Effective-medium properties of metamaterials: A quasimode theory

Shulin Sun,[1] S. T. Chui,[2] and Lei Zhou[1,*]
[1]Department of Physics and Surface Physics Laboratory (State Key Laboratory), Fudan University, Shanghai 200433, People's Republic of China
[2]Bartol Research Institute, University of Delaware, Newark, Delaware 19716, USA
(Received 1 March 2009; published 22 June 2009)

Under the generalized coherent-potential approximation, we established a "quasimode" theory to study the effective-medium properties of electromagnetic metamaterials. With this theory, we calculate the self-energy, density of states (DOS), and mean-free paths for optical modes traveling inside a metamaterial, and then determine the effective permittivity and permeability of the metamaterial by maximizing the DOS function. Compared with the traditional methods for calculating effective-medium parameters, the present approach could provide quantitative judgments on how meaningful are the obtained effective-medium parameters. As illustrations, we employed the theory to study the effective-medium properties of several examples including finite metallic wires and split ring resonators.

DOI: 10.1103/PhysRevE.79.066604 PACS number(s): 41.20.Jb, 78.20.Bh, 78.20.Ci

I. INTRODUCTION

There is much recent interest in artificial media with arbitrary permittivity ε and permeability μ, stimulated by many fascinating properties discovered based on such media, such as negative refraction [1,2], super lensing [3], and cloaking [4,5]. However, such unusual media do not exist readily in nature since ordinary materials do not exhibit magnetism at high frequencies [6]. It is only until recently that practical realizations of these unusual media (often called metamaterials) became possible, after Pendry proposed the famous split ring resonator (SRR) that possesses a magnetic response at any desired frequency [7]. The main idea to fabricate a metamaterial is to combine local resonance structures of electric and/or magnetic type to form a composite material. A standard method to determine the effective parameters of such composite medium is the so-called *S*-parameter retrieval method [8,9], which is to directly retrieve the effective ε and μ by comparing the transmission spectra of the realistic structure and the model medium. The retrieval method, together with its improved versions [10–14], has been successfully applied to determine the effective parameters of metamaterials in many cases. Other methods were also employed to calculate the effective parameters of metamaterials [7,15–22] with different advantages and limitations.

Despite the great successes achieved by these methods, there are still several problems. It is shown that the effective-medium parameters cannot be determined by standard methods in some cases even when the input wavelength λ_0 is much longer than the inhomogenity feature size (the lattice constant) in a metamaterial [23]. More mysteriously, in some cases, people found that the effective parameters obtained based on a *thin* metamaterial layer did not work for a *thick* sample possessing the same microstructure [24,25]. This is very intriguing at first sight, since in principle the effective parameters should be the *local* properties of a material and should *not* depend on the sample thickness. To address these problems, we feel that a theory that can be applied to justify the "quality" of the obtained effective parameters for a given metamaterial is highly desired.

In this paper, under the generalized coherent-potential approximation (CPA) [26], we establish a "quasimode" theory to study the effective-medium properties of metamaterials. Embedding the metamaterial under study into a reference medium whose permittivity ε_{ref} and permeability μ_{ref} can be tuned freely, we employ the Green's function (GF) theory to study the self-energy, the density of states (DOS), and the mean-free paths (MFP) for electromagnetic (EM) modes traveling inside the medium. We then determine the effective ε_{eff} and μ_{eff} of the metamaterial by varying the parameters of the reference medium to maximize the DOS function. We found that the theory can not only uniquely determine the effective-medium parameters of metamaterials (even approaching the resonance frequency), but more importantly, it also yields the MFP which can be used to judge the qualities of obtained effective parameters. A similar idea has been applied to study the *equivalent* parameters of a photonic crystal to mimic a homogeneous slab [27]. The main contributions of the present paper are the DOS function and the MFP that can help judge the qualities of the obtained effective media parameters.

The present paper is organized as follows. We will first present the basic formalisms of the theory in Sec. II, and then apply our theory to study three typical examples in Sec. III, including two basic building blocks of metamaterials—finite metallic wires and SRRs. Finally, we conclude our paper in Sec. IV.

II. THEORETICAL FORMALISMS OF THE QUASIMODE THEORY

Consider a metamaterial whose effective parameters are to be calculated. For simplicity and definiteness, we assume that the metamaterial is a periodic lattice of complex microstructures, which is the case for many practical situations.

*Author to whom correspondence should be addressed; phzhou@fudan.edu.cn

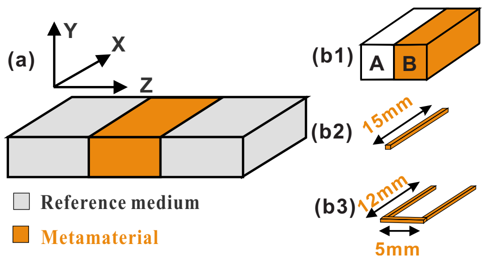

FIG. 1. (Color online) (a) Schematic illustration of the calculation strategy. Unit cells of three examples studied in present paper: (b1) 1D *AB* lattice; (b2) finite metallic wire; (b3) SRR. Here the cross section of the metallic wire in both (b2) and (b3) is 0.5 mm×0.2 mm.

Consider the wave propagations inside such a complex medium. To make the problem more tractable, we adopted the CPA concept to replace most part of metamaterial by a reference homogeneous medium with permittivity $\varepsilon_{\rm ref}$ and permeability $\mu_{\rm ref}$, and leave a slab of the realistic metamaterial embedded inside the reference medium, as shown in Fig. 1(a). The metamaterial slab should be thick enough so that the surface effects can be neglected. With this simplification, the EM wave propagations can be easily solved by a standard GF method following Ref. [26], which we recapitulate next.

Consider a fixed polarization and assume the propagation direction to be perpendicular to the slab [28], the problem is then reduced to a one-dimensional (1D) scalar problem. Define a GF satisfying

$$[\nabla^2+\varepsilon(\vec{r})\mu(\vec{r})k_0^2]G(\omega,\vec{r}-\vec{r}\,')=\delta(\vec{r}-\vec{r}\,'), \quad (1)$$

where $k_0^2=(\omega/c)^2$ in which c is the speed of light, and $\varepsilon(\vec{r})$ and $\mu(\vec{r})$ are the permittivity and permeability functions. Equation (1) can be solved as

$$G(\vec{r},\vec{r}\,')=G_0(\vec{r}-\vec{r}\,')+\int dr_1G_0(\vec{r}-\vec{r}_1)V(\vec{r})_1G(\vec{r}_1,\vec{r}\,'), \quad (2)$$

where $G_0(r-r')$ is the GF solution for the reference medium satisfying

$$[\nabla^2+\varepsilon_{\rm ref}\mu_{\rm ref}k_0^2]G_0(\omega,\vec{r}-\vec{r}\,')=\delta(\vec{r}-\vec{r}\,'), \quad (3)$$

and $V(\vec{r},\omega)=[\varepsilon(\vec{r})\mu(\vec{r})-\varepsilon_{\rm ref}\mu_{\rm ref}]k_0^2$ is the scattering potential [26]. Following Ref. [26], we rewrite Eq. (2) as a symbolic form,

$$G=G_0+G_0VG=G_0+G_0TG_0, \quad (4)$$

where $T=V+G_0VG_0+G_0VG_0VG_0+\cdots=V(1-G_0V)^{-1}$ is the standard T matrix. The configurational averaged GF is given by

$$\langle G\rangle_c=G_0+G_0\langle T\rangle_cG_0, \quad (5)$$

where $\langle T\rangle_c=\langle V(1-G_0V)^{-1}\rangle_c$ [29]. Now define a function Σ as

$$\sum=G_0^{-1}-\langle G\rangle_c^{-1}, \quad (6)$$

we can rewrite the final GF (after standard Fourier transformations) formally as

$$G_c(\omega,k)=\frac{1}{k_{\rm ref}^2(\omega)-k^2-\sum(\omega,k)}. \quad (7)$$

One immediately finds that Σ is nothing but the "self-energy" of the EM mode, analogous to the interacting electron case [30]. Equation (7) shows that an EM mode traveling inside such a complicated medium still behaves like a "free" mode except that there is a "self-energy" correction.

According to Ref. [26], in the weak-scattering limit, the self-energy can be expressed in terms of the forward-scattering amplitude as

$$\sum(\omega,k)\approx T(k,k)/L, \quad (8)$$

where L is the total size of the system used for normalization purpose only. The detailed derivation of Eq. (8) is summarized in the Appendix. We next evaluate the T matrix. The electric field, which satisfies the standard scalar wave equation $[\nabla^2+\varepsilon(\vec{r})\mu(\vec{r})(\omega/c)^2]\phi(\omega,\vec{r}-\vec{r}\,')=0$, can be written in term of the GF and the T matrix as

$$\begin{aligned}|\phi\rangle&=|\phi_0\rangle+G_0T|\phi_0\rangle=e^{ik_{\rm ref}z}-\frac{i}{2\kappa_0}\\&\quad\times\int\exp[ik_{\rm ref}|z-z_1|]T(z_1,z_2)e^{ik_{\rm ref}z_2}dz_1dz_2,\\&=e^{ik_{\rm ref}z}-\frac{i}{2\kappa_0}\exp[ik_{\rm ref}|z|]T\left(k_{\rm ref}\frac{|z|}{z},k_{\rm ref}\right), \quad (9)\end{aligned}$$

where $|\phi_0\rangle=\exp(ik_{\rm ref}r-\omega t)$ (with $k_{\rm ref}=\sqrt{\varepsilon_{\rm ref}\mu_{\rm ref}}k_0$) is the free wave solution inside the reference medium. Here we have omitted the common factor of $e^{-i\omega t}$. Suppose the scattering problem for the complex structure has been solved by some numerical methods, we have generally

$$\begin{aligned}\phi(z)&=S_{21}e^{ik_{\rm ref}z} & z\to\infty\\ \phi(z)&=e^{ik_{\rm ref}z}+S_{11}e^{-ik_{\rm ref}z} & z\to-\infty\end{aligned}, \quad (10)$$

where S_{11} and S_{21} are the standard S parameters. It is straightforward to obtain

$$T(k_{\rm ref},k_{\rm ref})=2k_{\rm ref}i(S_{21}-1),\quad T(-k_{\rm ref},k_{\rm ref})=2k_{\rm ref}iS_{11}, \quad (11)$$

through comparing Eqs. (9) and (10). Therefore, the self-energy Σ can be calculated from the S parameters, once the latter are obtained with numerical methods.

We now discuss how to determine the effective parameters of the target system. In the spirits of CPA, one needs to vary the reference medium properties $\varepsilon_{\rm ref}$ and $\mu_{\rm ref}$, so as to make the real part of self-energy Σ zero. However, this is not generally possible, especially in metamaterials near resonance frequencies. To determine the effective medium in such a situation, we employ the concept of generalized CPA as described in Ref. [26]. Let us define the DOS function,

$$\rho(\omega,k) = -\operatorname{Im} G_c(\omega,k) = -\operatorname{Im}\left[\frac{1}{k_{\mathrm{ref}}^2(\omega) - k^2 - \sum(\omega,k)}\right], \tag{12}$$

which describes the probability of finding a mode with frequency ω and wave-vector k in a medium. For a given frequency ω, the k value that yields the highest DOS defines a "quasimode" which has the highest probability to exist in such a complex medium. In clean systems with $\Sigma(\omega,k)=0$, the DOS function is just a collection of delta functions, which means that the mode is a *perfect* one and has an infinite lifetime. In a dirty system, the DOS function is no longer like a delta function and the resultant optical mode will be a *quasi*mode with a finite lifetime.

The DOS function $\rho(\omega,k)$ is also an implicit function of $\varepsilon_{\mathrm{ref}}$ and μ_{ref}, since both $k_{\mathrm{ref}}^2(\omega)$ and $\Sigma(\omega,k)$ are functions of $\varepsilon_{\mathrm{ref}}$ and μ_{ref}. Therefore, for a given frequency ω, we should in principle vary three quantities, $\varepsilon_{\mathrm{ref}}$, μ_{ref}, and k, to maximize the DOS function when searching for a mode. To make the calculations more tractable, we adopt a further approximation to simplify the searching process (See Sec. 3.9 of Ref. [26]). We put $k^2=k_{\mathrm{ref}}^2(\omega)=\varepsilon_{\mathrm{ref}}\mu_{\mathrm{ref}}(\frac{\omega}{c})^2$ into Eq. (12), and then define an effective DOS function as

$$\rho_{\mathrm{eff}}(\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}}) = -\operatorname{Im} G(\omega,k)|_{k^2=k_{\mathrm{ref}}^2} = \operatorname{Im}\frac{1}{\sum_{\mathrm{eff}}(\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}})} = \frac{-\operatorname{Im}\sum_{\mathrm{eff}}(\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}})}{[\operatorname{Im}\sum_{\mathrm{eff}}(\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}})]^2+[\operatorname{Re}\sum_{\mathrm{eff}}(\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}})]^2}, \tag{13}$$

where $\Sigma_{\mathrm{eff}}=\Sigma(\omega,k)|_{k^2=k_{\mathrm{ref}}^2}$ is the effective self-energy, which is a function of the reference medium parameters. Under this approximation, the DOS function now depends only on $\varepsilon_{\mathrm{ref}}$ and μ_{ref}. Therefore, we only need to vary these two parameters, $\varepsilon_{\mathrm{ref}}$ and μ_{ref} to maximize ρ_{eff} when determining the effective parameters (denoted by $\varepsilon_{\mathrm{eff}}$ and μ_{eff}) of the target metamaterial. This simplification would significantly save our computational time in practice. We note that such an approximation inevitably generates errors in estimating the DOS function. However, the induced error is significant only when the point $\{\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}}\}$ is far away from $\{\varepsilon_{\mathrm{eff}},\mu_{\mathrm{eff}}\}$ which yields the peak value of ρ_{eff}, but becomes less significant when the point $\{\varepsilon_{\mathrm{ref}},\mu_{\mathrm{ref}}\}$ approaches $\{\varepsilon_{\mathrm{eff}},\mu_{\mathrm{eff}}\}$ (see Sec. 3.9 of Ref. [26]). Therefore, adopting such an approximation would not affect our finding the peak position $\{\varepsilon_{\mathrm{eff}},\mu_{\mathrm{eff}}\}$ of the DOS function, which we really care about.

The approach described above can give us more information about the quasimode besides the effective-medium parameters $\varepsilon_{\mathrm{eff}}$ and μ_{eff}. Let us look at the dispersion of EM mode, which is determined by finding the pole of the GF,

$$\varepsilon_{\mathrm{eff}}\mu_{\mathrm{eff}}\left(\frac{\omega}{c}\right)^2 = k^2 - \sum\nolimits_{\mathrm{eff}}. \tag{14}$$

Apparently, the solution k of Eq. (14) must be a complex value. Define $k=k'+i\gamma$, we find that the imaginary part of k is given by

$$\gamma = \operatorname{Im}\sqrt{\varepsilon_{\mathrm{eff}}\mu_{\mathrm{eff}}\left(\frac{\omega}{c}\right)^2 + \sum\nolimits_{\mathrm{eff}}}. \tag{15}$$

The imaginary part of a wave vector usually characterizes the "damping" of a mode traveling inside a medium, which comes from both scatterings and absorptions. In our case, the damping is mainly caused by scatterings, and is present even in the absence of absorptions. The scatterings by the inhomogenity cause a traveling EM mode to lose its phase coherence. While such scattering loss is easy to understand in a disordered medium [26], its origin in a periodic system is not commonly appreciated. Let us look at the geometry shown in Fig. 1. When a plane EM wave with a definite $\vec{k}=\vec{k}_{\parallel,0}+k_z\hat{z}$ is incident on the metamaterial slab, within the effective-medium picture, the wave inside the slab (which is assumed homogeneous in effective-medium picture) should be a *single* mode with a definite wave-vector $\vec{k}_{\parallel,0}+k_{z,\mathrm{eff}}\hat{z}$. However, in realistic situations, the EM wave inside the metamaterial slab is a linear combination of *multiple* modes with different parallel wave-vectors $\vec{k}_{\parallel}=\vec{k}_{\parallel,0}+n\vec{G}$. Here $\vec{G}$ is the reciprocal vector of the periodic lattice on the x-y plane and n is an integer. Since each mode (i.e., high-diffraction order mode) possesses a *different* k value along the z axis, the whole wave function will gradually lose its phase coherence as a *single* mode in the traveling process, particularly in the case where the scattering to higher-order mode channel is significant. Such scattering loss is the origin of the "damping" in the wave vector of the quasimode, and has also been mentioned in Ref. [24]. In fact, such scatterings are sometimes termed as "Umklapp scattering" in electron case [31]. We note that the above discussions are general, and thus applicable to the normal-incidence case with $k_{\parallel,0}=0$.

Considering such scattering loss, we can explicitly define a MFP by

$$l(\omega) = \frac{1}{\gamma(\omega)}, \tag{16}$$

which has the physical interpretation of an "*effective distance*" to measure how long can an EM mode travel in the system before encountering a scattering. The MFP thus helps us justify how good the true system behaves as an effective medium, and how reasonable are the effective-medium parameters to describe the studied metamaterials.

III. APPLICATIONS OF THE THEORY

In this section, we employ our theory to study the effective-medium properties of various systems. We first study a simple 1D *AB* lattice as a benchmark test, and then apply our theory to study two basic constitutional elements of metamaterials—a finite metallic wire and a SRR. The polarization is the same for all three cases, with the electric field along x direction, magnetic field along y direction, and wave vector along z direction. The lattice constants of the metamaterials formed by finite metallic wires and SRRs are 16 mm × 6 mm × 7.5 mm along the x, y, and z directions, respectively.

Consider a 1D *AB* lattice consisting of two homogeneous dielectric slabs with parameters given by $\varepsilon_A=16$, $\mu_A=1$, and

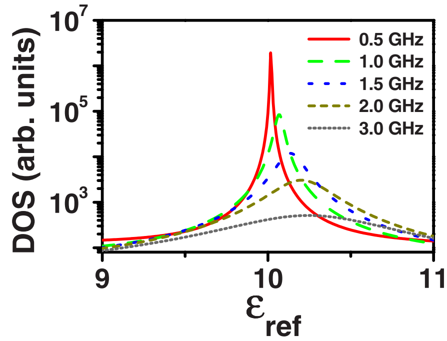

FIG. 2. (Color online) DOS (in arbitrary unit) as the function of ε_{ref} calculated at a series of frequencies for the 1D *AB* lattice structure. Here we set $\mu_{ref}=1$ in the calculations.

$d_A=3.75$ *mm*; $\varepsilon_B=4$, $\mu_B=1$, and $d_B=3.75$ *mm*. To study its effective-medium properties, we follow the established quasimode theory to embed a unit cell as shown in Fig. 1 (b1) in a reference medium, and employed the conventional transfer-matrix method to calculate the *S* parameters. Since there is no magnetism in this problem, we simply set $\mu_{ref}=1$ in the calculations. Figure 2 shows the DOS ρ as functions of ε_{ref} for several typical frequencies; we find that all the DOS functions are maximized around $\varepsilon_{ref}\sim 10$, coinciding well with the volume-averaged value predicted by the standard effective-medium theory. However, while at lower frequencies, the peak is very sharp and the maximum DOS value is very high indicating that the effective-medium description is good, at higher frequencies, the peak is obviously broadened with a decreasing maximum DOS value implying that the effective-medium description becomes bad.

We next employ our theory to study a metamaterial consisting of finite metallic wires. Each metallic wire is 15-mm-long and has a cross-section 0.5 mm$\times$0.2 mm [see inset to Fig. 1 (b2)]. In our calculations, the metamaterial slab that we took is 7.5-mm-thick and consists of one planar array of metallic wires. The scattering problem here is much more difficult to solve than the 1D *AB* lattice case, and we employed a full-wave finite element method [32] to compute the *S* parameters, from which we calculated the DOS and the MFP functions. We choose a typical frequency to illustrate how we determine the effective parameters. With the frequency fixed at $f=5.0$ GHz, we plotted in Figs. 3(a) and 3(b) the obtained DOS function ρ and the MFP function l vs ε_{ref} for different μ_{ref} [33]. We found that the DOS function is maximized at $\varepsilon_{ref}=2.793$ and $\mu_{ref}=0.906$ which are identified as the effective-medium parameters of the system at this frequency. Meanwhile, we found from Fig. 3(b) that the MFP also takes the maximum value at this position. This is reasonable, since with this particular medium as a reference, the scatterings will be mostly reduced, and thus the MFP is the longest. Compared with the standard *S*-parameter retrieval method, we note that the obtained effective medium is unique in our method, and the drawback of multiple solutions is overcome.

We repeated the calculations for eight different frequencies $f=1,2,3,\ldots,8$ GHz, and plotted the spectrum of DOS vs ε_{ref} for each frequency. For illustrative purposes, we stacked the eight spectra together in Fig. 4 [34]. We note that

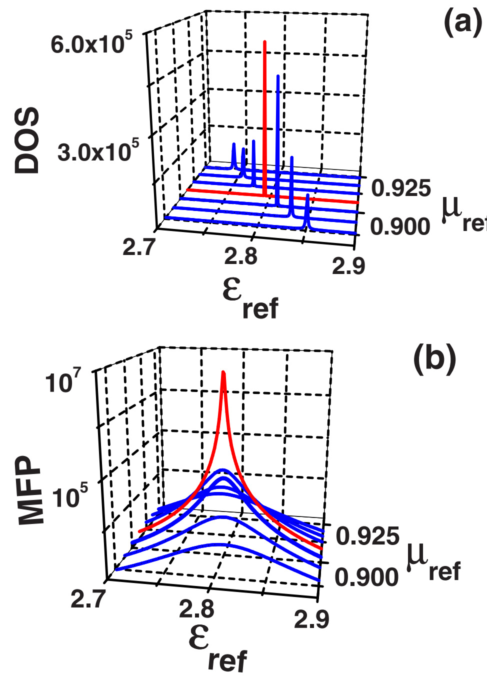

FIG. 3. (Color online) (a) DOS (in arbitrary unit) and (b) MFP (in unit of *a*: lattice constant along *z* direction) as function of ε_{ref} for different μ_{ref}, calculated at $f=5.0$ GHz for the finite metallic wire structure with geometry shown in Fig. 1 (b2).

such an illustration technique is widely adopted in literature to show the electronic quasiparticle dispersions [35]. It is shown that each spectrum exhibits a peak at different ε_{ref} values, which clearly illustrates the system's effective permittivity ε_{eff} as a function of frequency *f*. In fact, we can gain more physics from Fig. 4. We find that the peak in the DOS function is broadened and the maximum DOS value decreases as the frequency increases. Such a tendency is significantly enhanced when the frequency is higher than 7 GHz. Since the DOS function has the physical interpretation of the probability to find a mode, Fig. 4 suggests that the uncertainty region for the calculated ε_{eff} value is significantly enhanced as the frequency increases. In a homogeneous medium without scatterings, the DOS function is a delta function and thus the effective parameter takes a definite value

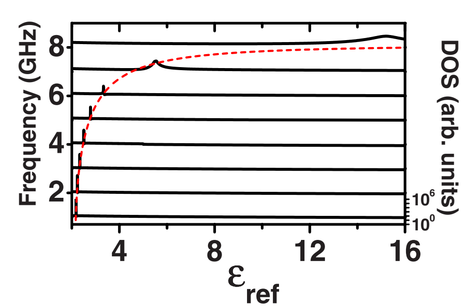

FIG. 4. (Color online) For the finite metallic wire structure as shown in Fig. 1 (b2), DOS$\sim\varepsilon_{ref}$ spectra (solid lines) calculated at frequencies 1, 2, 3, 4, 5, 6, 7, and 8 GHz, stacked from bottom to up with increasing frequency. Here each spectrum has the same labeling scale. The dashed line represents ε_{eff} as a function of frequency calculated by the retrieval method for the same system.

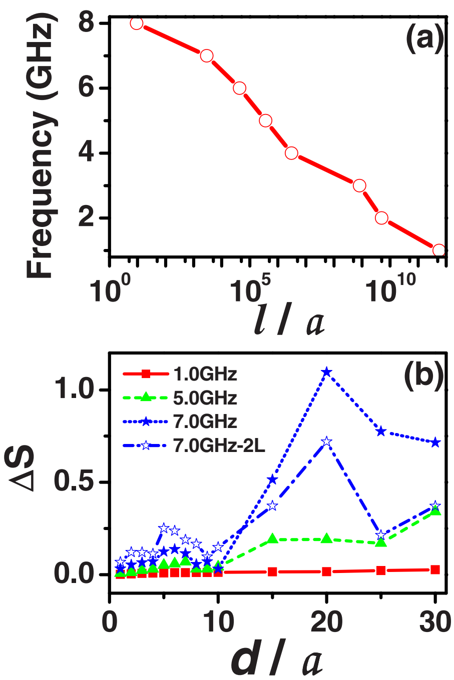

FIG. 5. (Color online) (a) Calculated MFP (denoted by l) as a function of frequency for the finite metallic wire structure; (b) ΔS as functions of the sample thickness calculated at three frequencies: 1, 5, and 7 GHz. The open stars represent ΔS as a function of the sample thickness calculated at $f=7$ GHz but with effective parameters calculated based on a two-layer sample.

without any uncertainty. Indeed, we found that the uncertainty range is small in the long-wavelength case. However, as frequency increases, particularly near the resonance frequency ($\sim$10 GHz here), even we can still get some effective medium to describe the realistic system, the uncertainty range of the obtained effective parameter increases drastically, and the effective-medium description deteriorates and gradually breaks down.

The result of the frequency dependence of ε_{eff} is also obtained by the retrieval method (short dash line in Fig. 4). While the retrieval results are generally in good agreements with ours, in fact our calculations show that the retrieved ε_{eff} have "bad" qualities at frequencies higher than 7 GHz.

The physics can be better understood through looking at the calculated MFP. We showed in Fig. 5(a) the calculated MFP l as a function of frequency for the present system. As expected, the MFP is a decreasing function of frequency, which means that the probability to encounter a scattering is enlarged as frequency increases, and in turn, the effective-medium properties become worse. We now quantitatively study the role played by the MFP. At a fixed frequency, we studied the transmission properties for a metamaterial slab with thicknesses d (here the reference medium is air), and define the calculated S parameters as S^{real}. Then we do the same calculations but with the realistic metamaterial slab replaced by a homogeneous slab of the same thickness and with effective parameters ε_{eff}, and μ_{eff}. The S parameters thus obtained are defined as S^{eff}. Let us now define a quantity ΔS as

$$\Delta S = \sqrt{|S_{11}^{\text{eff}} - S_{11}^{\text{real}}|^2 + |S_{21}^{\text{eff}} - S_{21}^{\text{real}}|^2}, \qquad (17)$$

which measures the *absolute* "differences" between the effective medium and the realistic system in terms of both transmission and reflection spectra [36]. Obviously, ΔS serves to testify the quality of the effective-medium description. The smaller the ΔS, the better the effective-medium description.

We have performed numerical calculations at three typical frequencies—1, 5, and 7 GHz, for the metamaterial slabs with different thicknesses d. The obtained ΔS for different frequencies are shown in Fig. 5(b) as functions of d/a [a(=7.5 mm) is the lattice constant along z direction for the metallic wire structure]. We find that the effective-medium description works very well in the low-frequency situation ($f=1$ GHz), and ΔS is very small (typically smaller than 0.03) for all the slab thicknesses considered. However, at modest frequency ($f=5$ GHz), it is found that while the effective-medium description is still good for thin metamaterial slabs, ΔS is significantly enhanced as d increased, indicating that the effective-medium description is no longer reasonable for thicker samples. Such a tendency is even more prominent for the case of $f=7$ GHz—while the effective-medium parameters work well to describe the EM properties of a *thin* metamaterial slab, the *same* effective-medium parameters cannot work to describe a *thick* metamaterial sample composed by the same type of unit cells. We note that similar observations were found in previous studies [24,25].

The physics behind such an intriguing effect can be understood from the MFP shown in Fig. 5(a). As we have discussed, the MFP has the physical significance of the "*effective distance*" for an EM mode traveling inside the metamaterial freely. For a thin metamaterial slab, its thickness d is always smaller than the MFP l, and therefore, the phase coherence of the EM quasimode is preserved when passing through the medium. That is why the effective-medium description is good for the thin-slab case. However, as the ratio of d/l increases, more scatterings are introduced so that the effective-medium description becomes bad. Apparently, such a tendency is less significant for the case of long MFP (say, $f=1$ GHz case), and the effective-medium description can sustain to thicker samples in such a case. Therefore, the MFP can help us judge the quality of the effective-medium description.

One may argue that the effective parameters may change for a thicker system. To clarify this point, we recalculated the effective parameter for the system at $f=7$ GHz using a two-layer sample ($d=2a$), and found that the effective-medium parameters are $\varepsilon_{\text{eff}}=5.200$ and $\mu_{\text{eff}}=0.658$ [quite close to the result calculated with the thin sample ($d=a$): $\varepsilon_{\text{eff}}=4.819$, $\mu_{\text{eff}}=0.699$]. With this new set of effective-medium parameters, we repeated the calculations for ΔS and plotted ΔS as a function of d/a in Fig. 5(b). We note that the hollow-star line has relatively smaller ΔS than the solid-star line when d/a increases. This is because the effective-medium parameters obtained with a two-layer film are more reasonable than that with a 1 layer film, since the former calculation has naturally taken more multiple-scattering effects into account. However, we note that significant errors still exist in thick samples. Therefore, this "improved" effective-medium description still cannot hold for thick samples, since the "quasi-

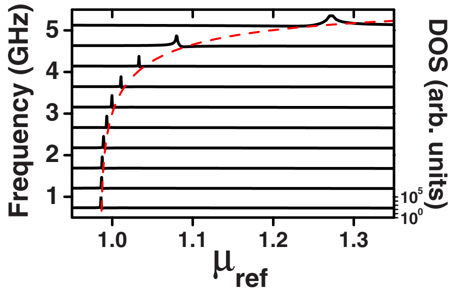

FIG. 6. (Color online) For SRR structure as shown in Fig. 1(b3), DOS spectra as function of μ_{ref} calculated at frequencies: 0.5, 1, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, and 5 GHz, stacked from bottom to up with increasing frequency. Here each spectrum has the same labeling scale. The dashed line represents μ_{eff} as a function of frequency calculated by the retrieval method for the same system.

modes" inside the samples *inherently* possess strong damping.

Our theory can be employed to study other metamaterials with more complex micro structures. Below we illustrate its applications to a SRR structure, with geometry shown in Fig. 1 (b3). Compared with the metallic wire structure, because of the polarization of the present calculation, the SRR structure mainly exhibits magnetic responses, although it also possesses electric resonances with different resonance frequencies. To illustrate the frequency dispersion of the SRR's magnetic permeability, we plotted the DOS function ρ vs μ_{ref} at a series of frequencies: 0.5, 1.0, 1.5, 2.0, ... ,5.0 GHz, and stacked these spectra together in Fig. 6 [37], which clearly illustrates the frequency dependence of μ_{eff}. For comparison, we again added the results obtained from the retrieval method in the same figure. Similar to the finite wire case, as a resonance is approached (at about 5.78 GHz), the uncertain regions of μ_{eff} become wider. Although one can still obtain some effective-medium parameters for the studied metamaterial both by the retrieval method and by our theory, the qualities of such effective parameters become bad; the effective description at higher frequency may not hold for thicker samples because such modes typically possess shorter mean-free paths.

IV. CONCLUSIONS

To summarize, under the generalized coherent-potential approximation, we established a "quasimode" theory to study the effective-medium properties of electromagnetic metamaterials. The main idea is to determine the effective parameters of the target medium through maximizing the DOS function, which has the physical interpretation of the existing probability of a particular EM mode. The most important output of our theory is the mean-free path of an EM mode, which measures how far can an EM mode travel "freely." Compared with some standard methods, the present approach is applicable to frequency region near resonances, and most importantly, provides quantitative judgments on how meaningful are the obtained effective-medium parameters. We found that a system with a larger MFP has a better effective-medium property, and its effective-medium description can hold for thicker samples. We have successfully employed the theory to study the effective-medium properties of both finite metallic wires and split ring resonators.

ACKNOWLEDGMENTS

We thank Professor P. Sheng and Professor C. T. Chan for many stimulating discussions. This work was supported by the China-973 Program (under Grant Nos. 2004CB719800 and 2006CB921701), the NSFC (under Grant No. 60725417), Shanghai science and technology committee, and PCSIRT. STC is supported by U.S. DOE.

APPENDIX: DERIVATION OF Eq. (8)

According to Ref. [26], Eq. (4) can be rewritten as

$$G(z,z') = G_0(z-z') + \int G_0(z-z_1)T(z_1,z_2)G_0(z_2-z')dz_1dz_2. \tag{A1}$$

Following Ref. [26], we need to perform configuration average for both $G(z,z')$ and $T(z_1,z_2)$. The configuration average is a necessary step in the homogenization, and includes: (a) average over all possible scatters; (b) average over different positions with the same source-detector distance. Consider that

$$G(z,z') = \int \frac{dk_1dk_2}{(2\pi)^2}G(k_1,k_2)e^{ik_1z}e^{-ik_2z'}$$
$$= \int \frac{dk_1dk_2}{(2\pi)^2}G(k_1,k_2)e^{i(k_1-k_2)Z}e^{i(k_1+k_2)\delta z/2}, \tag{A2}$$

Where $Z=(z+z')/2$, $\delta z=z-z'$, we find that averaging step (b) yields generally

$$G_c(z,z') = G_c(z-z') = \frac{1}{L}\int dZG(z,z')$$
$$= \frac{1}{L}\int \frac{dk}{2\pi}G_c(k,k)e^{ik(z-z')}. \tag{A3}$$

Here L is the total size of the studied system, which is a constant for normalization purpose only. Now that G_c is a function of δz only, we can define another quantity $G_c(k)$ such that

$$G_c(z-z') = \int \frac{dk}{2\pi}G_c(k)e^{ik(z-z')}/. \tag{A4}$$

Obviously, we get $G_c(k,k)=G_c(k)\cdot L$ by comparing Eq. (A3) with Eq. (A4). The same arguments apply to the T matrix and we get $T_c(k,k)=T_c(k)\cdot L$. Based on the Fourier-transformed form of Eqs. (5) and (6), we can easily find that

$$\sum(\omega,k) = T(k)[1+T(k)G_0(k)]^{-1}. \tag{A5}$$

In the weak-scattering limit, i.e., $T(k)G_0(k) \ll 1$, we finally get

$$\sum(\omega,k) \approx T(k) = T(k,k)/L. \tag{A6}$$

[1] D. R. Smith, W. J. Padilla, D. C. Vier, S. C. Nemat-Nasser, and S. Schultz, Phys. Rev. Lett. **84**, 4184 (2000).
[2] R. A. Shelby, D. R. Smith, and S. Schultz, Science **292**, 77 (2001).
[3] J. B. Pendry, Phys. Rev. Lett. **85**, 3966 (2000).
[4] J. B. Pendry, D. Schurig, and D. R. Smith, Science **312**, 1780 (2006).
[5] D. Schurig, J. J. Mock, B. J. Justice, S. A. Cummer, J. B. Pendry, A. F. Starr, and D. R. Smith, Science **314**, 977 (2006).
[6] L. D. Landau, E. M. Lifschitz, and L. P. Pitaevskii, *Electrodynamics of Continuous Media*, 2nd ed. (Pergamon, Oxford, 1984).
[7] J. B. Pendry, A. J. Holden, D. J. Robbins, and W. J. Stewart, IEEE Trans. Microwave Theory Tech. **47**, 2075 (1999).
[8] J. Baker-Jarvis, E. J. Vanzura, and W. A. Kissick, IEEE Trans. Microwave Theory Tech. **38**, 1096 (1990).
[9] D. R. Smith, S. Schultz, P. Markos, and C. M. Soukoulis, Phys. Rev. B **65**, 195104 (2002).
[10] P. Markos and C. M. Soukoulis, Opt. Express **11**, 649 (2003).
[11] D. R. Smith, D. C. Vier, T. Koschny, and C. M. Soukoulis, Phys. Rev. E **71**, 036617 (2005).
[12] X. Chen, B.-I. Wu, J. Au Kong, and T. M. Grzegorczyk, Phys. Rev. E **71**, 046610 (2005).
[13] O. Ouchetto, C. Qiu, S. Zouhdi, L. Li, and A. Razek, IEEE Trans. Microwave Theory Tech. **54**, 3893 (2006).
[14] L. Hou, J. Y. Chin, X. M. Yang, X. Q. Lin, R. Liu, F. Y. Xu, and T. J. Cui, J. Appl. Phys. **103**, 064904 (2008).
[15] D. R. Smith, D. C. Vier, N. Kroll, and S. Schultz, Appl. Phys. Lett. **77**, 2246 (2000).
[16] S. A. Cummer and B. I. Popa, Appl. Phys. Lett. **85**, 4564 (2004).
[17] B. Popa and S. A. Cummer, Phys. Rev. B **72**, 165102 (2005).
[18] D. R. Smith and J. B. Pendry, J. Opt. Soc. Am. B **23**, 391 (2006).
[19] M. Silveirinha, Phys. Rev. B **75**, 115104 (2007).
[20] Y. Wu, J. Li, Z. Q. Zhang, and C. T. Chan, Phys. Rev. B **74**, 085111 (2006).
[21] V. Fokin, M. Ambati, C. Sun, and X. Zhang, Phys. Rev. B **76**, 144302 (2007).
[22] S. T. Chui and Z. F. Lin, Phys. Rev. E **78**, 065601 (2008).
[23] See footnote [12] of J. Li, L. Zhou, C. T. Chan, and P. Sheng, Phys. Rev. Lett. **90**, 083901 (2003).
[24] C. Rockstuhl, T. Paul, F. Lederer, T. Pertsch, T. Zentgraf, T. P. Meyrath, and H. Giessen, Phys. Rev. B **77**, 035126 (2008).
[25] J. Zhou, T. Koschny, M. Kafesaki, and C. M. Soukoulis, Photonics Nanostruct. Fundam. Appl. **6**, 96 (2008).
[26] P. Sheng, *Introduction to Wave Scattering, Localization, and Mesoscopic Phenomena* (Academic Press, San Diego, 1995).
[27] T. Decoopman, G. Tayeb, S. Enoch, D. Maystre, and B. Gralak, Phys. Rev. Lett. **97**, 073905 (2006).
[28] One should redefine the metamaterial slab when calculating the effect parameters for another propagation direction.
[29] The configuration average is still meaningful even for a periodic metamaterial, since there are many different ways to realize the same configuration as shown in Fig. 1(a).
[30] G. D. Manhan, *Many Particle Physics* (Plenum, New York, 1990).
[31] J. M. Ziman, *Principles of the Theory of Solids*, 2nd ed. (Cambridge University Press, Cambridge, England, 1972).
[32] Comsol Multiphysics by COMSOL ©, ver. 3.5, network license (2008).
[33] Since the computations were rather time consuming, we only chose several typical values of μ_{ref} to calculate the DOS and MFP vs $\varepsilon_{\mathrm{ref}}$ in the regions far away from the highest peak of DOS. However, when approaching it, we have added much more μ_{ref} points to carefully identify the peak positions.
[34] Here, we set $\mu_{\mathrm{ref}}=\mu_{\mathrm{eff}}$ for each spectrum calculated at different frequencies.
[35] D. W. Shen, Y. Zhang, L. X. Yang, J. Wei, H. W. Ou, J. K. Dong, C. He, B. P. Xie, J. F. Zhao, B. Zhou, M. Arita, K. Shimada, H. Namatame, M. Taniguchi, J. Shi, and D. L. Feng, Phys. Rev. Lett. **101**, 226406 (2008).
[36] We note that typically only transmission spectrum is taken into account when one calculates the effective parameters in the standard retrieval method.
[37] Here, we set $\varepsilon_{\mathrm{ref}}=\varepsilon_{\mathrm{eff}}$ for each spectrum calculated at different frequencies.