Hybridization theory between localized mode and free propagating modes for light scattering from a dielectric sphere

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Light scattering from a homogeneous dielectric sphere is discussed in terms of hybridization between a localized mode excited inside the dielectric sphere and free propagating modes in vacuum. This theory is a photonic counterpart of the Anderson model in electron systems, yielding a rigorous theoretical foundation of the heavy photon concept, which was numerically proposed for almost flat photonic bands. The magnitude of the hybridization is analytically expressed. The localized mode is identified with the photon virtual bound state. In order to confirm the validity of the present theory, a comparison is made between the present theory and conventional numerical calculation for results of the photonic density of states.

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I. INTRODUCTION

The study of light scattering from a particle or an ensemble of particles has a long history over a century [1]. In particular, the scattering from a homogeneous dielectric sphere is one of the central issues. The exact solution for the scattering amplitude was obtained by Mie [2], which was represented in the form of an infinite series. Since the convergence of the series is not fast, extensive efforts to approximate Mie's result both for analytic and for numerical calculations are made to obtain formulas suitable for practical uses, depending on the specific regions of the plane of refractive index and size parameter [1,3–5]. The outcome leads to a basis for device development, such as a high-Q value microsphere resonator [6].

The study of light scattering from a homogeneous dielectric sphere is directed not only to practical purposes but also to fundamental issues even nowadays [7]. The fact that the extensive studies of fundamental issues have been kept shows that it is an inexhaustible spring. One example is the complex angular momentum method [8]. In the present paper, the subject is illuminated from another fundamental point of view, which is based on the heavy photon concept in photonic crystals (PCs) [9].

The heavy photon is an important concept to understand certain photonic bands. In a PC—defined as a system with periodic structure of dielectrics or metals [10–12]—the photon dispersion relation is modified to construct photonic bands. The photonic bands result from the interplay between the scattering from the individual scatterer and the scattering whose origin is the periodicity. The heavy photon is associated with the former aspect. Although details of the photonic band structures depend on both a lattice structure and refractive index, one can find typical features: the photonic bands that appear in a rather lower energy region are almost linear, which can be understood from the empty lattice picture. They are affected by the periodicity of the structure. On the other hand, in the higher energy region where diffraction channels open, there are almost flat photonic bands. The heavy photon concept was proposed for the almost flat photonic bands of PCs made up of dielectric spheres [9].[1] In Ref. [9], it was numerically revealed that certain flat photonic bands were characterized by a single eigenelectromagnetic mode of a single dielectric sphere. It was also reported that the width of such a photonic band agreed with the width of the photonic density of states (PDOS) in light scattering from a single dielectric sphere. Note that the PDOS characterizes the increase of the photon density of states owing to the introduction of the dielectric sphere into vacuum space. From these two findings, they proposed that such a flat photonic band formation results from repetition of the following single event: once a freely propagating mode enters a dielectric sphere by tunneling, it stays for a moment (localized mode, in a sense). It then escapes from the sphere and again freely propagates.

This scenario immediately reminds us of the heavy fermion, which is one of the important problems in electron systems [13]. In a typical case of a heavy fermion, a localized d state in a magnetic impurity atom hybridizes with the free s electrons in a host metal and obtains an itinerary to construct an almost flat electronic band. The flatness is the origin of the "heavy" quality. The hybridization is related to the finite lifetime of the localized state, which determines the Lorentzian width of the density of states. The essential point is that a localized mode is embedded in free continuous modes on the energy axis, which is described by the Fano model [14]. Analogously, the heavy photon concept is based on the view that a certain localized mode excited in a dielectric sphere is embedded in freely propagating modes and hybridizes with the free modes. The heavy photon concept is thus a vectorial extension of the heavy fermion and a quite interesting problem.

The modes on these flat photonic bands are expected to have several distinguished properties owing to the peculiar mechanism of band formation. Indeed, interesting properties of electromagnetic forces were reported for the photonic

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[1]The concept does not mean that the photon obtains mass.

bands characterized by the heavy photon, which is expected to play an essential role for fabrication of PCs [15]. Furthermore, the flatness of the photonic bands means considerable reduction of the light group velocity. It leads to the effective enhancement of the light-matter interaction. This enhancement is expected to be important for device development.

In spite of the importance of the heavy photon concept for both fundamental and application research, it is just an intuitive proposition based on numerical results with lack of a rigorous foundation. The purpose of this paper is to give a rigorous foundation to the heavy photon concept. Since the heavy photon concept is associated with the individual constituent scatterers of the PC, as stated previously, it is essential to discuss the single sphere problem. In order to establish the heavy photon concept, the following points should be discussed. The hybridization between a localized mode excited inside a dielectric sphere and freely propagating modes should be verified and the localized mode identified. The magnitude of the hybridization should be clarified. For demonstration of the validity of the present theory, the PDOS obtained from this theory should be compared with numerical results. All of these points are addressed in this study.

The organization of this paper is as follows. In Sec. II, the hybridization between a localized mode and free propagation modes is shown to be well defined by formulating the problem of light scattering from a homogeneous dielectric sphere into the Fano model. The analytic expressions of the magnitude of the hybridization are obtained. Section III gives a comparison of the PDOS given by the present theory with numerical results in order to verify the present theory, where special attention is paid to the width of the PDOS. The localized mode is identified. Finally, conclusions and future problems are given in Sec. IV. Derivations of several important equations and supporting materials are shown in the Appendixes.

II. THEORY

A. Summary of conventional method for electromagnetic wave in space including a dielectric sphere

For later use, the results are summarized for the propagation of electromagnetic waves in the geometry that a dielectric sphere with constant refractive index n and radius a is located at the center of a vacuum sphere with radius $R \gg a$.[2] The condition that electromagnetic wave should vanish at the vacuum sphere boundary $r=R$ is imposed. The equation that the transverse electric field obeys is

$$\nabla^2 \mathbf{E} + k^2 \mathbf{E} + U(r)\mathbf{E} = \mathbf{0}, \tag{1}$$

where k is the wave number of the electric field in vacuum. $U(r)$ denotes the "effective potential" caused by the dielectric sphere as $U=k^2(n^2-1)\theta(a-r)$, where $\theta(r)$ is the step function. The two independent solutions are the vector spherical waves, the **M** wave (TE mode) and **N** wave (TM mode), both of which are characterized by $R_{l,k}(r)$ satisfying [16]

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 + U(r)\right] R_{l,k}(r) = 0. \tag{2}$$

Two independent fundamental solutions for $R_{l,k}(r)$ are known to be the Riccati-Bessel functions $\psi_l(x) \equiv x j_l(x)$ and $\chi_l(x) \equiv -x n_l(x)$, where $j_l(x)$ and $n_l(x)$ are the lth order spherical Bessel and spherical Neumann functions, respectively [1].

Let us introduce the radial functions

$$R^{\lambda}_{l,k}(x) = \begin{cases} p^{\lambda}_{l,k}(r) & (r < a), \\ q^{\lambda}_{l,k}(r) & (r > a), \end{cases} \tag{3}$$

where λ indicates the TE (**M** wave) or TM (**N** wave) mode. From analyticity at the origin, the general solutions are written as

$$p^{\lambda}_{l,k}(r) = B^{\lambda}_{in} \psi_l(nkr), \tag{4}$$

$$q^{\lambda}_{l,k}(r) = B^{\lambda}_{out}[\beta^{\lambda}_l \psi_l(kr) + \chi_l(kr)], \tag{5}$$

respectively. The prefactors $B^{\lambda}_{in(out)}$ are not essential in the following discussion. The coefficient β^{λ}_l is determined by the boundary condition at $r=a$ as

$$\beta^{\lambda}_l = -\frac{\chi'_l(ka) - n^{\mu} D_l(nka)\chi_l(ka)}{\psi'_l(ka) - n^{\mu} D_l(nka)\psi_l(ka)}, \tag{6}$$

where $\mu = +1(-1)$ for $\lambda = \mathrm{TE}$ (TM), respectively, and $D_l(nka) \equiv \psi'_l(nka)/\psi_l(nka)$. It should be noted that β^{λ}_l is represented by the phase shift of a partial wave with angular momentum l as $\beta^{\lambda}_l = \cot \delta^{\lambda}_l$ [17]. The boundary condition that $q^{\lambda}_{l,k}(R) = 0$ gives $\beta^{\lambda}_l = -\chi_l(kR)/\psi_l(kR)$. Then the allowed k's in this geometry are determined. Remember that these results do not depend on the confinement nature of the electromagnetic wave inside the dielectric sphere.

B. Hybridization between a localized mode and free modes

This subsection, which is the main part of the present work, presents a hybridization theory between a localized mode inside the dielectric sphere and free propagating modes in vacuum space. For the purpose, the task is to rewrite the results summarized in the previous subsection into the equivalent form to the one derived from the Fano model [14]. After the foundation, the PDOS is analytically obtained. As for the localized state, the Mie resonant states are taken as the candidates, since wave functions for the Mie resonant states are known to be quite localized inside the dielectric sphere [18]. It should be refined later if it is necessary.

1. Wave function

In the first place, free modes in the vacuum sphere *without* the dielectric sphere are analyzed. Consider a function $\phi_{l,k}(r)$ that satisfies

[2] Since the procedure of this study is to express in terms of a phase shift how much free modes are affected by a localized mode, it is convenient to discretize the free modes.

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right]\phi_{l,k}(r) = 0, \tag{7}$$

under the boundary condition that $\phi_{l,k}(r=R)=0$ and the normalization condition that

$$\int_0^R \phi_{l,k}^2(r)dr = 1. \tag{8}$$

The boundary condition discretizes allowed k's as $k_s=(s+l/2)\pi/R$ with integer s, where the asymptotic form of the Riccati-Bessel function is used. The radial function characterizing free modes is then obtained as

$$\phi_{l,s}(r) = \sqrt{\frac{2}{R}}\psi_l(k_s r). \tag{9}$$

The main task for the present purpose is to expand $q_{l,k}^{\lambda}(r)$ in terms of $\phi_{l,s}(r)$'s. This is mathematically equivalent to the Fourier-Bessel expansion of $q_{l,k}^{\lambda}(r)$. Instead of directly performing the Fourier-Bessel expansion, we extend a convenient method proposed by Kondo [19] for the Anderson model in electron systems [13,20]. For the expansion, the following identity is used:

$$[q_{l,k}^{\lambda}(a)]' F_{l,k}(a,r) - q_{l,k}^{\lambda}(a)\frac{\partial}{\partial a}F_{l,k}(a,r) = \begin{cases} q_{l,k}^{\lambda}(r) & (r>a), \\ 0 & (r<a), \end{cases} \tag{10}$$

where $F_{l,k}(r,r')$ is defined as

$$F_{l,k}(r,r') \equiv \sum_s \frac{\phi_{l,s}(r')\phi_{l,s}(r)}{k^2 - k_s^2}. \tag{11}$$

The proof of this identity is given in Appendix A. Insertion of the definition of $F_{l,k}(r,r')$ yields for $r>a$

$$q_{l,k}^{\lambda}(r) = \sum_s \frac{[q_{l,k}^{\lambda}(a)]'\phi_{l,s}(a) - q_{l,k}^{\lambda}(a)\phi_{l,s}'(a)}{k^2 - k_s^2}\phi_{l,s}(r). \tag{12}$$

Remember that the right hand side of this equation identically vanishes for $r<a$, as is desired. Making use of the boundary conditions at $r=a$ that $q_{l,k}^{\mathrm{TE}}(a)=(1/n)p_{l,k}^{\mathrm{TE}}(a)$ and $[q_{l,k}^{\mathrm{TE}}(a)]'=(1/n)[p_{l,k}^{\mathrm{TE}}(a)]'$ for the TE mode, and $q_{l,k}^{\mathrm{TM}}(a)=p_{l,k}^{\mathrm{TM}}(a)$ and $[q_{l,k}^{\mathrm{TM}}(a)]'=(1/n^2)[p_{l,k}^{\mathrm{TM}}(a)]'$ for the TM mode, we replace $q_{l,k}^{\lambda}(a)$ and $[q_{l,k}^{\lambda}(a)]'$ in Eq. (12) with $p_{l,k}^{\lambda}(a)$ and $[p_{l,k}^{\lambda}(a)]'$, respectively.

Here let us consider such $p_{l,k}^{\lambda}(r)$'s that satisfy the condition that

$$\frac{\int_0^a |p_{l,k}^{\lambda}(r)|^2 dr}{\int_0^R |p_{l,k}^{\lambda}(r)|^2 dr} \cong 1. \tag{13}$$

In this case, one can safely add $p_{l,k}^{\lambda}(r)$ to $q_{l,k}^{\lambda}(r)$ obtained above to construct $R_{l,k}^{\lambda}(r)$ for $0<r<R$, since $p_{l,k}^{\lambda}(r)$ has negligible amplitude outside the dielectric sphere. Following the standard procedure [16], the spherical vector waves associated with the $R_{l,k}^{\lambda}(r)$'s are obtained as

$$\mathbf{M}[R_{l,k}^{\mathrm{TM}}(r)] = \mathbf{M}[p_{l,k}^{\mathrm{TE}}(r)] + \frac{1}{n} \times \sum_s \frac{[p_{l,k}^{\mathrm{TE}}(a)]'\phi_{l,s}(a) - p_{l,k}^{\mathrm{TE}}(a)\phi_{l,s}'(a)}{k^2 - k_s^2}\mathbf{M}[\phi_{l,s}(r)] \tag{14}$$

and

$$\mathbf{N}[R_{l,k}^{\mathrm{TM}}(r)] = \mathbf{N}[p_{l,k}^{\mathrm{TM}}(r)] + \sum_s \frac{n^{-2}[p_{l,k}^{\mathrm{TM}}(a)]'\phi_{l,s}(a) - p_{l,k}^{\mathrm{TM}}(a)\phi_{l,s}'(a)}{k^2 - k_s^2} \times \mathbf{N}[\phi_{l,s}(r)], \tag{15}$$

respectively.

The addition of $p_{l,k}^{\lambda}(r)$ to $q_{l,k}^{\lambda}(r)$ is expected to be valid for such $k=\{k_i^{\lambda}(k_1^{\lambda}<k_2^{\lambda}<\cdots)\}$ that satisfies the resonant condition $\beta_l^{\lambda}(k_i^{\lambda})=0$, or the Mie resonance condition $\delta_l^{\lambda}=\pi/2 \pmod{\pi}$ [1]. This is because the most part of the amplitude of the Mie resonant state is known to be within the region $r<a$ [18]. In the following discussion, $p_{l,k}^{\lambda}(r)$ is assumed to be the Mie resonant state.

2. Secular equation

The wave functions are represented in the form of hybridization between the localized mode characterized by $p_{l,k}^{\lambda}(r)$ and freely propagating modes characterized by $\phi_{l,s}(r)$'s in the previous subsection. It is, however, not sufficient for construction of the hybridization theory. Equivalence to the Fano model should be shown. For the purpose, we derive an equation equivalent to Eq. (6) by using $\phi_{l,s}(r)$ instead of both $\psi_l(kr)$ and $\chi_l(kr)$, which should have the equivalent form to the one derived from the Fano model. The equation obtained should determine the "eigenvalues" k's.

After some algebra, details of which are given in Appendix B, Eq. (6) is rewritten as

$$\sum_s \frac{[n^{\mu}kD_l(nka)\phi_{l,s}(a) - \phi_{l,s}'(a)]^2}{k^2 - k_s^2} = 0. \tag{16}$$

Let us expand $L_l^{\lambda}(k) \equiv n^{\mu}kD_l(nka)$ around $k=k_i^{\lambda}$ with application of the Wronski theorem, shown in Appendix C. Here k_i^{λ} satisfies the resonant condition $\beta_l^{\lambda}(k_i^{\lambda})=0$, resulting in the fact that the condition Eq. (C8) is well satisfied. From Eq. (C10), one has

$$L_l^{\lambda}(k) = L_l^{\lambda}(k_i^{\lambda}) - n^{1+\mu}\frac{k^2 - (k_i^{\lambda})^2}{\psi_l^2(nk_i^{\lambda}a)}. \tag{17}$$

In the following, $\Delta L_l^{\lambda} \equiv -n^{1+\mu}[k^2-(k_i^{\lambda})^2]/\psi_l^2(nk_i^{\lambda}a)$ is defined. Substituting Eq. (17) for Eq. (B21) and omitting higher order terms than $O((\Delta L)^2)$, then

$$[L_l^{\lambda}(k_i^{\lambda})]^2 F_{l,k}^A(a) - 2L_l^{\lambda}(k_i^{\lambda})F_{l,k}^B(a) + F_{l,k}^C(a) = -\Delta L_l^{\lambda}, \tag{18}$$

where Eqs. (B13) and (B16) are used. Using explicit forms of $F_{l,k}^A, F_{l,k}^B, F_{l,k}^C$, and $L_l^{\lambda}(k_i^{\lambda})$, Eq. (16) is rewritten as

$$E - E_i^\lambda = \sum_s \frac{[v_{l,s,i}^\lambda]^2}{E - E_s}, \tag{19}$$

where

$$v_{l,s,i}^\lambda = k_i^\lambda n^{(\mu-1)/2} \psi'_l(nk_i^\lambda a)\phi_{l,s}(a) - n^{-(\mu+1)/2}\psi_l(nk_i^\lambda a)\phi'_{l,s}(a), \tag{20}$$

$E=k^2$, $E_i^\lambda=(k_i^\lambda)^2$, and $E_s=k_s^2$. Remember that the form of $\sim 1/(k^2-k_s^2)$ is associated with the photon Green's function [21].[3]

Equations (14), (15), and (19) show that the formulation presented in this paper is equivalent to the Fano model [14], where a localized mode labeled with i is embedded in continuous free modes (labeled with s), and that the two modes are hybridized whose magnitude is denoted by $v_{l,s,i}^\lambda$. This equivalence is understood when one remembers the following simple fact. Consider the Fano model Hamiltonian $\mathcal{H}_\mathrm{F}$:

$$\mathcal{H}_\mathrm{F} = \sum_s \epsilon_s |s\rangle\langle s| + \epsilon_i |i\rangle\langle i| + \sum_s \left[V_s |s\rangle\langle i| + \mathrm{H.c.}\right]. \tag{21}$$

Here $|s\rangle$ and $|i\rangle$ denote continuous modes and a localized mode, respectively, and ϵ_s, ϵ_i, and V_s are the eigenenergy of $|s\rangle$, eigenenergy of $|i\rangle$, and magnitude of the hybridization of both modes, respectively. V_s is assumed to be real. In order to solve the eigenvalue problem $\mathcal{H}_\mathrm{F}|\Psi\rangle=\epsilon|\Psi\rangle$, consider an eigenfunction in the form of $|\Psi\rangle=|i\rangle+\Sigma_s c_s|s\rangle$. The coefficient is then determined as $c_s=V_s/(\epsilon-\epsilon_s)$, and the secular equation to determine ϵ is obtained as

$$\epsilon - \epsilon_i = \sum_s \frac{[V_s]^2}{\epsilon - \epsilon_s}. \tag{22}$$

One can easily see that this eigenvalue equation has the same form as Eq. (19). It is then concluded that Eq. (20) correctly represents the magnitude of hybridization between the ith localized mode inside the dielectric sphere and the freely propagating modes.

3. Photonic density of states

The PDOS is discussed in order to demonstrate the validity of the present formulation. The PDOS characterizes the increase of the number of the states owing to introduction of the dielectric sphere into vacuum. In order to obtain the PDOS from the present hybridization theory, one needs to perform the summation in Eq. (19). It is generally impossible to analytically perform the summation with respect to s because of the s dependence of the numerator $v_{l,s,i}^\lambda$. For analytic calculation, consider the states $\{k_s\}$ in the vicinity of such $k_{s_0}^\lambda$ that $k_{s_0}^\lambda \approx k_i^\lambda$, then it is shown that $v_{l,s,i}^\lambda$ does not depend on s, which is denoted by $V_{l,i}^\lambda$ in the following. The secular equation is then simplified as

$$E - E_i^\lambda = [V_{l,i}^\lambda]^2 \sum_s{}' \frac{1}{E - E_s}. \tag{23}$$

The prime shows that the summation with respect to s is restricted in the vicinity of $k_{s_0}^\lambda$. The explicit form of the hybridization $V_{l,i}^\lambda$ for each mode is now expressed as

$$V_{l,i}^\mathrm{TE} = k_i^\mathrm{TE}\psi'_l(nk_i^\mathrm{TE}a)\phi_{l,i}(a) - \frac{1}{n}\psi_l(nk_i^\mathrm{TE}a)\phi'_{l,i}(a), \tag{24}$$

$$V_{l,i}^\mathrm{TM} = k_i^\mathrm{TM}\frac{1}{n}\psi'_l(nk_i^\mathrm{TM}a)\phi_{l,i}(a) - \psi_l(nk_i^\mathrm{TM}a)\phi'_{l,i}(a), \tag{25}$$

respectively, where $\phi_{l,i}(a)$ is obtained by replacement of k_s in $\phi_{l,s}(a)$ with k_i^λ. The discretized states E_s's are represented as $E_s=s\Delta E$ with integer s and level separation $\Delta E=\pi k/R$. The "energy" E to be determined is the one that is energetically shifted from E_{s_0} as a result of being influenced by the embedded localized mode. The shift is related to a phase shift. One thus sets E in the denominator of Eq. (23) as $E=\Delta E(s_0-\delta_l^\lambda/\pi)$:

$$E - E_i^\lambda = [V_{l,i}^\lambda]^2 \sum_s{}' \frac{1}{\Delta E(s_0 - \delta_l^\lambda/\pi) - s\Delta E}. \tag{26}$$

Here one can allow removing the restriction of the summation because the contribution from s states far away from s_0 is negligible. This approximation enables one to analytically perform the summation to yield

$$E - E_i^\lambda = -\frac{\pi[V_{l,i}^\lambda]^2 \cot\delta_l^\lambda}{\Delta E}. \tag{27}$$

The derivative of δ_l^λ with respect to E is known to give the PDOS as a function of E, which is

$$\frac{d\delta_l^\lambda}{dE} = \frac{\Delta_{l,i}^\lambda}{(E - E_i^\lambda)^2 + [\Delta_{l,i}^\lambda]^2}. \tag{28}$$

The $\Delta_{l,i}^\lambda \equiv \pi[V_{l,i}^\lambda]^2/\Delta E$'s are represented as

$$\Delta_{l,i}^\mathrm{TE} = 2k_i^\mathrm{TE}\left[\psi'_l(nk_i^\mathrm{TE}a)\psi_l(k_i^\mathrm{TE}a) - \frac{1}{n}\psi_l(nk_i^\mathrm{TE}a)\psi'_l(k_i^\mathrm{TE}a)\right]^2, \tag{29}$$

$$\Delta_{l,i}^\mathrm{TM} = 2k_i^\mathrm{TM}\left[\frac{1}{n}\psi'_l(nk_i^\mathrm{TM}a)\psi_l(k_i^\mathrm{TM}a) - \psi_l(nk_i^\mathrm{TM}a)\psi'_l(k_i^\mathrm{TM}a)\right]^2, \tag{30}$$

respectively. When using the explicit form of the resonant conditions

$$\psi'_l(nk_i^\mathrm{TE}a)\chi_l(k_i^\mathrm{TE}a) - \frac{1}{n}\psi_l(nk_i^\mathrm{TE}a)\chi'_l(k_i^\mathrm{TE}a) = 0 \tag{31}$$

for the TE mode and

[3]Use of k^2 in this work is reasonable for the present purpose, in contrast to use of the dimensionless size parameter $x=ka$ which is generally used for the Mie scattering problem. The reason is as follows. The procedure for our purpose is to express how much free modes are affected by the induced localized mode, where the localized mode plays a role of an impurity scatterer for free modes. It is then appropriate to express the influence for free modes from the localized mode by the Green's function, as in the case of the Born series. For time delay and dwell time problems, the use of k^2 is discussed in [22].

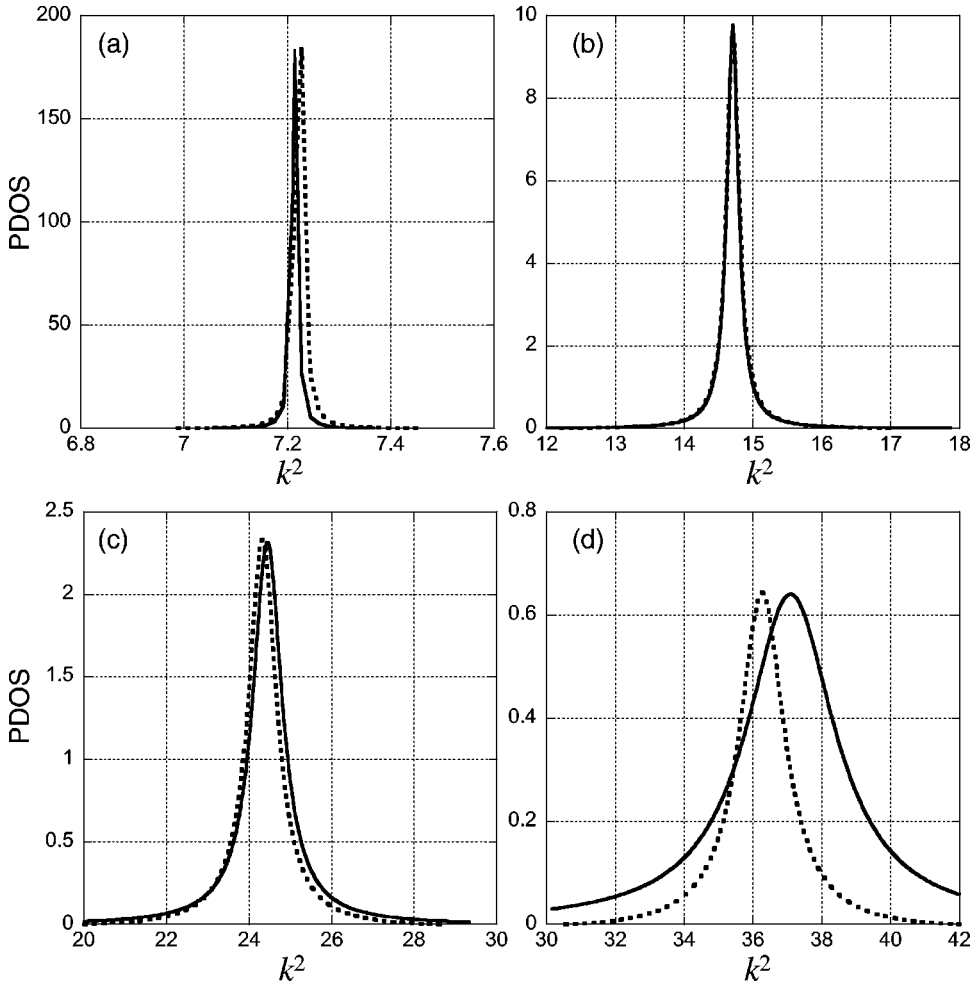

FIG. 1. PDOS with $(\lambda, l, i) = (\mathrm{TE}, 5, i)$, where $i=1$ (a), 2 (b), 3 (c), and 4 (d). The refractive index is set as $n=3.0$, and the radius of the dielectric sphere is taken as the unit length. The solid lines represent analytic results of the PDOS, the Lorentzian given by Eq. (28), and the dotted lines represent the numerically obtained PDOS, $d\delta^{\mathrm{TE}}_{l=5,\mathrm{num}}/dE$. It is clear that the first three peaks show good agreement. On the contrary, the fourth peak shows less agreement, although all these four peaks originate from Mie resonance. The unit of the horizontal (vertical) axis is $[\mathrm{length}]^{-2(+2)}$, e.g., $[\mathrm{mm}]^{-2(+2)}$ when $a=1$ mm.

$$\frac{1}{n}\psi'_l(nk_i^{\mathrm{TM}}a)\chi_l(k_i^{\mathrm{TM}}a) - \psi_l(nk_i^{\mathrm{TM}}a)\chi'_l(k_i^{\mathrm{TM}}a) = 0 \quad (32)$$

for the TM mode, those results are simplified as

$$\Delta^{\mathrm{TE}}_{l,i} = 2k_i^{\mathrm{TE}}\left[\frac{\psi_l(nk_i^{\mathrm{TE}}a)}{n\chi_l(k_i^{\mathrm{TE}}a)}\right]^2 \quad (33)$$

and

$$\Delta^{\mathrm{TM}}_{l,i} = 2k_i^{\mathrm{TM}}\left[\frac{\psi_l(nk_i^{\mathrm{TM}}a)}{\chi_l(k_i^{\mathrm{TM}}a)}\right]^2, \quad (34)$$

respectively. These are the formulas for the width of the PDOS. Note that there is no R dependence of the width. The fact that Eq. (28) is given by Lorentzian shows that the lifetime of the localized mode becomes finite as a result of hybridization with free modes [22].

III. DISCUSSION

A. Comparison of PDOS between analytic and numerical results

A comparison is made between the analytic result Eq. (28) and numerical results for the PDOS in order to check the validity of the present theory. In the following, the refractive index is set as $n=3.0$, and a is taken as the unit length. The numerical results of the PDOS are obtained from the derivative of the numerically obtained phase shift $\delta^{\lambda}_{l,\mathrm{num}}$ with respect to $E=k^2$. The phase shift $\delta^{\lambda}_{l,\mathrm{num}}$ of the partial wave of the λ mode with l is calculated by Eq. (6). The derivative of the phase shift gives peaks, each of which is numbered from $i=1$ in the manner that $k^{\lambda}_{i=1} < k^{\lambda}_{i=2} < \cdots$. Each peak of the PDOS is thus labeled by a set of (λ, l, i). The peaks are referred to as numerically obtained PDOS in the following.

Figures 1 and 2 are results of the comparison. Figures 1(a)–1(d) show the first four peaks of the PDOS from $i=1$ through $i=4$ for the TE mode with $l=5$. The solid line represents the Lorentzian obtained by the present theory, Eq. (28), and the dotted line represents the numerically obtained PDOS, $d\delta^{\lambda=\mathrm{TE}}_{l=5,\mathrm{num}}/dE$. One can see that the first three plots show good agreement between the present analytical and the numerical results. In contrast, the fourth one has a large deviation in spite of the fact that the peak in Fig. 1(d) also originates from the Mie resonance as well as the other peaks showing good agreement. The comparison for TM modes is shown in Figs. 2(a)–2(c), where the first three peaks of the PDOS from $i=1$ through $i=3$ for the mode with $l=5$ are presented. The first two peaks show good agreement with numerical results, $d\delta^{\lambda=\mathrm{TM}}_{l=5,\mathrm{num}}/dE$. The third one, however, shows disagreement, whose situation is similar to the case of the TE mode.

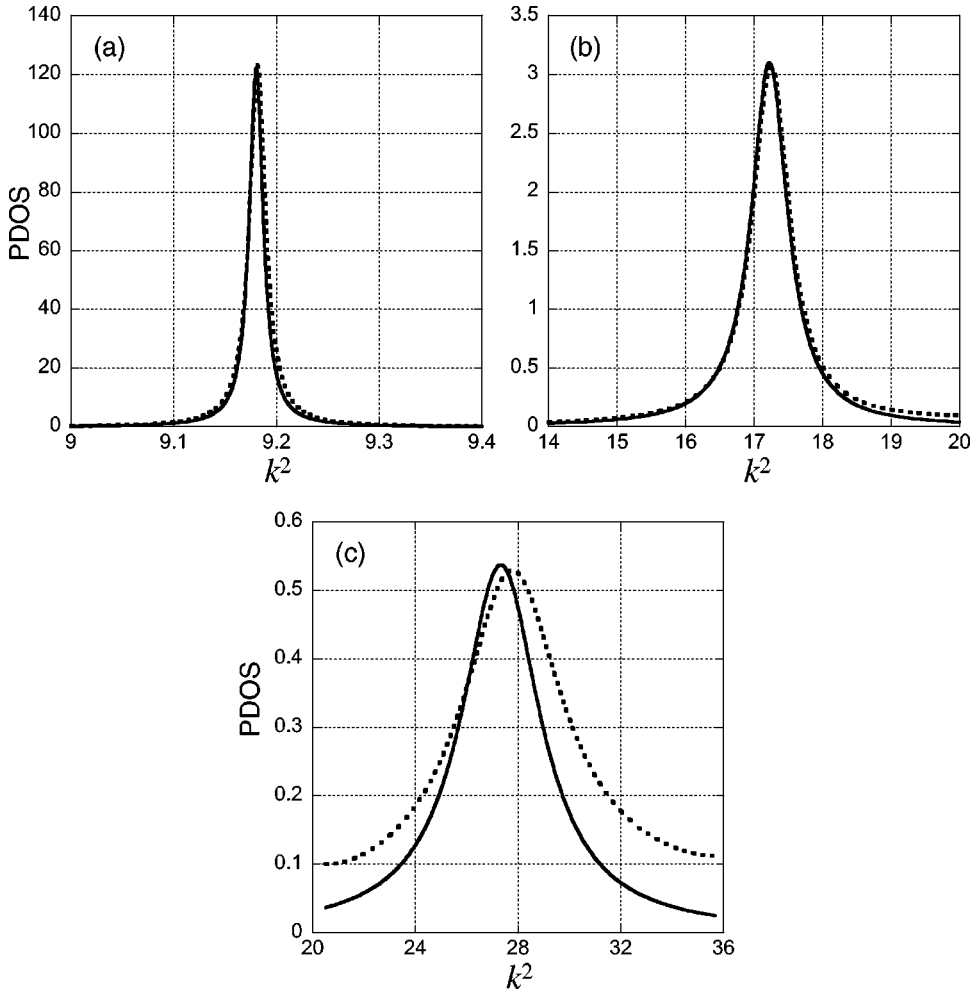

FIG. 2. PDOS with $(\lambda, l, i) = (\mathrm{TM}, 5, i)$, where $i=1$ (a), 2 (b), and 3 (c). Parameters are the same as the ones in Fig. 1. The solid lines represent analytic results of the PDOS, the Lorentzian given by Eq. (28), and the dotted lines represent the numerically obtained PDOS, $d\delta^{\mathrm{TM}}_{l=5,\mathrm{num}}/dE$. It is clear that the first two peaks show good agreement. On the contrary, the third peak shows less agreement, although all these three peaks originate from Mie resonance. For the unit of the axes, see the caption of Fig. 1.

For other l's, the similar behavior that the first few peaks show good agreement is observed for both TE and TM modes. Let us focus on the full width of the half maximum of the peaks (referred to as width, in the following) and discuss it quantitatively. The width of $d\delta^{\lambda}_{l,\mathrm{num}}/dE$ (the dotted lines in Figs. 1 and 2) is denoted as $D^{\lambda}_{l,i}$. $D^{\lambda}_{l,i}$ is evaluated by the Lorentzian fitting by using the least squares method. In order to measure the deviation between the Lorentzian width of the present theory $\Delta^{\lambda}_{l,i}$ and $D^{\lambda}_{l,i}$, the variance of the width is introduced, defined as

$$\sigma^{\lambda}_{l,i} \equiv \frac{D^{\lambda}_{l,i} - \Delta^{\lambda}_{l,i}}{D^{\lambda}_{l,i}}. \tag{35}$$

Figures 3 and 4 show the $\sigma^{\lambda}_{l,i}$'s against the peak numbers i with $l=1$, 3, 5, and 7 for TE and TM modes, respectively. Solid crosses are used for the peaks showing good agreement, and the dotted crosses are for ones with less agreement. Note that Figs. 3(c) and 4(c) correspond to Figs. 1 and 2, respectively. It is easy to see that the present theory shows good agreement with numerical results for the first several peaks, but not all. Remember that all peaks, whether showing good or less good agreement, satisfy the Mie resonant condition $\beta^{\lambda}_{l}(k^{\lambda}_{i}) = \cot \delta^{\lambda}_{l} = 0$, which are expected to have commonly quite localized nature inside a dielectric sphere. It is obvious that there is a criterion on the $E=k^2$ axis, beyond which Eq. (28) shows less agreement with numerical results, and that the criterion depends on l. Careful observation reveals that the condition $l/n < k^{\lambda}_{i} a < l$ is satisfied for the peaks showing good agreement. The states that satisfy both the Mie resonant condition and this inequality are the photon virtual bound states (PVBSs) [23]. Peaks showing good agreement with numerical results are then concluded to originate from PVBSs.

For completeness of the discussion, a brief summary of the PVBS is given. The details of the derivation are shown in Ref. [23]. The PVBS is defined as the state that satisfies both the Mie resonant condition $\cot \delta^{\lambda}_{l}(k) = 0$ and the inequality $l/n < ka < l$ simultaneously. Under the inequality, the resonant conditions are rewritten in the following form:

$$nka - \frac{l}{2}\pi = N\pi + \frac{l+1}{nka} \tag{36}$$

for the TE mode and

$$nka - \frac{l}{2}\pi = N\pi - \frac{nka}{n^2(l+1)} \tag{37}$$

for the TM mode with integer N. The meaning of "virtual" is the following: consider a gedanken case where an infinite barrier is located at the boundary of the dielectric sphere with

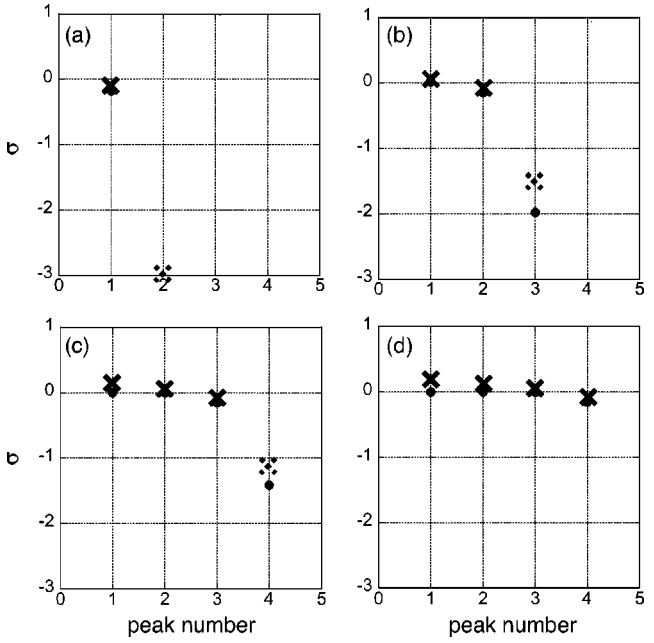

FIG. 3. Comparison of the width of the PDOS for the TE mode between the analytic result Eq. (33) and the numerically obtained results. The crosses show $\sigma_{l,i}^{\mathrm{TE}}$ plotted against the peak number i for $l=1$, 3, 5, and 7 in (a), (b), (c), and (d), respectively. Solid crosses are used for peaks showing good agreement and dotted crosses for peaks showing less agreement. Solid circles show $\tilde{\sigma}_{l,i}^{\mathrm{TE}}$ for comparison between the present theory and the previously reported results. Solid circle for $i=2$ in (a) is out of range; it is evaluated as $\tilde{\sigma}_{l=1,i=2}^{\mathrm{TE}}=-4.56$.

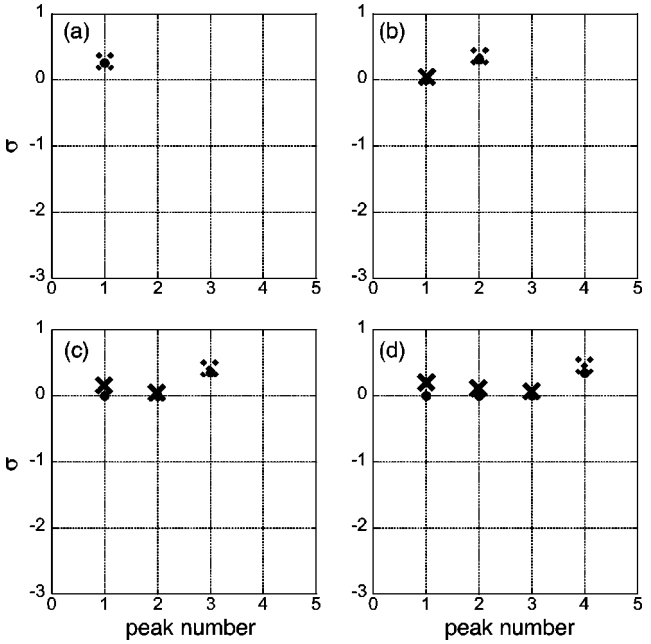

FIG. 4. Comparison of the width of the PDOS for the TM mode between the analytic result Eq. (34) and numerically obtained results. The crosses show $\sigma_{l,i}^{\mathrm{TM}}$ plotted against the peak number i for $l=1$, 3, 5, and 7 in (a), (b), (c), and (d), respectively. Solid crosses are used for peaks showing good agreement and dotted crosses for peaks showing less agreement. Solid circles show $\tilde{\sigma}_{l,i}^{\mathrm{TM}}$ for comparison between the present theory and the previously reported results.

radius a. In this case, the electromagnetic wave is completely bounded inside the dielectric sphere. The condition which determines the wave number is

$$nka-\frac{l}{2}\pi=N\pi. \tag{38}$$

This equation, the completely bound condition, should be compared with Eqs. (36) and (37). Both of the two equations have small correction terms, the second terms in the right hand sides, comparing with Eq. (38). Since the gedanken case will not occur for dielectrics, PVBSs are the most bounded states for actual electromagnetic wave for a dielectric sphere. Note that the condition $l/n<ka<l$ was presented *schematically* in Ref. [8]. For later convenience, the state that satisfies the Mie resonant condition but does not satisfy the inequality $l/n<ka<l$ is referred to as non-PVBS in the following.

Figures 3 and 4 show that the hybridization theory is valid for PVBSs but not for non-PVBSs. The reason of disagreement for non-PVBSs is that the assumption Eq. (13) breaks. The non-PVBSs are not influenced by the "confinement potential well" $l(l+1)/r^2-U(r)$ as PVBSs are [23]. The localized nature is thus poor. In addition, it is confirmed that the numerically obtained PDOS for a non-PVBS deviates from the Lorentzian form. Indeed, the Lorentzian fitting for non-PVBSs is not good. This is a numerical proof that the localized nature of the non-PVBS is quite poor. The hybridization theory is then not well defined for non-PVBSs.

It is not essential that only the cases with odd l's are presented here. The reason is that under the present parameter conditions the numbers of peaks showing good agreement for $l=2l_0-1$ and $2l_0$ are found to be the same. Note that the smallest angular momentum for the spherical vector wave is $l_0=1$. The hybridization theory does not depend on whether l is odd or even.

In Figs. 3 and 4, only one peak showing disagreement (dotted crosses) is presented for each l and there are no plots for further non-PVBSs. This is because there is no sense after breaking the basic assumption for the hybridization theory that the localized states should be localized.

In summary, the hybridization theory between the localized state and freely propagating modes for light scattering problem from a dielectric sphere is established for PVBSs and the localized mode is identified with a PVBS.

B. The relation to the result from the Breit-Wigner formula

One might think that the disagreement of the PDOS for non-PVBSs is caused by a lack of validity of the approximation for the summation in Eq. (26) used to have the analytic result of the PDOS, although the reason for the disagreement is discussed in the previous subsection. In order to reconfirm it, we refer to the previously reported results of the width for the Mie resonance obtained by Johnson [18]. For the purpose, Johnson's results are briefly mentioned in the following.

By expanding the phase shift around the resonance $x_i^\lambda = k_i^\lambda a$ as

$$\beta_l^\lambda(x) \cong [\beta_l^\lambda(x_i^\lambda)]'(x - x_i^\lambda), \tag{39}$$

one can obtain the PDOS with respect to x in the form of the Breit-Wigner formula

$$\frac{d\delta_l^\lambda}{dx} = \frac{1/[\beta_l^\lambda(x_i^\lambda)]'}{\{1/[\beta_l^\lambda(x_i^\lambda)]'\}^2 + (x - x_i^\lambda)^2}. \tag{40}$$

The Mie resonant width $w_{l,i}^\lambda \equiv 1/[\beta_l^\lambda(x_i^\lambda)]'$, coming from the resonance $x = x_i^\lambda$, is reduced to [18]

$$w_{l,i}^{\mathrm{TE}}(x_i^{\mathrm{TE}}) = \frac{1}{(n^2-1)\chi_l^2(x_i^{\mathrm{TE}})} \tag{41}$$

for the TE mode

$$w_{l,i}^{\mathrm{TM}}(x_i^{\mathrm{TM}}) = \frac{1}{(n^2-1)\chi_l^2(x_i^{\mathrm{TM}})[l(l+1)/(nx_i^{\mathrm{TM}})^2 + G_l^2(x_i^{\mathrm{TM}})]} \tag{42}$$

for the TM mode, where $G_l(x) \equiv \chi'_l(x)/\chi_l(x)$.

In order to relate $\Delta_{l,i}^\lambda$ to $w_{l,i}^\lambda$, multiply both sides of Eq. (39) by $x + x_i^\lambda$ and approximate $x + x_i \cong 2x_i^\lambda$ for x in the vicinity of x_i^λ; one can then obtain

$$\beta_l^\lambda(x_i^\lambda) \cong \frac{a}{2k_i w_{l,i}^\lambda}[k^2 - (k_i^\lambda)^2]. \tag{43}$$

Since our result is written as

$$\beta_l^\lambda = \frac{1}{\Delta_{l,i}^\lambda}[k^2 - (k_i^\lambda)^2], \tag{44}$$

the relation between the Lorentzian width $\Delta_{l,i}^\lambda$ and the Mie resonant width $w_{l,i}^\lambda(x_i)$ is obtained as

$$\Delta_{l,i}^\lambda = \frac{2k_i^\lambda}{a} w_{l,i}^\lambda(x_i^\lambda). \tag{45}$$

Here we introduce the variance of the width

$$\tilde{\sigma}_{l,i}^\lambda \equiv \frac{D_{l,i}^\lambda - (2k_i^\lambda/a)w_{l,i}^\lambda}{D_{l,i}^\lambda}, \tag{46}$$

in order to compare the numerically obtained width $D_{l,i}^\lambda$ and $w_{l,i}^\lambda$. The variance $\tilde{\sigma}_{l,i}^\lambda$ for both TE and TM modes is superimposed as solid circles in Figs. 3 and 4, respectively. The overall behavior of the circles and the crosses, not only the solid crosses but also the dotted ones, is quite similar. This fact shows that disagreement between $\Delta_{l,i}^\lambda$ and $D_{l,i}^\lambda$ for non-PVBSs is not caused by the approximation used for the analytic calculations and that the present hybridization theory is valid for PVBSs.

C. Identities from Green's theorem

The magnitude of hybridization is intuitively related to a volume integral between inside and outside "wave functions" multiplied by a "potential." In this subsection, the relation between the rigorous results for the hybridization and the intuition for the light scattering problem is discussed. The subject in this context for the electron problems is discussed in Ref. [24].

The expressions for the magnitude of hybridization between the PVBS and free modes, Eqs. (24) and (25), remind us of the surface integral. A surface integral should be related to the corresponding volume integral through the Green's theorem. In order to clarify the relation, let us start the equations for a free transverse electric field $\nabla^2\mathbf{E}^{(0)} + k^2\mathbf{E}^{(0)} = \mathbf{0}$ and for the electric field $\mathbf{E}$ influenced by the potential $U(r)$, $\nabla^2\mathbf{E} + k^2\mathbf{E} + U(r)\mathbf{E} = \mathbf{0}$. After eliminating the terms including k^2 and performing the volume integral for both sides over the range of $r < a$ with use of the divergence-free condition, one then obtains

$$-\int_{r\le a} \mathbf{E}^{(0)} \cdot U(r)\mathbf{E}\, d^3r = \int_{r=a} d\mathbf{\Omega} \cdot [\mathbf{E}^{(0)} \times (\nabla \times \mathbf{E}) - \mathbf{E} \times (\nabla \times \mathbf{E}^{(0)})]. \tag{47}$$

The surface integral in the right hand side results from applying Green's theorem for vector fields [25]:

$$\int_V d^3r[\mathbf{A} \cdot \nabla^2\mathbf{B} - \mathbf{B} \cdot \nabla^2\mathbf{A}] = \int_S d\mathbf{\Omega} \cdot [\mathbf{A} \times (\nabla \times \mathbf{B}) + \mathbf{A}(\nabla \cdot \mathbf{B}) - \mathbf{B} \times (\nabla \times \mathbf{A}) - \mathbf{B}(\nabla \cdot \mathbf{A})], \tag{48}$$

where both $\mathbf{A}$ and $\mathbf{B}$ are arbitrary vectors.

Consider the case of the TE mode where the electric field is represented by $\mathbf{M}$. Using the identities of the spherical vectors $\nabla \times \mathbf{M}^{(0)} = k\mathbf{N}^{(0)}$ and $\nabla \times \mathbf{M} = nk\mathbf{N}$, and integrating out the angular components in the surface integral, one then has the identity

$$-\int_{r\le a} \mathbf{M}^{(0)} \cdot U(r)\mathbf{M}\, d^3r = \frac{l(l+1)}{k^2}\left[k\psi'_l(nka)\phi_l(a) - \frac{1}{n}\psi_l(nka)\phi'_l(a)\right]. \tag{49}$$

Note that the equation obtained holds *identically* for arbitrary k's.

Here, let us introduce the localized state. Set $k = k_i^{\mathrm{TE}}$ for a given l which yields one of the PVBSs, then the right hand side (RHS) of Eq. (49) is identified as

$$(\mathrm{RHS}) = \frac{l(l+1)}{(k_i^{\mathrm{TE}})^2} V_{l,i}^{\mathrm{TE}}. \tag{50}$$

Since $\mathbf{M}$ in the volume integral now represents the PVBS characterized by $k = k_i^{\mathrm{TE}}$, the field is quite well localized for $r < a$ and the following approximation is allowed:

$$-\int_{r\le a} \mathbf{M}^{(0)} \cdot U(r)\mathbf{M}\, d^3r \cong -\int_{r\le R} \mathbf{M}^{(0)} \cdot U(r)\mathbf{M}\, d^3r. \tag{51}$$

One eventually obtains

$$V_{l,i}^{\mathrm{TE}} = -\frac{(k_i^{\mathrm{TE}})^2}{l(l+1)} \times \int_{r\leqslant R} d^3r\, \mathbf{M}^{(0)} \times [\phi_{l,k_i^{\mathrm{TE}}}(r)] \cdot U(r)\mathbf{M}[\psi_l(nk_i^{\mathrm{TE}}r)]. \quad (52)$$

For the TM mode (**N** field), a similar procedure with the use of $\nabla\times\mathbf{N}^{(0)}=k\mathbf{M}^{(0)}$ and $\nabla\times\mathbf{N}=nk\mathbf{M}$ yields the identity

$$V_{l,i}^{\mathrm{TM}} = -\frac{(k_i^{\mathrm{TM}})^2}{l(l+1)} \times \int_{r\leqslant R} d^3r\, \mathbf{N}^{(0)} \times [\phi_{l,k_i^{\mathrm{TM}}}(r)] \cdot U(r)\mathbf{N}[\psi_l(nk_i^{\mathrm{TM}}r)]. \quad (53)$$

It is true that the results derived through the vectorial Green's theorem Eqs. (52) and (53) contain the identical forms of $V_{l,i}^{\mathrm{TE}}$ and $V_{l,i}^{\mathrm{TM}}$ obtained in Sec. II. The results through the Green's theorem are, however, nothing but identities. One can thus not immediately obtain the Fano model that a localized state (a PVBS, in the present case) is embedded into free continuous modes and cannot verify the hybridization. In order to conclude that the hybridization is well defined for the identified localized states, the discussion presented in Sec. II is inevitable.

IV. CONCLUDING REMARKS

The theory presented in this work corresponds to a photonic counterpart of the Anderson model in electron systems, where a magnetic impurity atom is located in a host metal [13,20]. The essential point is the fact that a localized mode is embedded in free continuous modes, that is, the Fano model. The key for the present work is to regard the dielectric sphere as the impurity "atom" for free modes. As for a localized mode, the PVBSs in the present study correspond to *d* states in the impurity atom. Free propagating lights correspond to *s* electrons in the host metal. There is complete one-to-one correspondence between photonic and electron problems. In this sense, we can conclude that the present theory is a photonic Anderson model, which is an extension from scalar to vectorial wave functions [26].

The fact that a dielectric *sphere* is treated in this study is not essential for the present formulation, which was also reported in Ref. [9]. A part of the reason to use a sphere is that we follow the original proposal in Ref. [9]. In addition there are advantages in using spherical systems as a convenience of analytical handling and the capability of regarding the sphere as an impurity "atom." For the case of dielectrics with other shapes, the essential points are common with the present work, although the difficulty of analytic treatment depends on the shape.

The present paper deals with the most fundamental problem for establishment of the heavy photon concept. Although it is essential, the following point should also be discussed to demonstrate the usefulness of the heavy photon in PCs: a comparison of the photonic bandwidth calculated by "first principles methods" and by a tight binding model formulated through hybridization theory. In order to solve this problem, one has to derive the effective coupling between the PVBSs excited in spheres. For the purpose it is needed to eliminate the photon degrees of freedom in the hybridization theory. The PVBSs are expected to be represented by two-level systems, since they are localized excitations. The hybridization is then represented as a coupling between the Pauli matrix and Bose operators which denote free photons. A second order perturbation, such as the Born-Markov method, is one of the procedures to eliminate the photon degrees of freedom and obtain an effective coupling of two-level systems. If the effective interaction is short range, the tight binding coupling between the localized excitations in the dielectric spheres is found [27]. The magnitude of the coupling should be directly compared with the width of the flat photonic bands. This scenario will be addressed in the near future.

In conclusion, light scattering from a homogeneous dielectric sphere is formulated in terms of the hybridization between the localized mode excited in the dielectric sphere and freely propagating modes. This theory is a photonic counterpart of the Anderson model in electron systems. The purpose of this work is fulfilled by showing that the light scattering problem is formulated in a theory equivalent to the Fano model. The analytic expression of the magnitude of the hybridization is obtained. The localized mode is identified with a PVBS, which satisfies the Mie resonant condition and the inequality $l/n<ka<l$ simultaneously. The comparison between the PDOS represented by the Lorentzian Eq. (28) and numerical results shows good agreement for the PVBSs, which guarantees validity of the present theory. This hybridization theory yields a rigorous foundation for the heavy photon concept for flat photonic bands.

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APPENDIX A: PROOF OF EQ. (10)

Consider the inhomogeneous differential equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right] F_{l,k}(r,r') = \delta(r-r'). \quad (A1)$$

The solution is known to be written in terms of eigenfunctions of the corresponding homogeneous differential equation [28]. The homogeneous differential equation is

$$\mathcal{L}[\phi(r)] \equiv \frac{d^2\phi(r)}{dr^2} - \frac{l(l+1)}{r^2}\phi(r) + k^2\phi(r) = 0. \quad (A2)$$

Two independent fundamental solutions of this equation are the Riccati-Bessel functions $\psi_l(kr)$ and $\chi_l(kr)$. Let $r \in [0,R]$ and $R\gg 1$. The boundary conditions that $|\phi(r=0)| < \infty$ and $\phi(R)=0$ are imposed and the normalization condition

$$\int_0^R |\phi(r)|^2 dr = 1 \quad (A3)$$

is assumed. One can then obtain the following eigenfunctions:

$$\{\phi_{l,s}(r)\} = \left\{ \sqrt{\frac{2}{R}}\psi_l(k_s R) \right\}. \tag{A4}$$

This is a complete function set. Since $R \gg 1$, one can write the eigenvalues by using the asymptotic form of ψ_l as

$$k_s = \frac{\pi}{R}\left(s + \frac{l}{2}\right), \tag{A5}$$

with integer s.

Here we expand $F_{l,k}(r,r')$ in terms of the complete set $\{\phi_{l,s}(r)\}$ as

$$F_{l,k}(r,r') = \sum_s c_s(r')\phi_{l,s}(r); \tag{A6}$$

then the following identity holds:

$$\mathcal{L}[F_{l,k}(r,r')] = \sum_s c_s(r')(k^2 - k_s^2)\phi_{l,s}(r). \tag{A7}$$

It reduces the inhomogeneous differential equation to

$$\sum_s c_s(r')(k^2 - k_s^2)\phi_{l,s}(r) = \delta(r - r'). \tag{A8}$$

Using the orthogonality

$$\int_0^R \phi_s(r)\phi_{s'}(r)dr = \delta_{ss'}, \tag{A9}$$

the expansion coefficient $c_s(r')$ is determined as

$$c_s(r') = \frac{\phi_{l,s}(r')}{k^2 - k_s^2}. \tag{A10}$$

The solution is obtained as

$$F_{l,k}(r,r') = \sum_s \frac{\phi_{l,s}(r')\phi_{l,s}(r)}{k^2 - k_s^2}. \tag{A11}$$

On the other hand, one can derive another form of $F_{l,k}(r,r')$. For $r \neq r'$, the inhomogeneous differential equation is reduced to

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right]F_{l,k}(r,r') = 0. \tag{A12}$$

Considering the boundary condition that $F(r_<, r_> = R) = 0$ and the symmetry for r and r', one can write the general solution

$$F_{l,k}(r,r') = C\psi_l(kr_<)[\beta_l^\lambda \psi_l(kr_>) + \chi_l(kr_>)], \tag{A13}$$

where C is a coefficient to be determined, and $r_{<(>)}$ denotes the smaller (larger) one among r and r'. The boundary condition gives $\beta_l^\lambda = -\chi_l(kR)/\psi_l(kR)$. Integrate the inhomogeneous differential equation from $r = r' - \epsilon$ to $r = r' + \epsilon$ and take the limit $\epsilon \to 0$; then

$$\left.\frac{dF}{dr}\right|_{r=r'+\epsilon} - \left.\frac{dF}{dr}\right|_{r=r'-\epsilon} = 1. \tag{A14}$$

Substitution of Eq. (A13) turns Eq. (A14) into

$$Ck[\psi_l(kr)\chi'_l(kr) - \psi'_l(kr)\chi_l(kr)] = 1. \tag{A15}$$

Using the identity $\psi\chi' - \psi'\chi = -1$, C is determined as

$$C = -\frac{1}{k}. \tag{A16}$$

Since one has obtained the two equivalent forms of $F_{l,k}(r,r')$, one can now prove that the identity Eq. (10) holds for

$$q_{l,k}^\lambda(r) = B_{out}^\lambda[\beta_l^\lambda \psi_l(kr) + \chi_l(kr)]. \tag{A17}$$

Using the form

$$F_{l,k}(r_<, r_>) = -\frac{1}{k}\psi_l(kr_<)[\beta_l^\lambda \psi_l(kr_>) + \chi_l(kr_>)], \tag{A18}$$

one can show for $r > a$ that

$$\left.\frac{\partial F_{l,k}(r_<, r_>)}{\partial r_<}\right|_{r_<=a} \equiv \frac{\partial}{\partial a}F_{l,k}(a,r) = -\psi'_l(ka)[\beta_l^\lambda \psi_l(kr_>) + \chi_l(kr_>)]. \tag{A19}$$

The derivative of $q_{l,k}^\lambda$ is

$$[q_{l,k}^\lambda(a)]' \equiv \left.\frac{\partial q_{l,k}^\lambda(r)}{\partial r}\right|_{r=a} = B_{out}^\lambda k[\beta_l^\lambda \psi'_l(ka) + \chi'_l(ka)]. \tag{A20}$$

Using the above equations, one can obtain the following identity:

$$[q_{l,k}^\lambda(a)]' F_{l,k}(a,r) - q_{l,k}^\lambda(a)\frac{\partial}{\partial a}F_{l,k}(a,r) = B_{out}^\lambda[\beta_l^\lambda \psi_l(kr) + \chi_l(kr)]. \tag{A21}$$

Similarly for $r < a$

$$\left.\frac{\partial F_{l,k}(r_<, r_>)}{\partial r_>}\right|_{r_>=a} \equiv \frac{\partial}{\partial a}F_{l,k}(r,a) = -\psi_l(kr_<)[\beta_l^\lambda \psi'_l(ka) + \chi'_l(ka)]. \tag{A22}$$

Straightforward calculation yields

$$[q^\lambda{}_{l,k}(a)]' F_{l,k}(a,r) - q_{l,k}^\lambda(a)\frac{\partial}{\partial a}F_{l,k}(a,r) = 0. \tag{A23}$$

One has consequently the identity Eq. (10).

APPENDIX B: DERIVATION OF EQ. (16)

In Appendix A, we showed that

$$F_{l,k}(r,r') \equiv \sum_s \frac{\phi_{l,s}(r)\phi_{l,s}(r')}{k^2 - k_s^2} = -\frac{1}{k}\psi_l(kr_<)[\beta_l^\lambda \psi_l(kr_>) + \chi_l(kr_>)].$$

One can define similar functions $F_{l,k}^A(r), F_{l,k}^{B_1}(r), F_{l,k}^{B_2}(r)$, and $F_{l,k}^C(r)$ and prove similar identities. The proof is parallel with the one for $F_{l,k}(r,r')$. The definitions and the identities are listed:

$$F_{l,k}^A(r) \equiv \sum_s \frac{\phi_{l,s}(r)\phi_{l,s}(r)}{k^2 - k_s^2} \tag{B1}$$

$$\equiv -\frac{1}{k}\psi_l(kr)[\beta_l^{\lambda}\psi_l(kr)+\chi_l(kr)], \tag{B2}$$

$$F_{l,k}^{B_1}(r) \equiv \left.\frac{\partial}{\partial r}F_k(r,r+\epsilon)\right|_{\epsilon\to 0} \tag{B3}$$

$$=-\psi'_l(kr)[\beta_l^{\lambda}\psi_l(kr)+\chi_l(kr)], \tag{B4}$$

$$F_{l,k}^{B_2}(r) \equiv \left.\frac{\partial}{\partial r}F_k(r,r-\epsilon)\right|_{\epsilon\to 0} \tag{B5}$$

$$=-\psi_l(kr)[\beta_l^{\lambda}\psi'_l(kr)+\chi'_l(kr)], \tag{B6}$$

$$F_{l,k}^{C}(r) \equiv \frac{\partial^2}{\partial r\,\partial r'}F_k(r,r') \tag{B7}$$

$$=\sum_s \frac{\phi'_{l,s}(r)\phi'_{l,s}(r)}{k^2-k_s^2} \tag{B8}$$

$$=-k\psi'_l(kr)[\beta_l^{\lambda}\psi'_l(kr)+\chi'_l(kr)], \tag{B9}$$

$$F_{l,k}^{B}(r,r') \equiv \left.\frac{\partial}{\partial r'}F_k(r,r')\right|_{r'=r} \tag{B10}$$

$$=\sum_s \frac{\phi_s(r)\phi'_s(r)}{k^2-k_s^2}. \tag{B11}$$

From simple calculations, the following identities are obtained:

$$F_{l,k}^{B_1}(r)-F_{l,k}^{B_2}(r)=-1, \tag{B12}$$

$$F_{l,k}^{B_1}(r)F_{l,k}^{B_2}(r)=F_{l,k}^{A}(r)F_{l,k}^{C}(r), \tag{B13}$$

$$F_{l,k}^{B}(r)-F_{l,k}^{B_1}(r)=F_{l,k}^{B_2}(r)-F_{l,k}^{B}(r)=\frac{1}{2}. \tag{B14}$$

From these results, we can obtain Eq. (16) as follows. Using the identity for the Riccati-Bessel functions $\psi\chi'-\psi'\chi=-1$, Eq. (6) is rewritten as

$$[\chi_l(ka)+\beta_l^{\lambda}\psi_l(ka)]\times[n^{\mu}D_l(nka)\psi_l(nka)-\psi'_l(nka)]=-1. \tag{B15}$$

This is turned into

$$n^{\mu}kD_l(nka)F_{l,k}^{A}(a)-F_{l,k}^{B1}(a)=1, \tag{B16}$$

by using $F_{l,k}^{A}$ and $F_{l,k}^{B_1}$. Multiplying Eq. (B16) by $F_{l,k}^{C}(a)$ and using the identities Eqs. (B12) and (B13), one has

$$F_{l,k}^{B_2}[nkD_l(nka)F_{l,k}^{B_1}-F_{l,k}^{C}]=0. \tag{B17}$$

Since $F_{l,k}^{B_2}\neq 0$, use of Eq. (B12) gives

$$n^{\mu}kD(nka)F_{l,k}^{B_2}(a)-F_{l,k}^{C}(a)=n^{\mu}kD(nka). \tag{B18}$$

Eliminating $F_{l,k}^{B_2}$ by using Eq. (B14), one can obtain

$$n^{\mu}kD_l(a)F_{l,k}^{B}(a)-F_{l,k}^{C}(a)=\frac{1}{2}n^{\mu}kD_l(nka). \tag{B19}$$

From Eq. (B14), Eq. (B16) is also expressed in another form as

$$n^{\mu}kD_l(nka)F_{l,k}^{A}(a)-F_{l,k}^{B}(a)=\frac{1}{2}. \tag{B20}$$

Substrate Eq. (B20) multiplied by $n^{\mu}kD_l(nka)$ from Eq. (B19), then

$$\{n^{\mu}kD_l(nka)\}^2F_{l,k}^{A}(a)-2n^{\mu}kD_l(nka)F_{l,k}^{B}(a)+F_{l,k}^{C}(a)=0. \tag{B21}$$

Substitution of the eigenfunction representations of $F_{l,k}^{A}, F_{l,k}^{B}$, and $F_{l,k}^{C}$ yields

$$\sum_s \frac{[n^{\mu}kD_l(nka)\phi_{l,s}(a)-\phi'_{l,s}(a)]^2}{k^2-k_s^2}=0. \tag{B22}$$

APPENDIX C: WRONSKI THEOREM [29]

Let $r\in[0,R]$. Consider the following two equations:

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2+u(r)k^2\right]\varphi_k(r)=0, \tag{C1}$$

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k'^2+u(r)k'^2\right]\varphi_{k'}(r)=0, \tag{C2}$$

where

$$u(r)=\theta(a-r)(n^2-1). \tag{C3}$$

Impose that $\varphi(r=0)=0$ and that

$$\int_0^R|\varphi(r)|^2dr=1. \tag{C4}$$

Substrate Eq. (C2) multiplied by φ_k from Eq. (C1) multiplied by $\varphi_{k'}$, then

$$\frac{d}{dr}[\varphi_{k'}(r)\varphi'_k(r)-\varphi'_{k'}(r)\varphi_k(r)] + (k^2-k'^2)[1+u(r)]\varphi_k(r)\varphi_{k'}(r)=0. \tag{C5}$$

Integrating from $r=0$ to a, one can obtain

$$\varphi_k(a)\varphi'_{k'}(a)-\varphi'_k(a)\varphi_{k'}(a)=n^2(k^2-k'^2)\int_0^a\varphi_k(r)\varphi_{k'}(r)dr. \tag{C6}$$

Suppose that $k\approx k'$, then one can approximate

$$\int_0^a\varphi_k(r)\varphi_{k'}(r)dr\approx\int_0^a[\varphi_{k'}(r)]^2dr. \tag{C7}$$

When $\varphi_{k'}(r)$ is quite localized in the region $r<a$, that is,

$$\int_0^a|\varphi_{k'}(r)|^2dr\cong\int_0^R|\varphi_{k'}(r)|^2dr=1, \tag{C8}$$

Eq. (C6) is turned into

$$\varphi'_k(a)\varphi_{k'}(a) - \varphi_k(a)\varphi'_{k'}(a) = -n^2(k^2 - k'^2). \quad \text{(C9)}$$

Dividing both sides by $\varphi_k(a)\varphi_{k'}(a)$, one can obtain the final form as

$$\frac{\varphi'_k(a)\varphi_{k'}(a) - \varphi_k(a)\varphi'_{k'}(a)}{\varphi_k(a)\varphi_{k'}(a)} = -n^2\frac{k^2 - k'^2}{\varphi_k(a)\varphi_{k'}(a)} \approx -n^2\frac{k^2 - k'^2}{\varphi^2_{k'}(a)}. \quad \text{(C10)}$$

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