Spatial dispersion in lattices of split ring resonators with permeability near zero

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We demonstrate that metamaterials formed by split ring resonators may exhibit strong spatial dispersion when the effective permeability is near zero. It is shown that the nonlocal effects can be characterized using a generalized Clausius-Mossotti formula. The proposed theory is verified using full wave simulations.

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Currently the most popular approach to create materials with a magnetic response is based on split ring resonators (SRRs). These particles are formed either by a pair of coplanar metallic rings,[1] or alternatively, in order to eliminate the bianisotropic response,[2] by two parallel rings (see Fig. 1). Lattices of SRRs are widely used as components of left-handed materials[3] and indefinite media.[4] Their response is usually assumed to be local. In this work, we demonstrate that orthorhombic and bcc lattices of SRRs cannot be described by local material parameters when the effective permeability is near zero. It is shown that in such regime it is necessary to take into account spatial dispersion effects in order to properly describe wave propagation. It is proven that such nonlocal effects can be characterized using a generalized Clausius-Mossotti (CM) formula with the interaction constant dependent on the wave vector.

Let us consider an orthorhombic lattice of SRRs (see Fig. 1), which traditionally is described as a uniaxial material with the effective parameters:

$$\bar{\bar{\varepsilon}} = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \bar{\bar{\mu}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mu \end{pmatrix}. \tag{1}$$

The magnetic response of a generic SRR can be characterized by the magnetic polarizability α, which relates the induced magnetic dipole moment m and the local induction field $\mathbf{B}_{\text{loc}}(\mathbf{r})$:

$$m = \alpha \langle B_{\text{loc},z} \rangle, \quad \alpha = \left[\left(\frac{\omega_r^2}{\omega^2} - 1 \right) \frac{L}{\mu_0 S^2} \right]^{-1}, \tag{2}$$

where $\langle B_{\text{loc},z} \rangle = \frac{1}{S} \int \mathbf{B}_{\text{loc}}(\mathbf{r}) . \mathbf{ds}$ represents the local field averaged over the area $S = \pi R^2$ of the SRR, $\omega_r = 1/\sqrt{LC}$ is the resonant frequency, and L and C are the self-inductance and capacitance given by:

$$C = \frac{\varepsilon_0 \pi R (\varphi - \pi)}{\cosh^{-1}\left(\frac{d^2}{2r^2} - 1 \right)}, \quad L = \mu_0 R \left[\ln\left(\frac{8R}{r} \right) - 2 \right]. \tag{3}$$

These parameters are obtained as in Ref. 5 but taking also into account the value of the ring angular width φ.

The classical CM formula yields the following estimation for the effective permeability:

$$\mu(\omega) = 1 + \frac{1}{a_z a^2} \frac{1}{\alpha^{-1}(\omega) - C}. \tag{4}$$

Here C is an interaction constant given explicitly in Ref. 6, p. 758. It is well-known that for a simple cubic lattice, $C = 1/3a^3$. Since the magnetic response can be enhanced by closely packing the inclusions, here we will consider an orthorhombic lattice such that $a_z = 0.5a$. In this case, the interaction constant is equal to $C = 3.1/a^3$. This classical interaction constant is obtained under the approximation that the local field is uniform and does not vary from cell to cell. Such approximation typically yields satisfactory results, especially in the long wavelength limit. However, in our previous work,[7] it was demonstrated that near a resonance the classical theory does not fully describe all the physics and phenomena. Here, we will demonstrate that a similar situation occurs when the effective permeability is near zero.

Following Ref. 7 the Clausius-Mossotti formula can be generalized to

$$\mu(\omega, \mathbf{k}) = 1 + \frac{1}{a_z a^2} \frac{1}{\alpha^{-1}(\omega) - C(\omega, \mathbf{k})}, \tag{5}$$

where $\mathbf{k} = (k_x, k_y, k_z)$ is the wave vector, and $C(\omega, \mathbf{k})$ is the spatially averaged (over the area of the SRR in the unit cell) zz component of the interaction dyadic $\bar{\bar{\mathbf{C}}}_{\text{int}}(\mathbf{r}; \omega, \mathbf{k})$ defined in Ref. 7.

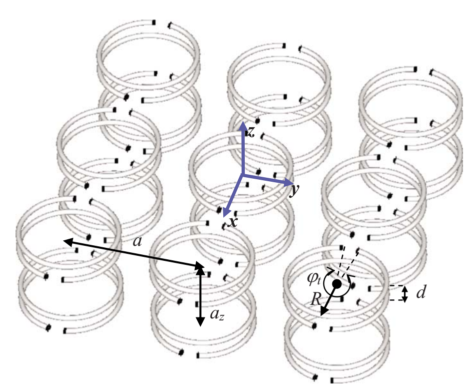

FIG. 1. (Color online) Geometry of an orthorhombic lattice $a \times a \times a_z$ of broadside coupled SRRs. Each ring covers an angular sector defined by the angle φ and has mean radius R. The rings are made of metallic wires with radius r. The mean distance between rings is d.

$$C(\omega,\mathbf{k}) = \frac{1}{\pi R^2}\int_S C_{\mathrm{int}}^{zz}(\mathbf{r};\omega,\mathbf{k})ds. \quad (6)$$

Unlike classical theory, the results of Ref. 7 fully take into account the dependence of the interaction constant on frequency and wave vector. Since the SRRs considered in this work are relatively large, the interaction constant is averaged over the area of the ring. In fact, for the lattices considered here, the interaction constant varies significantly over the unit cell and thus the approximation $\bar{\bar{\mathbf{C}}}_{\mathrm{int}}(\mathbf{r};\omega,\mathbf{k}) \approx \bar{\bar{\mathbf{C}}}_{\mathrm{int}}(0;\omega,\mathbf{k})$ used in Ref. 7 may be highly inaccurate for large rings.

In general, $C(\omega,\mathbf{k})$ has to be evaluated numerically for each $(\omega,\mathbf{k})$. Nevertheless, we found out that for lattices with $a_z < a$, $C(\omega,\mathbf{k})$ depends mainly on the parameters ω and k_z, and can be fairly well approximated by the analytical expression,

$$C(\omega,\mathbf{k}) \approx \left\{C_0 + C_1[\cos(k_z a_z) - 1] + C_2\left(\frac{\omega a}{c}\right)^2\right\}\frac{1}{a^3}, \quad (7)$$

where the constants C_0, C_1, and C_2 depend on the lattice structure and on the radius R of the SRRs. These constants can be determined numerically following ideas similar to those described in Ref. 7. For example, for an orthorhombic lattice with $a_z=0.5a$ and for SRRs with mean radius $R=0.4a$, it can be verified that $C_0=1.64$, $C_1=0.43$, and $C_2=-0.12$.

The value of the constants C_i $(i=1,2,3)$ may depend appreciably on the radius R of the particles. Indeed, for point particles with vanishingly small radius R, we obtain $C_0=3.1$, $C_1=1.7$, and $C_2=-0.07$. This significant dependence on R is a consequence of the local field varying very intensely near a lattice point for orthorhombic lattices with $a_z \ll a$, as mentioned before. Notice that for rings with very small radius, formula (5) reduces to the classical CM formula (4) when $\omega=0$ and $\mathbf{k}=0$.

The physical reason for the emergence of spatial dispersion is the intrinsic granularity of the composite material which may cause the dipole-like interactions (described by the interaction constant) to depend appreciably on the specific phase shift between adjacent particles. Notice that within the approximation (7), the permeability depends only on ω and k_z, and thus for propagation along directions parallel to the xoy plane the structured material has a local response.

In order to check the accuracy of the analytical model [Eq. (5)], we used the full wave homogenization method proposed in Ref. 8 to extract the effective parameters of a lattice of SRRs with the parameters indicated in the legend of Fig. 2. The extracted effective permeability (solid black line) and permittivity (solid dashed line) are depicted in Fig. 2 as a function of normalized frequency. The effective permeability has a resonance at $\omega a/c=0.76$. These local effective parameters are meaningful only when the spatial dispersion effects are weak. It is thus interesting to compare the extracted μ with the values predicted by the classical CM formula (solid red line) and the nonlocal homogenization model [Eq. (5)] (solid blue line). Figure 2 shows that the

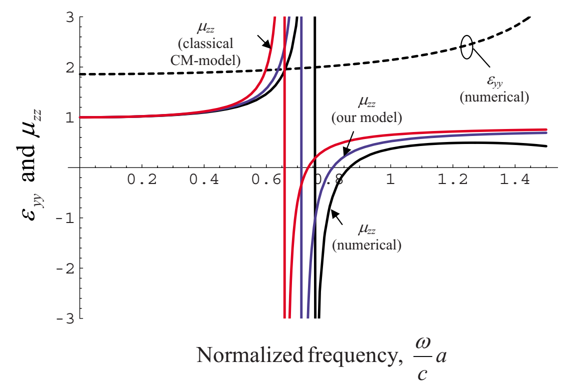

FIG. 2. (Color online) Effective permittivity and permeability of a lattice of SRRs with $r_w=0.005a$, $d=0.04a$, $\varphi=350°$, $R=0.4\ a$, and $a_z=0.5a$.

classical CM formula does not predict accurately the resonance frequency because it overestimates the interaction between the rings. The results obtained with our new model are significantly better.

To assess the effect of possible spatial dispersion effects, we have calculated the band structure of the material using the full wave hybrid plane-wave-integral-equation method proposed in Ref. 9 along the $Z\Gamma$ and ΓX segments of the Brillouin zone, where $X=(\pi/a,0,0)$ and $Z=(0,0,\pi/a_z)$. The dispersion diagram of the first few modes is shown in the left panel of Fig. 3 (solid black lines) and compared to results predicted by the nonlocal homogenization model [Eq. (5)] (solid blue lines) and by the CM-classical formula [Eq. (4)] (dashed green lines). These analytical results were obtained by solving the well-known dispersion equation for transverse electric (TE^z) waves in uniaxial media,

$$k_x^2 + k_y^2 + \mu k_z^2 = \varepsilon\mu\left(\frac{\omega}{c}\right)^2. \quad (8)$$

As illustrated in Fig. 2, the permittivity varies slowly in the considered frequency range, and thus for simplicity we have approximated it by its static value: $\varepsilon \approx 1.9$.

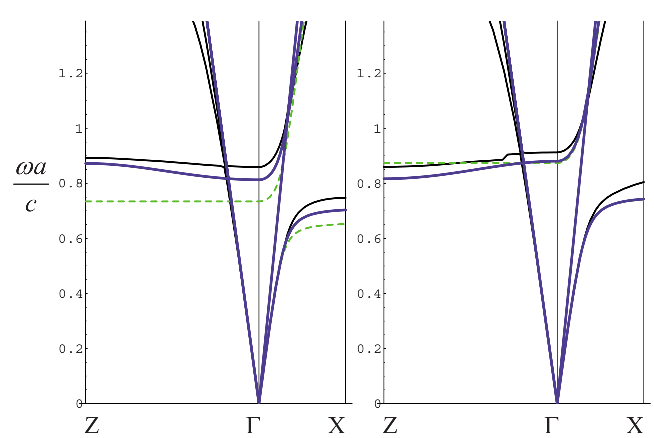

FIG. 3. (Color online) Left panel: Dispersion diagram for an orthorhombic lattice of SRRs. Right panel: Dispersion diagram for a bcc lattice of SRRs. The SRRs have the same parameters as in Fig. 2. Dashed (green/light gray) lines: CM-classical model. Solid (thick) blue/dark gray lines: nonlocal homogenization model. Solid (thin) black lines: full wave simulations.

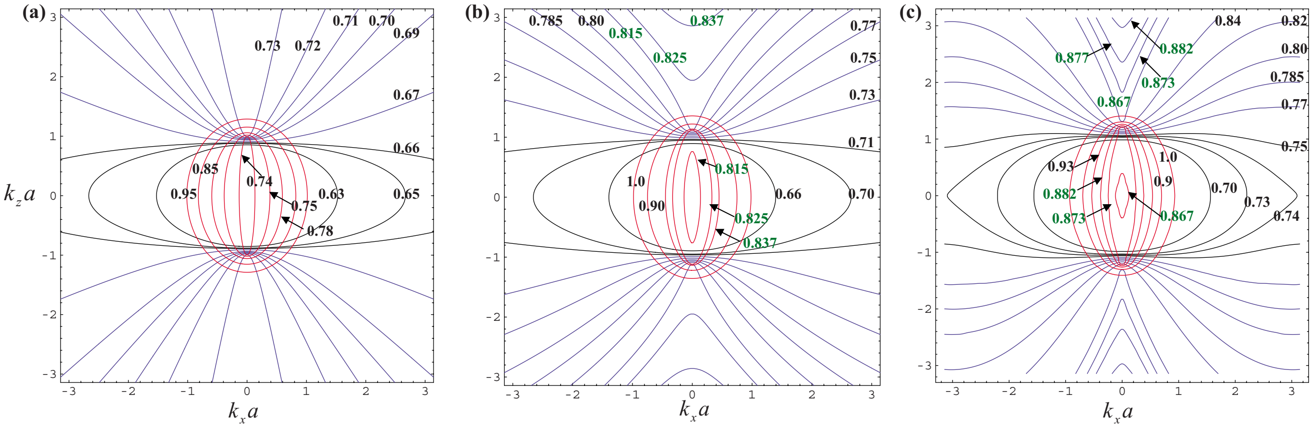

FIG. 4. (Color online) Isofrequency contours for an orthorhombic lattice of SRRs with the same parameters as in Fig. 2: (a) local model, (b) nonlocal model, and (c) full wave simulation. The insets indicate the value of the corresponding normalized frequency $\omega a/c$.

As seen in Fig. 3, a good qualitative agreement is obtained between our nonlocal homogenization model and the full wave results. Apart from the shift of the resonance frequency, the main difference between the classical CM theory and the nonlocal homogenization results is the nearly flat line in the $Z\Gamma$ segment. It can be easily verified from Eq. (8) that this line corresponds to longitudinal modes (magnetic field is along the direction of propagation z) with the dispersion characteristic $\mu=0$. The classical model [Eq. (4)] predicts that the dispersion relation of these modes is completely flat, since μ does not depend on the wave vector. In a different manner, the nonlocal model [Eq. (5)] predicts that the band associated with longitudinal modes has a positive slope. This is consistent with the full wave results (solid black lines), even though the full wave results predict a slightly smaller slope than that yielded by our homogenization model. These results indicate that spatial dispersion effects may be important at the plasma frequency for which $\mu=0$, especially for propagation along directions close to the z axis.

In order to further investigate these effects, we have calculated the isofrequency contours in the plane $X\Gamma Z$ (Fig. 4). The insets in the graphics indicate the values of the associated normalized frequency $\omega a/c$. Panel (a) shows the contours predicted by the classical CM model. For frequencies below the resonance frequency the contours are elliptic (black contours, e.g., $\omega a/c=0.63$). For frequencies very close to the resonance ($\mu=\infty$), the contours are nearly flat (e.g., $\omega a/c=0.66$). Above the resonance the effective permeability becomes negative and the medium is indefinite with hyperbolic contours (blue contours). As the effective permeability approaches zero, the asymptotes of the hyperbolas are closer and closer to the z axis, and when the permeability is exactly zero the dispersion contour collapses into the z axis. For frequencies corresponding to permeability values above zero (red contours, e.g., $\omega a/c=0.74$), the contours become again elliptic.

It is interesting to compare the isofrequency contours predicted by the classical CM model, with the results obtained using the nonlocal theory [panel (b) of Fig. 4]. A simple inspection of the two plots shows that the isofrequency contours are completely different for frequencies in the range $0.80<\omega a/c<0.90$, i.e., for frequencies such that $\mu\approx 0$. In particular the contours associated with the green insets ($\omega a/c=0.815, 0.825, 0.837$) are neither elliptic nor hyperbolic, but instead have both elliptic and hyperbolic components. This indicates that at these frequencies two different eigenwaves with the same (TE^z) polarization can propagate in the material. This phenomenon was originally reported in Ref. 10 and is a consequence of the nonlocal material response. It is important to underline that in general the modes associated with these contours are not longitudinal, and thus it is expected that both modes can be excited in typical configurations, as the analysis of Ref. 11 suggests.

The described results are completely consistent with full wave simulations[9] [panel (c) in Fig. 4]. In fact, apart from a slight difference between the frequency values associated with contours, the qualitative variation with frequency of the contours of panels (b) and (c) is very similar. This confirms the existence of significant spatial dispersion effects in metamaterials formed by SRRs. Our simulations (not shown here) indicate that these effects are increasingly important when a_z/a is decreased. On the other hand, for very long wavelengths $a/\lambda \ll 0.1$, the effects of spatial dispersion may become less relevant because the interaction constant becomes independent of k_z in the limit $a\to 0$ and thus the material response may become nearly independent of the wave vector, even for values of $k_z c/\omega$ that are relatively large. However, in practice it is extremely difficult to design SRRs with a sufficiently high capacitance that may enable a strong magnetic response at the required low values of a/λ, particularly at the infrared and optical regimes.

We have also analyzed the effect of shifting adjacent planes of SRRs by the half-lattice constant along the x- and y-directions, so that the primitive vectors of the lattice become $\mathbf{a}_1=(1,0,0)a$, $\mathbf{a}_2=(0,1,0)a$, and $\mathbf{a}_3=(0.5,0.5,0.5)a$. It can be verified that for such primitive vectors the particles are packed into a bcc lattice. The classical interaction constant for point particles arranged into a bcc lattice is $C=1/(3V_{\text{cell}})=0.67/a^3$, where $V_{\text{cell}}=0.5a^3$ is the volume of the unit cell. On the other hand, for SRRs with radius $R=0.4a$, our theory predicts that the averaged interaction constant is described to a first approximation by Eq. (7) with $C_0=0.72$, $C_1=-0.45$, and $C_2=-0.17$. Notice that the coefficient C_1, which describes the effects of spatial dispersion, has a differ-

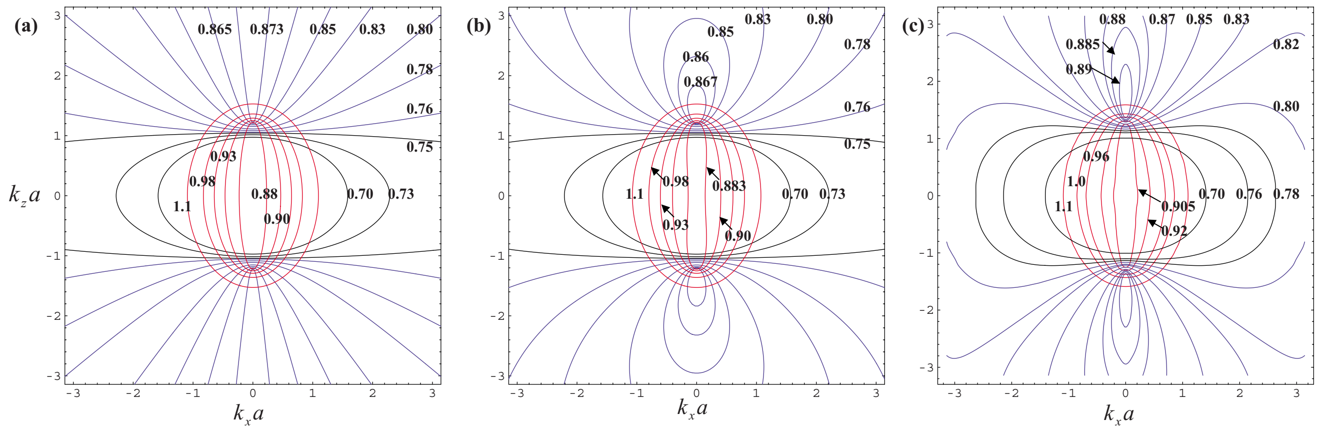

FIG. 5. (Color online) Isofrequency contours for a bcc lattice of SRRs: (a) local model, (b) nonlocal model, and (c) full wave simulation. The insets indicate the value of the corresponding normalized frequency $\omega a/c$.

ent sign as compared to the coefficient C_1 associated with the orthorhombic lattice considered previously. This change of sign has an important consequence: The longitudinal modes become backward waves. This phenomenon is clear from the band structure diagram in the right-hand side panel of Fig. 3 and is also completely supported by full wave simulations.

It is also evident from Fig. 3 that the classical CM model is more accurate for a bcc lattice than for an orthorhombic lattice, predicting almost exactly the resonance and plasma frequencies of the material. In fact, for a bcc lattice, the classical value of C is almost coincident with the value of C_0 given by our nonlocal model, showing that the despite the large diameter of the rings, the SRRs can be accurately modeled as point particles.

The isofrequency contours for the bcc lattice are depicted in Fig. 5. It is remarkable how different the contours are as compared to the orthorhombic case. Indeed, slightly below the plasma frequency the hyperbolic contours become ellipses that shrink into a point as $\mu \to 0^-$ and transform into a line segment when $\mu=0^+$. When the permeability becomes slightly positive, $\mu=0^+$, the isofrequency contours are very similar to those predicted by the classical local model. Thus, for a bcc lattice the spatial dispersion effects seem to be more important in the regime where the structure behaves as an indefinite medium $\mu<0$, being not so relevant when $\mu>0$. In particular, unlike in the case of an orthorhombic lattice, in the regime $\mu>0$ only a single propagating mode can be excited. This suggests that the increased symmetry of the bcc lattice may help to some extent to make the response of the material local.

In conclusion, it was demonstrated that metamaterials formed by magnetic scatterers may suffer from strong spatial dispersion in the regime where μ is near zero. Such effects can be accurately described by a generalized Clausius-Mossotti formula. These findings are confirmed by full wave simulations.

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[1] J. Pendry, A. Holden, D. Robbins, and W. Stewart, IEEE Trans. Microwave Theory Tech. **47**, 2075 (1999).
[2] R. Marqués, F. Medina, and R. Rafii-El-Idrissi, Phys. Rev. B **65**, 144440 (2002).
[3] D. R. Smith, W. J. Padilla, D. C. Vier, S. C. Nemat-Nasser, and S. Schultz, Phys. Rev. Lett. **84**, 4184 (2000).
[4] D. R. Smith and D. Schurig, Phys. Rev. Lett. **90**, 077405 (2003).
[5] J. D. Baena, L. Jelinek, R. Marqués, and M. Silveirinha, arXiv:0711.4215 (unpublished).
[6] R. Collin, *Field Theory of Guided Waves* (IEEE, Piscataway, NJ, 1990).
[7] M. G. Silveirinha, Phys. Rev. B **76**, 245117 (2007).
[8] M. G. Silveirinha, Phys. Rev. B **75**, 115104 (2007).
[9] M. G. Silveirinha and C. A. Fernandes, IEEE Trans. Microwave Theory Tech. **52**, 889 (2004).
[10] P. A. Belov and C. R. Simovski, Phys. Rev. E **72**, 026615 (2005).
[11] A. B. Kozyrev, C. Qin, I. V. Shadrivov, Y. S. Kivshar, I. L. Chuang, and D. W. van der Weide, Opt. Express **15**, 11714 (2007).