Journal of Luminescence 129 (2009) 1718–1721

Contents lists available at ScienceDirect

Journal of Luminescence

journal homepage: www.elsevier.com/locate/jlumin

Photon localization and tunneling in a disordered nanostructure

Arata Sato [a,*], Yuji Tanaka [a], Fujio Minami [a], Kiyoshi Kobayashi [a,b,1]

[a] Department of Physics, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo 152-8551, Japan
[b] CREST, Japan Science and Technology, 4-3-11 Takeda, Kofu, Yamanashi 400-8511, Japan

ARTICLE INFO

Available online 7 April 2009

PACS:
63.22.−m
68.37.Uv
78.67.−n

Keywords:
Disordered nanostructure
Dressed photon
Near field
Photon localization
Phonon
Polariton

ABSTRACT

A simple but flexible 2D lattice model is proposed to discuss localization and tunneling of a dressed photon in disordered nanomaterial systems. It is shown that a 1D finite disordered system with site-dependent masses is obtained after the contraction from 2D to 1D. A dressed photon description for a photon-electronic polarization–phonon interacting system is used to examine the spatial distribution of a dressed photon associated with coherent phonons in such a system. The temporal and tunneling behaviors of a dressed photon between two closely separated nanosystems are also investigated numerically. The model proposed is applicable to an arbitrary shape of nanostructure, and photon localization and tunneling inherent in the shape of the nanostructure is expected to be applied to the local manipulation of quantum states of nanostructure in excitation transfer processes, including spin and phonon degrees of freedom.

1. Introduction

Optical near fields (ONFs) that are localized close to the surfaces of materials originating in light-matter interactions are free from the diffraction limits of light, and have been applied in a variety of nanoscale spectroscopy and photochemical reactions. These studies have revealed the unique properties and the importance of phonons at the nanoscale [1,2], which arise from the spatial localization of ONFs. In a near-field photodissociation process, for example, molecules are dissociated even if the energy of incident light is lower than the dissociation energy, which is impossible when a far field with the same energy and intensity is used, and suggests that phonons in an optically excited probe system might assist the dissociation process in a non-adiabatic way.

In order to clarify the phonon's role at the nanoscale and the relationship with ONFs, as well as to explore the possibility of them, we discuss the mechanism of spatial localization and tunneling of photons associated with phonons depending on the shape of nanostructure, with the help of a quantum-theoretical method. First, we model a nanostructure like an ONF probe tip as a 2D lattice system with a varying site-interval less than the coherence length of phonons. Reducing from the 2D to 1D disordered finite system, we show that photons localize at the edge of the system affected by the phonons' localization, in terms of a dressed photon description. Then, we evaluate the penetration length of ONFs, i.e., tunneling probability of dressed photons as a function of the distance between them, locating another nanosystem close to the ONF probe tip, e.g., a molecule, a quantum dot, or a bow tie-shaped 2D lattice system.

The paper is organized as follows. The model and formulation are outlined in the next section. Numerical results and discussion on localization behavior and temporal behavior of a dressed photon in two separated nanosystem are given in Section 3, followed by concluding remarks in Section 4.

2. Model and formulation

We are interested in a system where incident photons, electronic polarizations, and phonons are interacting one another in the nanoscale region. A simple 2D finite lattice system, as shown in Fig. 1, is considered for a nanostructure like an optical near-field probe tip. The electronic polarizations induced in the nanomaterial system are treated together with incident photons as a quasiparticle which is hereafter called a photon [1]. We first examine the vibrational (phonon) modes in the 2D nanomaterial system, and then behavior of the photon–phonon interacting finite system.

The model Hamiltonian $\hat{H}$ for the 2D nanomaterial system is expressed in terms of site $\mathbf{i} = (i_x, i_y)$ by

$$\hat{H} = \hat{H}_X + \sum_{i_x=0}^{N_x-1} \hat{H}_{y,i_x} + \sum_{i_x=0}^{N_x-1} \hat{H}_{xy,i_x}, \quad (1)$$

* Corresponding author. Tel.: +81 3 5734 2446; fax: +81 3 5734 2751.
E-mail address: sato@nfo-titech.jp (A. Sato).
[1] Current address: Department of Electrical and Electric Engineering, University of Yamanashi.

0022-2313/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.jlumin.2009.02.032

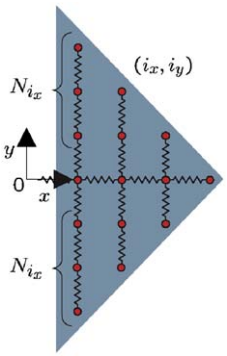

Fig. 1. A simple 2D finite lattice system considered for a nanostructure like an optical near-field probe tip. Each site is expressed by (i_x, i_y) in the coordinate system shown.

where $\hat{H}_x$ represents the coupled oscillators on the x-axis, while $\hat{H}_{y,i_x}$ and $\hat{H}_{xy,i_x}$ designate the coupled oscillators in the y direction at site i_x and the interaction to exchange momenta of the x and y directions at site $(i_x, 0)$, respectively. Here N_x means the number of sites in the x direction. Explicit expressions for $\hat{H}_{y,i_x}$ and $\hat{H}_{xy,i_x}$ are given by

$$\hat{H}_{y,i_x} = \sum_{i_y=-N_{i_x}}^{N_{i_x}} \frac{\hat{p}_{y,i_y}^2}{2m} + \frac{g}{2m} \sum_{i_y=-N_{i_x}}^{N_{i_x}-1} \hat{p}_{y,i_y}\hat{p}_{y,i_y+1} + \frac{k}{2} \sum_{i_y=-N_{i_x}}^{N_{i_x}} \hat{y}_{i_y}^2 \tag{2a}$$

$$= \hat{\mathbf{P}}_y \cdot M_{2N_{i_x}+1}^{-1} \cdot \hat{\mathbf{P}}_y + \frac{k}{2}\hat{\mathbf{Y}} \cdot \mathrm{I} \cdot \hat{\mathbf{Y}}, \tag{2b}$$

$$\hat{H}_{xy,i_x} = 2g_0\hat{p}_{x,0}\hat{p}_{y,0} = 2\hat{\mathbf{\Pi}}_x \cdot \hat{\mathbf{P}}_y, \tag{2c}$$

where $\hat{p}_{y,i_y}$ is the momentum at site i_y conjugate to the coordinate $\hat{y}_{i_y}$ while m, g, and k are mass, coupling constant for the momentum exchange, and spring constant of the oscillators, respectively. Eqs. (2b) and (2c) were expressed in the compact form, with the help of the following matrix representations as:

$$M_{2N_{i_x}+1}^{-1} = \frac{1}{4m} \underbrace{\begin{pmatrix} 2 & -g & 0 & \cdots & 0 \\ -g & 2 & -g & & 0 \\ 0 & -g & 2 & \ddots & 0 \\ \vdots & & \ddots & \ddots & -g \\ 0 & 0 & 0 & -g & 2 \end{pmatrix}}_{2N_{i_x}+1},$$

$$\hat{\mathbf{P}}_y = \begin{pmatrix} \hat{p}_{y,N_{i_x}} \\ \vdots \\ \hat{p}_{y,0} \\ \vdots \\ \hat{p}_{y,-N_{i_x}} \end{pmatrix}, \quad \hat{\mathbf{\Pi}}_x = \begin{pmatrix} 0 \\ \vdots \\ g_0 p_{x,0} \\ \vdots \\ 0 \end{pmatrix}, \tag{3}$$

and the unit matrix I.

To clarify the 2D effects, we reduce the system dimension from 2D to 1D by integrating the y directional degrees of freedom. Noticing that the $\hat{\mathbf{P}}_y$-dependent terms in Eqs. (2b) and (2c) can be written as

$$-\hat{\mathbf{\Pi}}_x \cdot M_{2N_{i_x}+1} \cdot \hat{\mathbf{\Pi}}_x = -g_0^2 (M_{2N_{i_x}+1})_{00} \hat{p}_{x,0}^2, \tag{4}$$

they can be renormalized as mass correction factors, resulting in the kinetic energy of a 1D Hamiltonian as

$$\hat{H}_{\mathrm{kin}} = \frac{\hat{p}_{x,0}^2}{2m} - g_0^2 (M_{2N_{i_x}+1})_{00} \hat{p}_{x,0}^2 \sim \frac{\hat{p}_{x,0}^2}{2m(1 + 2mg_0^2 (M_{2N_{i_x}+1})_{00})} \equiv \frac{\hat{p}_{x,0}^2}{2m_{i_x}}. \tag{5}$$

It follows from Eq. (5) that the 1D system has site-dependent masses, m_{i_x}, or it becomes a finite disordered system of coupled oscillators.

In addition, introducing the coherence length of phonons, L_c, we allow the couplings more than the nearest neighbor sites, and finally obtain the effective 1D Hamiltonian as

$$\hat{H}_{1D} = \sum_{i=0}^{N_x-1} \frac{\hat{p}_i^2}{2m_i} + \frac{k\,\mathrm{e}^{-a/L_c}}{2}\hat{x}_0^2 + \frac{k\,\mathrm{e}^{-a/L_c}}{2}\hat{x}_{N_x-1}^2 + \frac{k}{2} \sum_{i=0}^{N_x-2} \sum_{n=1}^{N_x-i-1} \mathrm{e}^{-na/L_c} (\hat{x}_{i+n} - \hat{x}_i)^2, \tag{6}$$

where $\hat{p}_i$ denotes the momentum conjugate to the coordinate $\hat{x}_i$, and a represents the distance between two nearest neighbor sites. According to Refs. [2,3], we have normal vibrational modes of the system, or phonons after the quantization of the field [4].

Following the procedure described in Ref. [2], we can obtain the Hamiltonian for a photon-electronic polarization–phonon interacting finite system as

$$\hat{H} = \sum_{i=0}^{N_x-1} \hbar(\omega - \omega_i)\hat{\alpha}_i^\dagger \hat{\alpha}_i + \sum_{i=0}^{N_x-2} \hbar J_i (\hat{\alpha}_i^\dagger \hat{\alpha}_{i+1} + \hat{\alpha}_{i+1}^\dagger \hat{\alpha}_i), \tag{7}$$

where $\hbar$ and ω are the Planck constant divided by 2π and the frequency of a photon, respectively. The operator $\hat{\alpha}_i$, transformed from a photon $\hat{a}_i$, represents a photon dressed by coherent phonons which is written by

$$\hat{\alpha}_i = \hat{a}_i \exp\left\{ \sum_{p=1}^{N_x} \frac{\chi_{ip}}{\Omega_p} (\hat{b}_p^\dagger - \hat{b}_p) \right\}, \tag{8}$$

and the Hermitian conjugate of $\hat{\alpha}_i$ is denoted by $\hat{\alpha}_i^\dagger$. Here χ_{ip} and Ω_p are the photon–phonon coupling constant depending on site i and phonon mode p and the frequency of the phonon specified by mode number p, respectively. The creation (annihilation) operator of a phonon in mode p is denoted by $\hat{b}_p^\dagger$ ($\hat{b}_p$). The site-dependent frequency of a dressed photon originating from the photon–phonon coupling is denoted by ω_i, while the site-dependent hopping constant of a dressed photon due to the photon–phonon coupling is expressed by J_i [2].

Since the Hamiltonian in Eq. (7a) is diagonalized by using an orthogonal matrix, temporal evolution of the number operator of a dressed photon, $\hat{N}_i(t)$, and the probability finding a dressed photon at site i after a dressed photon is initially incident at site j can be easily obtained.

3. Numerical results

Based on the formulation developed in Section 2, we present typical numerical results to discuss the spatial distribution, the temporal and tunneling behavior of a dressed photon in 1D finite nanosystems.

Fig. 2 shows the mass correction $(M_{2N_{i_x}+1})_{00}$ as a function of site number in the y direction. As the number of oscillators in the y direction increases, the absolute value of the mass correction also increases, which is true regardless of the coupling constant g.