\psi_{-k}^{(0)}\rangle, \tag{A6}$$

where

$$V=V_{\mathrm{bg}}+H_{\mathrm{I}} \tag{A7}$$

and

$$G_0^{(+)}(E_k)=\frac{1}{E_k+\mathrm{i}0^+-H_0} \tag{A8}$$

is the free Green's operator. Below we will use Eqs. (A5) and (A6).

A2. Proof of Eq. (15)

Equation (A5) yields

$$\langle l|\psi_k^{(+)}\rangle=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}kl}+\sum_{l'}\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k'\frac{\mathrm{e}^{\mathrm{i}k'(l-l')}}{E_k+\mathrm{i}0^+-E_{k'}}\langle l'|V|\psi_k^{(+)}\rangle. \tag{A9}$$

On the other hand, we have the relation[8]

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k'\frac{\mathrm{e}^{\mathrm{i}k'(l-l')}}{E_k+\mathrm{i}0^+-E_{k'}}=-\mathrm{i}\frac{\mathrm{e}^{\mathrm{i}k|l-l'|}}{\xi\sin k} \tag{A10}$$

for $\xi>0$ and $k>0$. Substituting Eq. (A10) into Eq. (A9), and using the result $\langle l|V=0$ for $l<0$, we find that for $l<0$ we have

$$\langle l|\psi_k^{(+)}\rangle=\frac{1}{\sqrt{2\pi}}\left[\mathrm{e}^{\mathrm{i}kl}-\frac{2\pi\mathrm{i}}{\xi\sin k}\langle\psi_{-k}^{(0)}|V|\psi_k^{(+)}\rangle\mathrm{e}^{-\mathrm{i}kl}\right]. \tag{A11}$$

Comparing this result with Eqs. (8) and (11), we obtain

$$r(k)=-\frac{2\pi\mathrm{i}}{\xi\sin k}\langle\psi_{-k}^{(0)}|V|\psi_k^{(+)}\rangle. \tag{A12}$$

Similarly, when $\Omega_1=\Omega_2=0$, we have

$$r_{\mathrm{bg}}(k)=-\frac{2\pi\mathrm{i}}{\xi\sin k}\langle\psi_{-k}^{(0)}|V_{\mathrm{bg}}|\psi_k^{(\mathrm{bg}+)}\rangle. \tag{A13}$$

Substituting Eqs. (A4) into Eq. (A12) and using Eq. (A13), we obtain

$$r(k)=r_{\mathrm{bg}}(k)-\frac{2\pi\mathrm{i}}{\xi\sin k}t'(k), \tag{A14}$$

with

$$t'(k)=\sum_{j=1,2}\alpha_j\Omega_j^*\left[\langle\psi_{-k}^{(0)}|V_{\mathrm{bg}}G_{\mathrm{bg}}^{(+)}(E_k)|n_j\rangle+\langle\psi_{-k}^{(0)}|n_j\rangle\right]. \tag{A15}$$

On the other hand, using Eq. (A6), we can re-write the function $t'(k)$ as

$$t'(k) = \sum_{j=1,2} \alpha_j \Omega_j^* \left[\langle \psi_{-k}^{(\mathrm{bg}-)} | n_j \rangle \right]. \tag{A16}$$

Substituting Eq. (A15) into Eq. (A14), we obtain Eq. (15) in the main text.

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