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Quantum walk calculations of dressed-photon–phonon transfer in a single nanometer-sized particle

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Abstract

This paper analyzes temporal variations of the light originating from a dressed-photon–phonon (DPP) and emitted from a single nanometer-sized particle (NP). Numerical calculations are carried out by using a quantum walk (QW) model. Photon breeding (PB) with respect to momentum is discussed by analyzing the calculated dependences of the slope S and the ratio I_+/I_- of the two emitted light intensities $I_\pm$ on a physical parameter χ/J. It is confirmed that I_+/I_- is larger than unity at $\chi/J > \sqrt{2}$, which corresponds to the PB with respect to momentum.

1 Introduction

A previous paper analyzed the time dependence of the intensity of light emitted as a result of dressed-photon–phonon (DPP) transfer between two nanometer-sized particles (NPs) and subsequent energy relaxation under optical pulse irradiation [1]. It should be noted that the phonon is a quantum of the crystal lattice vibration that induces non-adiabatic (thermal) energy relaxation.

By noting that a random walk (RW) process lies behind the quantum walk (QW) process, the time evolution operator $\mathcal{L}$ for the interpolation model was used. It was represented by the sum of those of the QW and RW evolution operators, $\mathcal{L}^{\mathrm{QW}}$ and $\mathcal{L}^{\mathrm{RW}}$, respectively:

$$\mathcal{L} = (1-p)\mathcal{L}^{\mathrm{QW}} + p\mathcal{L}^{\mathrm{RW}}, \tag{1}$$

where p $(0 \le p \le 1.0)$ is a probability [2].

For the calculation, $\mathcal{L}^{\mathrm{QW}}$ was chosen with probability $1-p$, while $\mathcal{L}^{\mathrm{RW}}$ was chosen with probability p at each time step, independently. The ratio χ / J between the dressed-photon (DP) hopping energy J and the DP-phonon coupling energy χ was used as a physical parameter.

The calculation results were as follows:

(1) In a time span shorter than t_x immediately after optical pulse irradiation, the emitted light intensities decreased and pulsated due to nutation of the DPP transfer. Since this decrease originates from the non-thermal (adiabatic) energy relaxation, the temporal variations of the emitted light intensities were reproduced by the QW model. The slope S_{QW} of the reproduced curve of this variation was large, and thus, the time constant τ_{QW} of the intensity decrease was short.

(2) In the time span longer than t_x, the emitted light intensities decreased due to the thermal (nonadiabatic) energy relaxation, and these were reproduced by the RW model. The slope S_{RW} of the curve was small, and thus, the time constant τ_{RW} of the intensity decrease was long.

(3) The crossover time t_x and the slopes of the curves depended on the values of p and χ / J.

Although results (1)–(3) suggested the presence of photon breeding (PB) with respect to the DPP momentum [3], detailed discussions on the origin of the PB were difficult due to the complicated feature of the nutation. In order to overcome this difficulty, this paper assumes a single NP to analyze the time-dependence of the emitted light intensities.

2 Numerical calculation method

Figure 1 schematically explains the QW model for a single NP. This section reviews the mathematical formulation that has been presented in ref. [4]. That is, the state of the DPP is represented by a vector

$$\vec{\Psi}_{t,(x,y)} = \begin{bmatrix} y_{DP+} \\ y_{DP-} \\ y_{Phonon} \end{bmatrix}_{t,(x,y)} . \tag{2}$$

Here, y_{DP+} and y_{DP-} are the creation probability amplitudes of the DPs that hop in directions that are parallel and antiparallel to the direction of the incident optical pulse propagation, respectively. y_{Phonon} is the creation probability amplitude of the phonon that is localized at the NP.

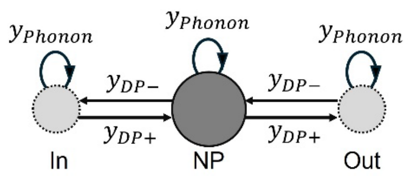

Fig. 1 A QW model for a single NP.

The coefficient matrix in the tempo-spatial evolution equation for eq. (2) is

$$U = \begin{bmatrix} -\cos^2\theta & \sin^2\theta & \frac{\sin 2\theta}{\sqrt{2}} \\ \sin^2\theta & -\cos^2\theta & \frac{\sin 2\theta}{\sqrt{2}} \\ \frac{\sin 2\theta}{\sqrt{2}} & \frac{\sin 2\theta}{\sqrt{2}} & \cos 2\theta \end{bmatrix}. \tag{3}$$

It is also represented by the DP hopping energy J and the DP-phonon coupling energy χ as

$$U = \begin{bmatrix} \varepsilon_+ & J & \chi \\ J & \varepsilon_- & \chi \\ \chi & \chi & \varepsilon_0 \end{bmatrix} , \tag{4}$$

where ε_+, ε_- and ε_0 are the eigen-energies of y_{DP+}, y_{DP-}, and y_{Phonon}, respectively. These equations indicate that the ratio χ/J is represented by

$$\chi/J = \sqrt{2}/\tan\theta \qquad . \qquad (5)$$

3 Results

Section 3.1 presents the results of numerical calculations which were derived by using eqs. (1)-(5). Their analytical expressions are given in Section 3.2. They present the values of the emitted output light intensities $I_+(=|y_{DP+}|^2)$ and $I_-(=|y_{DP-}|^2)$.

3.1 Results of numerical calculations

Figure 2 shows the results of numerically calculated time-dependences of $I_\pm$ in the case of θ=54.8 (deg.) and χ/J=1.0. Red and blue curves are for I_+ and I_-, respectively. They overlap with each other in this figure because their values are nearly equal except in the very early time span immediately after the optical pulse irradiation. Since these values are independent of the value of p, the case of p=0 is picked up to show the dependences of the slopes S of the curve on θ and χ/J in Figs. 3(a) and (b).

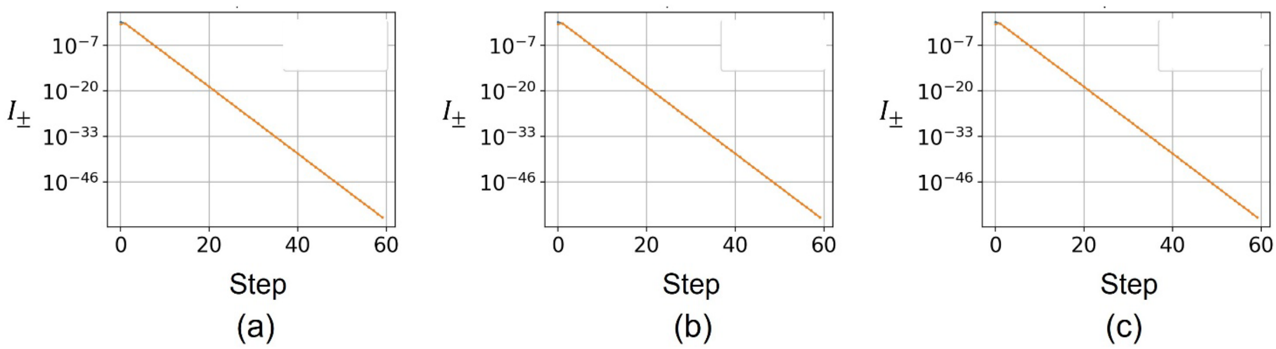

Fig. 2 Time-dependence of I_+ and I_-.

θ=54.8 (deg.) and χ/J=1.0. Red and blue curves are for I_+ and I_-, respectively.

(a) p=0, (b) p=0.6, (c) p=1.0.

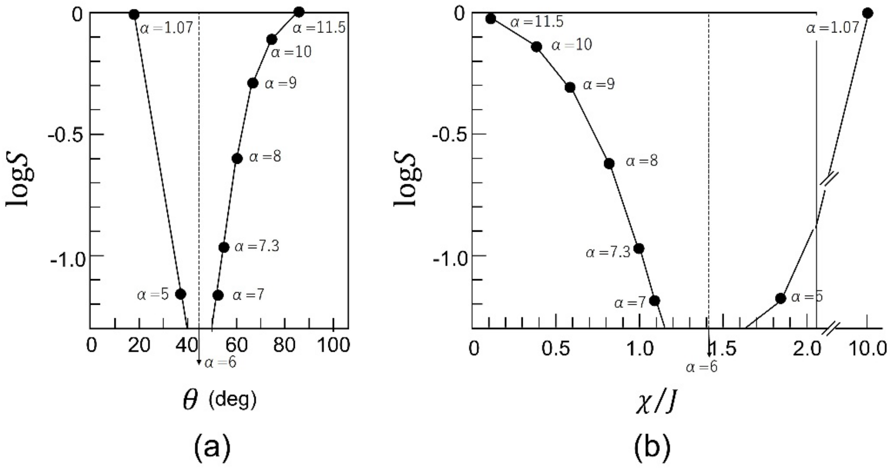

Fig. 3 Dependences of slopes S on θ (a) and on χ / J (b).

p =0 . The quantity α is defined as $\alpha \equiv \theta(\text{deg.}) / 7.5(\text{deg.})$

In order to analyze the time-dependence in the short time span immediately after the optical pulse irradiation, steps 1–5 in Fig. 2 are shown in Fig. 4. The values at step 1 indicate that $I_+ > I_-$ for $\chi / J > \sqrt{2}$ (Fig. 4(a)), which represents PB with respect to momentum. For comparison, Figs. 4(b) and (b) show that $I_+ = I_-$ at $\chi / J = \sqrt{2}$ and $I_+ < I_-$ for $\chi / J < \sqrt{2}$, respectively.

Figure 5 summarizes the dependence of I_+/I_- on χ / J at step 1, from which it is confirmed that $\chi / J = \sqrt{2}$ is the threshold of the advent of PB.

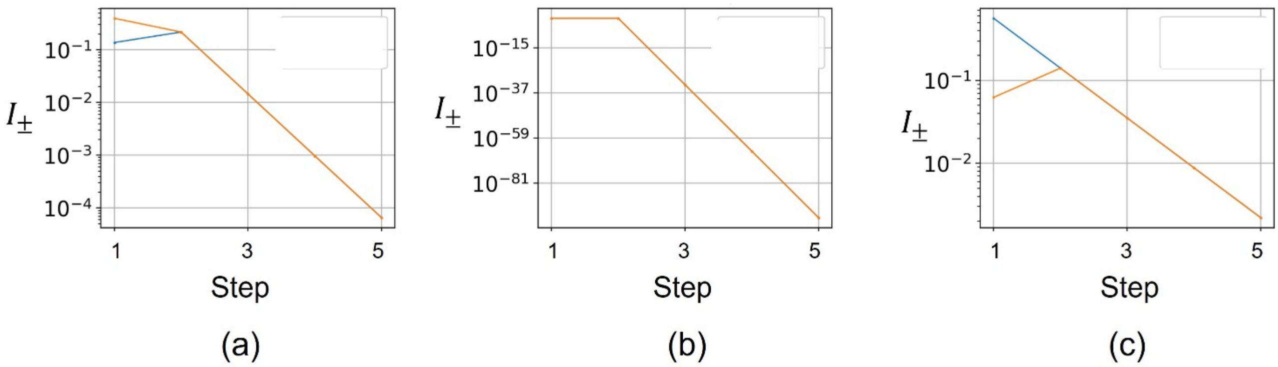

Fig. 4 Time-dependence of I_+ and I_- at steps 1-5 (p =0).

Red and blue curves are for I_+ and I_-, respectively.

(a) θ=37.5 (deg.) and χ / J=1.84, (b) θ=45 (deg.) and $\chi / J = \sqrt{2}$, (c) θ=60 (deg.) and χ / J=0.81.

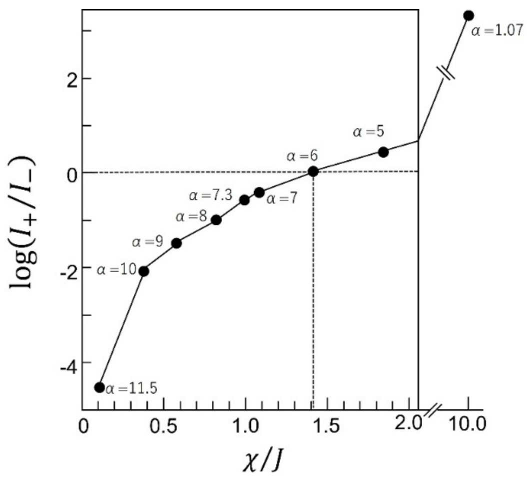

Fig. 5 Dependence of I_+/I_- on χ / J at step 1 of Fig. 4.

3.2 Analytical expressions

By eqs. (3) and (5), the state of the DPP at step 1 is analytically expressed as

$$\vec{\psi}_{1,(x,y)} = \begin{bmatrix} y_{DP+} \\ y_{DP-} \\ y_{Phonon} \end{bmatrix}_{1,(x,y)} = \begin{bmatrix} -\cos^2\theta \\ \sin^2\theta \\ 2^{-1/2}\sin 2\theta \end{bmatrix}. \tag{6}$$

Furthermore, at step n ($n \geq 2$), it is

$$\vec{\psi}_{n,(x,y)} = \begin{bmatrix} y_{DP+} \\ y_{DP-} \\ y_{Phonon} \end{bmatrix}_{n,(x,y)} = \begin{bmatrix} \frac{1}{2}\sin^2 2\theta \cos^{n-2} 2\theta \\ \frac{1}{2}\sin^2 2\theta \cos^{n-2} 2\theta \\ \frac{1}{\sqrt{2}}\sin 2\theta \cos^{n-1} 2\theta \end{bmatrix}. \tag{7}$$

Equation (7) indicates that $y_{DP+} = y_{DP-}$ ($I_+ = I_-$), which is the origin of overlapping of the red and blue curves at $n \geq 2$ in Figs. 2 and 4.

The values of $I_\pm$ decrease with increasing step number n and the analytical expression of the slope S of the curve is

$$\log S = \cos^2 2\theta . \quad (8)$$

Figures 6(a) and (b) shows the dependences of this value on θ and χ/J, respectively. They are consistent with Figs. 3(a) and (b).

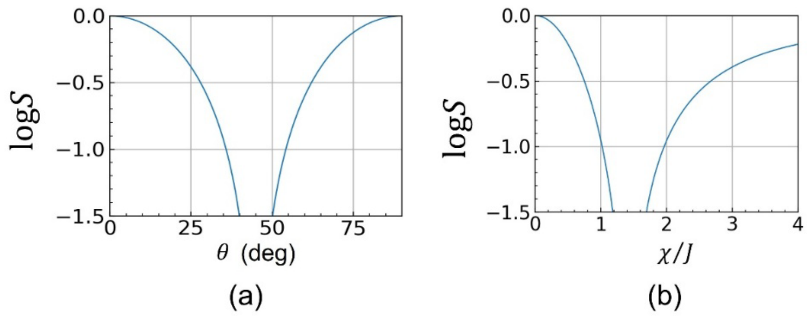

Fig. 6 Dependences of the analytically derived values on θ (a) and on χ/J (b).

An analytical expression of the ratio I_+/I_- at step 1 is derived from eq. (6) and is expressed as

$$I_+/I_- = \left|y_{DP+}/y_{DP-}\right|^2 = 1/\tan^4\theta = \left(\chi/J\right)^4/4. \qquad (9)$$

Its dependence on χ/J is shown by Fig. 7, which is consistent with Fig. 5.

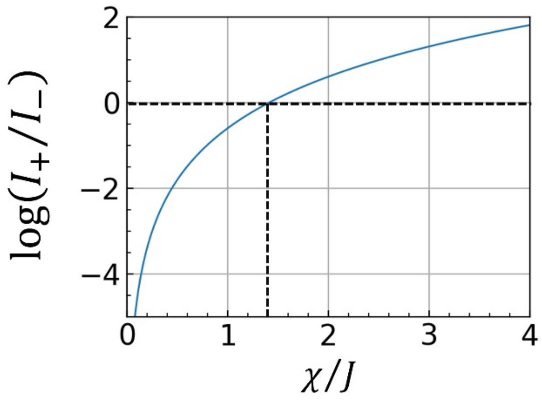

Fig. 7 Analytically derived dependence of I_+/I_- on χ/J at step 1 in Fig. 4 .

4 Discussions

This section discusses the dependences of the slope S and the ratio I_+/I_- on χ/J by referring to the results in Section 3.

[Slope S]

In the case of $\theta = 45\,(\text{deg.})$ ($\chi/J = \sqrt{2}$ by eq. (5)), eq. (6) indicates that $\vec{\psi}_{1,(x,y)} = \left[-1/2 \quad 1/2 \quad 1/\sqrt{2}\right]^T$ at step 1 ($n=1$). By eq. (7), $\vec{\psi}_{2,(x,y)} = \left[1/2 \quad 1/2 \quad 0\right]^T$ at step 2 ($n=2$). After step 3 ($n \geq 3$), $\vec{\psi}_{n,(x,y)} = \left[0 \quad 0 \quad 0\right]^T$ by eq. (7). These values indicate that the values of $I_\pm$ at steps 1 and 2 are both 1/4. However, $I_\pm$ =0 from step 3 ($n \geq 3$). Thus, the value of $I_\pm$ decreases rapidly between steps 2 and 3, as is schematically indicated by the broken line in Fig. 8. This decrease can be recognized by noting that the values of the vertical axis in Fig. 4(b) (10^{-15} – 10^{-81}) are much smaller than those of Figs. 4(a) (10^{-1} – 10^{-4})

and (c) (10^{-1} – 10^{-2}). This also corresponds to the extremely large value of $|\log S|$ in Figs. 3 and 6. The reason why $y_{Phonon} = 0$ after step 2 ($n \geq 2$) is because $\varepsilon_0 \left(= \cos 2\theta\right) = 0$ in eq. (3).

In the case of $\theta \neq 45$(deg.) ($\chi/J \neq \sqrt{2}$), Figs. 3(a) and 6(b) show that the dependence of S on χ/J is nearly symmetric with respect to $\chi/J = \sqrt{2}$.

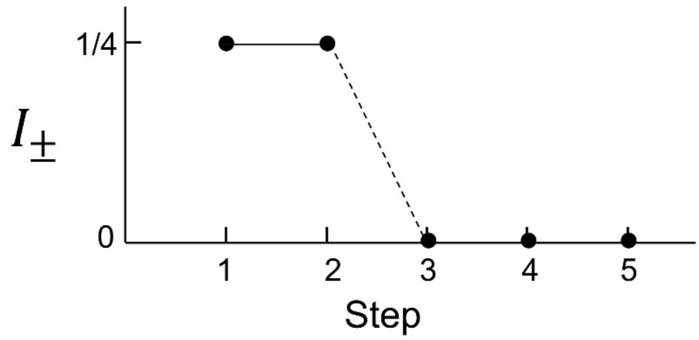

Fig. 8 Dependence of $I_\pm$ on step n.

[Ratio I_+/I_- at step 1]

Figures 5 and 7 show that the ratio I_+/I_- increases with χ/J, and reaches unity ($I_+/I_- = 1$) at $\chi/J = \sqrt{2}$. In the case of $\chi/J > \sqrt{2}$, it is larger than unity ($I_+/I_- > 1$), which corresponds to PB with respect to momentum.

It should be noted that the time constant of the temporal decrease of $I_\pm$ (the time constant τ_{QW} in ref. [1] and in (1) in Section 1) is inversely proportional to the slope S_{QW}. Therefore, increases of χ/J in Figs. 3(b) and 6(b) increase the time span during which the relation $I_+/I_- > 1$ is maintained. This means that the duration of PB increases, which is advantageous for reliable operation of nanometer-sized devices using the DPP transfer. Actually, the previous numerical calculation [3] for B atom-pairs in a Si crystal confirmed that the efficiency of the PB generation increased with increasing χ/J. The monotonic increase of I_+/I_- in Figs. 5 and 7 is consistent with the result of this confirmation.

5 Summary

This paper presented the results of numerical calculations of temporal variations of the intensities of light originating from the dressed-photon–phonon (DPP). A single nanometer-sized particle (NP) was assumed, and photon breeding (PB) with respect to momentum was discussed by analyzing the calculated dependences of the slope S and the ratio I_+/I_- of the emitted light intensities on the physical parameter χ/J. It was confirmed that I_+/I_- was larger than unity at $\chi/J > \sqrt{2}$, which corresponded to PB with respect to momentum.

Acknowledgements

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References

[1] M. Ohtsu, E. Segawa, K. Yuki and S. Saito, "Non-adiabatic relaxation process that lies behind the adiabatic relaxation dressed-photon–phonon transfer," *Off-shell Archive* (December 2025) Offshell: 2512O.001.v1. **DOI** 10.14939/2512O.001.v1, https://rodrep.or.jp/en/offshell/original_2512O.001.v1.html

[2] S. Yoshino, H. Shiratori, T. Yamagami, R. Horisaki, and E. Segawa, "Normal variance mixture with arcsine law of an interpolating walk between persistent random walk and quantum walk," *Entropy* 2025, **27**(7), 670; https://doi.org/10.3390/e27070670.

[3] M. Ohtsu, E. Segawa, K. Yuki, and S. Saito, "Spatial distribution of dressed-photon–phonon confined by an impurity atom-pair in a crystal," *Off-shell Archive* (January, 2023) Offshell: 2301O.001.v1. **DOI** 10.14939/2301O.001.v1 https://rodrep.or.jp/en/off-shell/original_2301O.001.v1.html

[4] M. Ohtsu, "A Quantum Walk Model for Describing the Energy Transfer of a Dressed Photon," *Off-shell Archive* (September, 2021) OffShell: 2109R.001.v1. **DOI** 10.14939/2109R.001.v1, http://offshell.rodrep.org/?p=345