

**QUASI-SEPARABLE T-SCATTERING OPERATOR APPROACH
TO LOCAL FIELD DIRECT CALCULATIONS
IN MULTIPLE SCATTERING PROBLEMS**

Yu. N. Barabanenkov¹, M. Yu. Barabanenkov²

¹ **V.A. Kotelnikov Institute of Radioengineering and Electronics of RAS, Moscow**

² **Institute of Microelectronics Technology of RAS, Chernogolovka, Moscow Region**

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Abstract. We present analytic solution to fundamental in wave multiple scattering theory Lippmann-Schwinger (LS) integral equation for electric field quantum mechanical type tensor T- scattering operator by nonmagnetic arbitrary shaped particle with given scalar dielectric permittivity and specific conductivity in free space. The solution is obtained with the aid of a vector expansion functions' basis and Galerkin method and written as sum of separable scattering operators weighted by inverse of a generating matrix, which is expressed through matrix describing wave coupling between the particle elements. Similar quasi-separable (QS) form is obtained for T-scattering operator of coupled particles' ensemble, when generating matrix is related with matrix describing wave coupling between particles; an equations' system for self consistent currents excited inside coupled particles is derived on this way also. Having given directly the current excited inside particle, T-scattering operator should be closed connected with wave spatial dispersion effect in homogenized electromagnetic crystal structure. Really, we show the rigorously defined a periodic structure effective dielectric permittivity tensor is exactly expressed by unit cell QS T- scattering operator, with generating matrix related to matrix of wave coupling between unit cell particles directly and via crystal. In order to test and apply the QS T-scattering operator approach, some different choosing the vector expansion functions are considered. In the case of vector spherical wave functions' basis the QS T-scattering operator gives the Mie solution for incident plane wave scattering from and transmitted into a spherical particle. The another

basis vector expansion functions defined on finite elements of particle volume is consistent with QS approximation of particle scattering potential operator, for which the LS equation is resolved exactly. Next, an asymptotic formula is obtained for contribution of spatially resonant coupling between two small spherical plasmonic particles inside unit cell of electromagnetic crystal into the structure effective magnetic permeability. We study at last some simple low dimensional ordered periodic arrays of particles, with particles' coupling matrix obeying a stochastic property for the case of specifically linearly polarized wave electric field, and find corresponding stochastic and overtone eigenmodes and method of their excitation. Exact and asymptotic formulas are found also for standing and propagating wave transfer of currents' exciting along a strait linear chain of particles with Jacobi's coupling matrix.

Keywords: electromagnetic wave field, arbitrary shaped nonmagnetic coupled particles, multiple scattering, T-scattering operator, Lippmann-Schwinger integral equation, analytic solution, currents excited inside particles, electromagnetic crystal structures, low dimension arrays of particles.

1. Introduction

Theory of electromagnetic waves' multiple scattering by dielectric and conducting nonmagnetic particles appears at present as tool for numerous studies of artificial materials and especially of microsized particles' assemblies, which are useful in variety of optical applications because of their resonant interaction with a visible and infrared light. Between these studies there are the following interesting examples. Microstructured periodic materials known as "metamaterials", with negative effective dielectric permittivity and/or negative effective magnetic permeability being derived either by spatially averaging the Maxwell equations on base of a self-consistent rigorous approach[1]or via so called full-wave dispersion relation [2,3] describing small nanoparticles in terms of their dipolar polarizability and using the local field approach. Contribution of coupled magnetic dipole

resonances in small dielectric spheres' clusters into the effective permittivity and permeability, being evaluated with the aid of classical Clausius-Mossotti homogenization formula [4]. Previously space-group resonance in clusters of nonresonant particles was considered [5, 6]. The coupling between optical waveguides and high-quality resonators, which can be created within a photonic crystal structure with modified some unit cells [7]. High quality optical modes in low dimensional arrays of dielectric nanoparticles studies within the coupled dipole approach [8, 9]. Earlier similar modes were studied in theory of coupled parallel antennas [10].

Turn directly to main subject of our paper concerning with itself theory of electromagnetic waves' multiple scattering by dielectric and conducting particles. This theory can be started with Lippmann-Schwinger (LS) integral equation for electric wave field tensor (dyadic) T- scattering operator by a particle, written similarly to the quantum mechanical case [11-14]. Having given directly the field and current excited inside a particle [15] as well as the field scattered by the particle, the T-scattering operator technique has been applying successfully for a long time. As early as 1967, a derivation was proposed [16] (see also [17,18]) of the phenomenological radiative transfer equation in a discrete randomly inhomogeneous medium, with due regard for correlation of particles in all orders and wave coupling between particles within the same cluster of particles. The Dyson and Bethe-Salpeter equations were used in the single- group approximation. Latter there were derived [19] exact self-consistent Dyson and Bethe-Salpeter equations (relations) for evaluating the ensemble averaged wave electric field and coherence function of wave electric field inside dense discrete random media, with random mass and intensity operators having been under averaging sign and written in terms of the particles' correlations functions of all orders and particles' clusters random group T-scattering operators. A group T-scattering operator was constructed via special group operation from T-scattering operators of cluster particles, with T-scattering operator of a particle set having been satisfied a self consistent LS equation, integral term of which

included exact random Green function and described particle coupling via the random medium. These self-consistent Dyson and Bethe-Salpeter equations gave all known approximations for wave multiple scattering in random media including the single group approximation. Ward-Takahashi identity for two-frequency combination of T-scattering operators was proved [20] to derive the radiative transfer equation with time delay via effect of pulse entrapping in a resonant random media. Mentioned above [7] scattering theory analysis of waveguide-resonator coupling was based on T-scattering operator, actually. Artificial magnetism in theory of wave multiple scattering by random discrete nonmagnetic conducting media [21] was considered with the aid of Dyson equation technique and generalized Lorentz –Lorenz formula including the Fourier transform of T-scattering operator of a particle. Referred to metamaterial effective permittivity derivation by spatially averaging the Maxwell equations [1] was performed with the aid of Lippmann-Schwinger integral equation for electric wave field inside periodic media that directly connected , actually, to a T-scattering operator of a periodically structure cell. Recently [22] the T-scattering operator technique was used to phenomenon study of virtual singular scattering of electromagnetic wave on a dielectric scatterer embedded into a flat left handed material slab (Veselago lens). Watson composition rule [12,17] of T-scattering operators was reformulated [23] in terms of virtual splitting the volume or surface inhomogeneous dielectric structure into a stack of elementary layers and the system of recurrent equations of invariant imbedding method [24] type obtained for changing the reflection and transmission coefficients of stack of N layers at (N+1)-st layer attachment.

Despite of enumerated T-scattering operator direct applications, to the best of our knowledge, there is no still sufficient attention on systematic method of solution to LS equation for this operator and instead that the Waterman transition matrix [14, 25-27] in the form, as one can verify, a simple combination from electric wave field dyadic Green function in free space and T-scattering operator widely has been using. The transition matrix technique expands the incident and the scattered

electromagnetic waves by a particle in vector spherical wave functions, with expressing the expanding coefficients of scattered wave through the expanding coefficients of incident wave with the aid of the transition matrix. As making so, the transition matrix is written with the help of the extended boundary condition technique in terms of surface integrals from vector spherical functions' bilinear combinations along the particle surface. A substantial progress has been achieved during last one and half decade in the form of new recursive transition matrix method for calculating local electromagnetic fields inside of spheres, system of which is subject to strong dependent scattering [28,29]. Though this achieving, the transition matrix technique needs in some improvement at present that is returning our attention to T-scattering operator. Really, using the spherical wave functions in the case of particles with complicate shape becomes nonrational, evidently. T-scattering operator gives directly the field inside a particle, whereas the transition matrix technique implies additional application of Mie internal field coefficients for evaluating the field in the interior of a particle [29]. Application the transition matrix technique can be difficult for rigorous evaluating an electromagnetic crystal structure effective dielectric permittivity [1] that directly connected with T-scattering operator of the structure unit cell.

The aim of our paper consists in considering a systematic method on practical solution to LS equation for electric wave field dyadic T-scattering operator in the form of quasi-separable (QS) approach. This approach adopted from the quantum mechanical scattering potential approximation as sum of separable potentials in nuclear physics [30]. In electromagnetics the separable approximation for small particle scattering potential was used at study the radiative transfer with time delay via effect of pulse entrapping in resonant random media [20] as well as the wave virtual singular scattering by scatterer inside Veselago lens [22]. We apply a vector expansion functions' basis and Galerkin technique [28,31,32] exploited [1] to evaluate a metamaterial effective dielectric permittivity and employ by us to solve the LS equation for dyadic T-scattering operator in QS form as sum of separable

scattering operators weighted by inverse of a generating matrix, which is expressed through wave coupling between the particle elements' matrix. One can apply various vector expansion functions' bases. In the case of vector spherical wave functions the QS T- scattering operator gives the well known Mie solution for incident plane wave scattering from and transmitted into a spherical particle. We show that a basis vector expansion functions defined on finite elements of particle volume in spirit of general finite element method [33] and used more earlier by Haar [34] enables one to verify that QS T-scattering operator corresponds really to a QS approximation of particle scattering potential operator, for which the LS equation is resolved exactly. Next our goal consists in constructing the QS T-scattering operator for coupled particles' ensemble with generating matrix related with wave coupling between particles, that we make by exact solving the Watson composition rule [12] of T-scattering operators. On this way we exploit the invariant imbedding method idea [23,24] to a recursive procedure creation for QS T- scattering operator generating matrix inversion, by attaching to N coupled particles a (N+1)-st particle and using the Frobenius formula [35] for inversion of 2×2 block's matrix. Side by side with this recursive procedure for inversion of the QS-T-scattering operator generating matrix, we consider an equations' system for self consistent currents excited inside coupled particles and apply this system to study new effects for some simple low dimensional ordered particles' arrays in the form of periodic polygon chain [9,10] as well as strait linear chain [3]. We show the particles' coupling matrix of periodic polygon chain obeys a stochastic property [35] and find corresponding stochastic eigenmodes and overtone ones and method of their excitation. For strait linear chain [3] with Jacobi's particles' coupling matrix rising to Rayleigh's book [36] yet we derive exact and asymptotic formulas for standing and propagating wave transfer of currents' exciting along the strait linear chain. Our last general result concerns the deriving an electromagnetic crystal structure unit cell QS T-scattering operator, with generating matrix related with matrix of wave coupling between the unit cell particles directly and via crystal electric field dyadic Green function. This QS T-scattering operator we

apply to analytic consideration of space–group resonance effect [5,6] between the unit cell small plasmonic particles contribution into the structure effective magnetic permeability, without applying a priory of Clausius-Mossotti homogenization formula.

The organization of the paper is as follows. In Section 2 the starting LS equation for dyadic T-scattering operator of a particle is resolved in QS form. Section 3 contains deriving the QS T-scattering operator for ensemble of N coupled particles, by resolving the Watson composition rule of T-scattering operators. The recursive procedure for QS T-scattering operator generating matrix inversion is created in Section 4. Section 5 includes consideration an equations' system for self consistent currents excited inside ensemble of coupled particles The QS T-scattering operator for electromagnetic crystal unit cell is derived in Section 6, with getting an exact formula for metamaterial effective dielectric permittivity in terms of the unit cell QS T-scattering operator. Applications of the QS T–scattering operator are placed in the Section 7. In Section 8 we conclude. Appendices A, B and C consist of details related to spherical particle QS T-scattering operator generating matrix, finite element vector expansions' functions and strait linear chain with Jacobi's particles' coupling matrix, respectively. Some preliminary results of this paper were reported to recent PIERS symposium [37].

2. Quasi-separable T-scattering operator of particle in free space

2.1. Lippmann-Schwinger equation

We start with Lippmann-Schwinger (LS) integral equation for total electric field $\vec{E}(\vec{r})$ of monochromatic electromagnetic wave outside and inside of a nonmagnetic particle with given scalar dielectric permittivity $\mathcal{E}(\vec{r})$ and specific conductivity $\sigma(\vec{r})$, the particle being placed in homogeneous nonmagnetic background (free space) with dielectric permittivity ϵ_0 and the electromagnetic field

source volume current density $\vec{j}^{src}(\vec{r})$. The LS equation for the total electric field has in dyadic denotation form

$$\vec{E}(\vec{r}) = \vec{E}^{(0)}(\vec{r}) + \int d\vec{r}' \overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}') V(\vec{r}') \vec{E}(\vec{r}') \quad (1)$$

Here $\vec{E}^{(0)}(\vec{r})$ denotes the incident on particle electric field given by

$$\vec{E}^{(0)}(\vec{r}) = \frac{4\pi\omega}{ic^2} \int d\vec{r}' \overline{\overline{G}}^{(0)}(\vec{r}, \vec{r}') \vec{j}^{src}(\vec{r}') \quad (2)$$

The symbol $\overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}')$ denotes the electric field dyadic Green function in free space of a form

$$\overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}') = \left(\overline{\overline{I}} + \frac{1}{k_0^2} \nabla \nabla \right) G_0(\vec{r} - \vec{r}') \quad (3)$$

with $\overline{\overline{I}}$ and $k_0 = (\omega/c) \epsilon_0^{1/2}$ and $G_0(r) = \exp(ik_0 r)/(-4\pi r)$ being the unit dyad and free space wave number and free space scalar Green function, respectively. The quantity $V(\vec{r})$ is named as particle scattering potential and defined in terms of particle complex permittivity $\hat{\epsilon} = \epsilon + i(4\pi\sigma/\omega)$ by $V(\vec{r}) = -\frac{\omega^2}{c^2}(\hat{\epsilon} - \epsilon_0)$. The

Gaussian system of units is used and c denotes the light speed in vacuum and ω denotes wave frequency. The magnetic permeability is supposed to be $\mu = 1$ everywhere. The LS-equation derivation from Maxwell equations has been given in [14,38] with the aid of vector Green theorem and accounting the boundary conditions.

Solution to the LS equation (1) for total electric field is written in terms of dyadic T-scattering operator as

$$\vec{E}(\vec{r}) = \vec{E}^{(0)}(\vec{r}) + \int d\vec{r}' \int d\vec{r}'' \overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}') \overline{\overline{T}}(\vec{r}', \vec{r}'') \vec{E}^{(0)}(\vec{r}'') \quad (4)$$

Comparison of this equality with integral Eq. (1) gives LS integral equation for T-scattering operator

$$\bar{\bar{T}}(\vec{r}, \vec{r}') = V(\vec{r}) \bar{\bar{I}} \delta(\vec{r} - \vec{r}') + V(\vec{r}) \int d\vec{r}'' \bar{\bar{G}}^{(0)}(\vec{r} - \vec{r}'') \bar{\bar{T}}(\vec{r}'', \vec{r}') \quad (5)$$

From equations (1) and (5) one gets [15] the following physically transparent relations

$$\begin{aligned} \vec{J}(\vec{r}) = V(\vec{r}) \vec{E}(\vec{r}) &\equiv \frac{4\pi\omega}{ic^2} \left[\sigma + \frac{\omega}{4\pi i} (\hat{\epsilon} - \epsilon_0) \right] \vec{E}(\vec{r}) \equiv \frac{4\pi\omega}{ic^2} \vec{j}(\vec{r}) \\ &= \int d\vec{r}' \bar{\bar{T}}(\vec{r}, \vec{r}') \vec{E}^{(0)}(\vec{r}') \\ \nabla \vec{J}(\vec{r}) &= 0 \end{aligned} \quad (6)$$

These relations show that one can evaluate the total electric field $\vec{E}(\vec{r})$ as well as the complete current $\vec{j}(\vec{r})$ excited inside particle, having known the particle T-scattering operator. We see also from Eq. (4) that convolution $\bar{\bar{G}}^{(0)} \bar{\bar{T}}$ of the electric wave field dyadic Green function in free space with T-scattering operator gives, actually, the Waterman transition matrix [14, 25-27]. The last divergence Eq.(6) imposes a solenoidal restriction on T-scattering operator, provided the complex dielectric permittivity has constant value inside particle.

2.2. Quasi-separable solution to Lippmann-Schwinger equation

Let us apply to solution of LS integral equation (5) for T-scattering operator a Galerkin technique [1,28,]. With this aim we choose a vector expansion functions' basis $\vec{t}_n(\vec{r})$, $n=1,2,3,\dots$. Dividing dyadic Eq.(5) by potential $V(\vec{r})$ and multiplying result on vector $\vec{t}_n(\vec{r})$ from the left side and integrating with respect to \vec{r} gives

$$\int d\vec{r} \frac{1}{V(\vec{r})} \vec{t}_n(\vec{r}) \bar{\bar{T}}(\vec{r}, \vec{r}') = \vec{t}_n(\vec{r}') + \int d\vec{r} \int d\vec{r}'' \vec{t}_n(\vec{r}) \bar{\bar{G}}^{(0)}(\vec{r} - \vec{r}'') \bar{\bar{T}}(\vec{r}'', \vec{r}') \quad (7)$$

We seek a solution to obtained equation in a form of dyadic expansion

$$\bar{\bar{T}}(\vec{r}, \vec{r}') = \sum_n \vec{t}_n(\vec{r}) \otimes \vec{t}_n(\vec{r}') \quad (8)$$

with $\tilde{t}_n(\vec{r}')$ being a set of unknown vectors and symbol \otimes denoting the dyadic product of two vectors. Substituting (8) into Eq. (7) leads to an algebraic equations' system for unknown vectors

$$\sum_m \langle n | \chi^{(0)} | m \rangle \tilde{t}_m(\vec{r}') = \vec{t}_n(\vec{r}') \quad (9)$$

The generating matrix $\langle n | \chi^{(0)} | m \rangle$ under left hand side (LHS) sum of Eq. (9) is defined by expression of two terms

$$\langle n | \chi^{(0)} | m \rangle = \int d\vec{r} \frac{1}{V(\vec{r})} \vec{t}_n(\vec{r}) \vec{t}_m(\vec{r}) - \langle n | g^{(0)} | m \rangle \quad (10)$$

the second of which describes wave coupling between the particle elements in free space according to

$$\langle n | g^{(0)} | m \rangle = \int d\vec{r} \int d\vec{r}' \vec{t}_n(\vec{r}) \overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}') \vec{t}_m(\vec{r}') \quad (11)$$

Resolving equations' system (9) with the aid of inverse matrix $\langle n | \chi^{(0)-1} | m \rangle$ as

$$\tilde{t}_n(\vec{r}') = \sum_m \langle n | \chi^{(0)-1} | m \rangle \vec{t}_m(\vec{r}') \quad (12)$$

and substituting the resolution result into dyadic expansion (8) right hand side (RHS) leads us to quasi-separable (QS) solution to LS integral equation (5) for T-scattering operator of a particle $\overline{\overline{T}}^{(0)}(\vec{r}, \vec{r}')$ in free space

$$\overline{\overline{T}}^{(0)}(\vec{r}, \vec{r}') = \sum_{nm} \langle n | \chi^{(0)-1} | m \rangle \vec{t}_n(\vec{r}) \otimes \vec{t}_m(\vec{r}') \quad (13)$$

The reciprocity of the electric field dyadic Green function in free space $\overline{\overline{G}}^{(0)}(\vec{r}, \vec{r}') = \overline{\overline{G}}^{(0)t}(\vec{r}', \vec{r})$ where the superscript t refers to the transpose dyadic, leads to the symmetrical property of the particle coupling matrix elements $\langle n | g^{(0)} | m \rangle = \langle m | g^{(0)} | n \rangle$ and the generating matrix $\langle n | \chi^{(0)} | m \rangle = \langle m | \chi^{(0)} | n \rangle$. The inverse matrix

symmetry property $\langle n | \mathcal{X}^{(0)-1} | m \rangle = \langle m | \mathcal{X}^{(0)-1} | n \rangle$ agrees with the T-scattering operator reciprocity $\overline{\overline{T}}^{(0)}(\vec{r}, \vec{r}') = \overline{\overline{T}}^{(0)t}(\vec{r}', \vec{r})$.

3. Quasi-separable T-scattering operator of particle's ensemble in free space

Having obtained QS T-scattering operator (13) of a single particle, one can get automatically QS T-scattering operator of N coupled particles' ensemble, with their centers being placed at $\vec{r}_1, \dots, \vec{r}_N$ points. To this end we start with Watson composition rule [12] for T-scattering operators in a form

$$\overline{\overline{T}}(\vec{r}, \vec{r}') = \sum_{j=1}^N \overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}') \quad (14)$$

and

$$\begin{aligned} \overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}') &= \overline{\overline{T}}^{(0)}(\vec{r} - \vec{r}_j, \vec{r}' - \vec{r}_j) \\ &+ \int d\vec{r}'' \int d\vec{r}''' \overline{\overline{T}}^{(0)}(\vec{r} - \vec{r}_j, \vec{r}'' - \vec{r}_j) \overline{\overline{G}}^{(0)}(\vec{r}'' - \vec{r}''') \sum_{j' \neq j} \overline{\overline{T}}^{(j')}(\vec{r}''', \vec{r}') \end{aligned} \quad (15)$$

Here $\overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}')$ and $\overline{\overline{T}}^{(0)}(\vec{r} - \vec{r}_j, \vec{r}' - \vec{r}_j)$ are self consistent and single T-scattering operators of ensemble j -th particle, respectively.

Substituting QS T-scattering operators (13) into Eqs. (15) RHS leads to exact solution of this equations' system. We seek such solution in a form of dyadic expansion

$$\overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}') = \sum_n \vec{t}_n(\vec{r} - \vec{r}_j) \otimes \tilde{\overline{\overline{T}}}_n^{(j)}(\vec{r}') \quad (16)$$

similar to (8). For unknown vectors $\tilde{\overline{\overline{T}}}_n^{(j)}(\vec{r}')$, $j=1, \dots, N$, one gets an equations' system

$$\tilde{T}_n^{(j)}(\vec{r}') = \tilde{t}_n(\vec{r}' - \vec{r}_j) + \sum_m \sum_{j' \neq j} \langle nj | \tilde{g}^{(0)} | mj' \rangle \tilde{T}_m^{(j')}(\vec{r}') \quad (17)$$

with inhomogeneous terms being defined by (12) and matrix elements under double sum given by

$$\langle nj | \tilde{g}^{(0)} | mj' \rangle = \sum_{m'} \langle n | \chi_1^{(0)-1} | m' \rangle \langle m' j | g^{(0)} | mj' \rangle \quad (18)$$

where the matrix of particles' coupling

$$\langle nj | g^{(0)} | mj' \rangle = \int d\vec{r} \int d\vec{r}' \tilde{t}_n(\vec{r} - \vec{r}_j) \overline{G}^{(0)}(\vec{r} - \vec{r}') \tilde{t}_m(\vec{r}' - \vec{r}_{j'}) \quad (19)$$

is similar to (11). The quantity $\chi_1^{(0)}$ denotes the generating matrix (10) of single particle.

The dyadic expansion (16) and relations (6) show that Eqs.(17) system is basic one to evaluate the total electric fields and complete currents excited inside coupled particles. To avoid in the second sum of Eqs.(17) system RHS restriction $j' \neq j$ one can put conditionally $\langle nj | \tilde{g}^{(0)} | mj' \rangle = 0$ if $j = j'$ and introduce next unit matrix $\langle nj | I | mj' \rangle = \delta_{nm} \delta_{jj'}$ and matrix A_N with elements

$$\langle nj | A_N | mj' \rangle = \langle nj | I | mj' \rangle - \langle nj | \tilde{g}^{(0)} | mj' \rangle \quad (20)$$

that is the Eqs. (17) system matrix. With the aid of resolvent matrix $R_N = A_N^{-1}$ the solution to Eqs. (17) system is written as

$$\tilde{T}_n^{(j)}(\vec{r}') = \sum_{mj'} \langle nj | R_N | mj' \rangle \tilde{t}_m(\vec{r}' - \vec{r}_{j'}) \quad (21)$$

Substituting this solution into dyadic expansion (16) RHS and denoting

$$\langle nj | \chi_N^{(0)-1} | mj' \rangle = \sum_{m'} \langle nj | R_N | m' j' \rangle \langle m' | \chi_1^{(0)-1} | m \rangle \quad (22)$$

gives the self consistent T-scattering operator of ensemble j th particle

$$\overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}') = \sum_{nmj'} \langle nj | \chi_N^{(0)-1} | mj' \rangle \vec{t}_n(\vec{r} - \vec{r}_j) \otimes \vec{t}_m(\vec{r}' - \vec{r}_{j'}) \quad (23)$$

The last step with using the Eq. (14) leads to desired QS T-scattering operator of particles' ensemble in free space

$$\overline{\overline{T}}(\vec{r}, \vec{r}') = \sum_{nmj'} \langle nj | \chi_N^{(0)-1} | mj' \rangle \vec{t}_n(\vec{r} - \vec{r}_j) \otimes \vec{t}_m(\vec{r}' - \vec{r}_{j'}) \quad (24)$$

The inverse $\langle nj | \chi_N^{(0)} | mj' \rangle$ to the matrix (22) is the generating matrix for N coupled particles' ensemble.

Note while particles' coupling matrix (19) is symmetrical one $\langle nj | g^{(0)} | mj' \rangle = \langle mj' | g^{(0)} | nj \rangle$ the transformed particles' coupling matrix (18) is not symmetrical unless the matrices (10) and (19) commute.

4. Quasi-separable recursive procedure for resolvent matrix evaluation

4.1. Recurrent equations with a particle attachment

Return to Watson composition rule for T-scattering operators in Eqs. (14) and (15) and consider a special case of two “particles”, with first complicate particle consisting , actually, the N coupled particles' ensemble, the T- scattering operator of which (24) we denote temporally $\overline{\overline{T}}_{1N}$, and a single $(N+1)$ -st particle, the T –

scattering operator of which we denote temporarily $\overline{\overline{T}}_{N+1N+1}$. In this special case Watson composition rule takes a form

$$\overline{\overline{T}}_{1N+1} = \overline{\overline{T}}_{1N}^{(1)} + \overline{\overline{T}}_{N+1N+1}^{(2)} \quad (25)$$

and

$$\begin{aligned} \overline{\overline{T}}_{1N}^{(1)} &= \overline{\overline{T}}_{1N} + \overline{\overline{T}}_{1N} \overline{\overline{G}}^{(0)} \overline{\overline{T}}_{N+1N+1}^{(2)} \\ \overline{\overline{T}}_{N+1N+1}^{(2)} &= \overline{\overline{T}}_{N+1N+1} + \overline{\overline{T}}_{N+1N+1} \overline{\overline{G}}^{(0)} \overline{\overline{T}}_{1N}^{(1)} \end{aligned} \quad (26)$$

Eqs. (25) and (26) system describes physically a changing T-scattering operator of N coupled particles' ensemble at attachment a single $(N+1)$ -st particle to this ensemble. These equations' system was used in Ref. [23] to study of changing the reflection and transmission coefficients of N layers' stack at $(N+1)$ -st infinitesimal thin layer attachment. One can recognize a using the Eqs. (25) and (26) system in Refs. [28,29] at elaborating the recursive transition matrix method for calculating local electromagnetic fields inside of coupled spheres. Nevertheless, analytic investigation of Eqs. (25) and (26) system shows that there is not more complicate and perhaps more simple alternative recursive method to evaluate T-scattering operator $\overline{\overline{T}}_{1N+1}$ of $N+1$ coupled particles at attachment a single $(N+1)$ -st particle to known T scattering operator $\overline{\overline{T}}_{1N}$ of N coupled particles. The alternative method is based on the basic Eqs. (17) system matrix (20) block splitting and the Frobenius formula [34] application for the block matrix inversion.

4.2. Matrix A_{N+1} block splitting

Turn to matrix (20) in the case of $N+1$ coupled particles and write of this one in details as a table matrix

$$\begin{aligned}
 & A_{N+1} \\
 = & \left[\begin{array}{cccc|c}
 \delta_{nm} & -\langle n1|\tilde{g}^{(0)}|m2\rangle & \dots & \dots & -\langle n1|\tilde{g}^{(0)}|mN\rangle & -\langle n1|\tilde{g}^{(0)}|mN+1\rangle \\
 -\langle n2|\tilde{g}^{(0)}|m1\rangle & \delta_{nm} & & & -\langle n2|\tilde{g}^{(0)}|mN\rangle & -\langle n2|\tilde{g}^{(0)}|mN+1\rangle \\
 \vdots & \vdots & \ddots & & & \vdots \\
 \vdots & \vdots & & \ddots & & \vdots \\
 -\langle nN|\tilde{g}^{(0)}|m1\rangle & -\langle nN|\tilde{g}^{(0)}|m2\rangle & & & \delta_{nm} & -\langle nN|\tilde{g}^{(0)}|mN+1\rangle \\
 \hline
 -\langle nN+1|\tilde{g}^{(0)}|m1\rangle & -\langle nN+1|\tilde{g}^{(0)}|m2\rangle & & & -\langle nN+1|\tilde{g}^{(0)}|mN\rangle & \delta_{nm}
 \end{array} \right] \quad (27)
 \end{aligned}$$

According to vertical and horizontal lines one can understand this matrix as 2×2 block matrix of the form

$$A_{N+1} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \quad (28)$$

Here the left up corner block matrix is appeared to be $A \equiv A_N$ and the right down corner block matrix coincides with matrix element $\langle nN+1|I|mN+1\rangle = \delta_{nm}$ of unit matrix. The block one column B and one row C matrices are given by

$$\langle nj|B|mj'\rangle = -\langle nj|\tilde{g}^{(0)}|mN+1\rangle \delta_{j'N+1}; \quad j = 1, \dots, N \quad (29)$$

and

$$\langle nj|C|mj'\rangle = -\langle nN+1|\tilde{g}^{(0)}|mj'\rangle \delta_{jN+1}; \quad j' = 1, \dots, N \quad (30)$$

Next we are interesting in resolvent matrix $R_{N+1} = A_{N+1}^{-1}$ corresponding to the case of $N+1$ particles and obtaining by the matrix (28) inversion. According to the Frobenius formula [35], the seeking resolvent matrix has 2×2 block matrix structure similar to (28) that we write as

$$R_{N+1} = \begin{bmatrix} R_{N+1(11)} & R_{N+1(12)} \\ R_{N+1(21)} & R_{N+1(22)} \end{bmatrix} \quad (31)$$

with blocks given by

$$\begin{aligned}
 R_{N+1(11)} &= R_N + R_N B H^{-1} C R_N, & R_{N+1(12)} &= -R_N B H^{-1} \\
 R_{N+1(21)} &= -H^{-1} C R_N, & R_{N+1(22)} &= H^{-1}
 \end{aligned}
 \tag{32}$$

Here the block matrix of principle H is defined by $H = D - C R_N B$ and has due to Eqs. (29) and (30) the right down corner block matrix form

$$\begin{aligned}
 &\langle nN + 1 | H | mN + 1 \rangle \\
 &= \delta_{nm} - \sum_{m'j'm''} \langle nN + 1 | \tilde{g}^{(0)} | m'j' \rangle \langle m'j' | R_N | m''j'' \rangle \langle m''j'' | \tilde{g}^{(0)} | mN + 1 \rangle
 \end{aligned}
 \tag{33}$$

The inverse matrix H^{-1} has similar right down corner block form . The nonzero elements of block matrices (32) can be evaluated as follows

$$\begin{aligned}
 &\langle nj | R_{N+1(11)} | mj' \rangle = \langle nj | R_N | mj' \rangle \\
 &+ \sum_{m'm''} \langle nj | R_{N+1(12)} | m'N + 1 \rangle \langle m'N + 1 | H | m''N + 1 \rangle \langle m''N + 1 | R_{N+1(21)} | mj' \rangle
 \end{aligned}
 \tag{34}$$

$$\begin{aligned}
 &\langle nj | R_{N+1(12)} | mN + 1 \rangle \\
 &= \sum_{m'j'm''} \langle nj | R_N | m'j' \rangle \langle m'j' | \tilde{g}^{(0)} | m''N + 1 \rangle \langle m''N + 1 | H^{-1} | mN + 1 \rangle
 \end{aligned}
 \tag{35}$$

$$\begin{aligned}
 &\langle nN + 1 | R_{N+1(21)} | mj' \rangle \\
 &= \sum_{m'm''j''} \langle nN + 1 | H^{-1} | m'N + 1 \rangle \langle m'N + 1 | \tilde{g}^{(0)} | m''j'' \rangle \langle m''j'' | R_N | mj' \rangle
 \end{aligned}
 \tag{36}$$

$$\langle nN + 1 | R_{N+1(22)} | mN + 1 \rangle = \langle nN + 1 | H^{-1} | mN + 1 \rangle
 \tag{37}$$

Eqs. (34)--(37) enables one to evaluate the blocks of resolvent matrix (31) in the case of $N + 1$ particles, provided one knows the resolvent matrix for N particles. That is a recursive procedure based on Frobenius formula in matrix algebra.

5. Self consistent currents excited inside coupled particles in quasi-separable approach

As was mentioned in Sec.3, Eqs. (17) system is basic one to evaluate the currents excited inside coupled particles, in the framework of quasi-separable approach. Consider this notice in more details.

According to Eqs. (6), (14) and (15) the self consistent current $\vec{J}^{(j)}(\vec{r})$ excited inside of ensemble j -th particle is defined by

$$\vec{J}^{(j)}(\vec{r}) = \int d\vec{r}' \overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}') \vec{E}^{(0)}(\vec{r}') \quad (38)$$

with the ensemble incident electric field $\vec{E}^{(0)}(\vec{r})$ giving in Eq. (2). The QS self consistent T-scattering operator of ensemble j -th particle $\overline{\overline{T}}^{(j)}(\vec{r}, \vec{r}')$ is presented as dyadic expansion (16) . Therefore denoting

$$\tilde{J}_n^{(j)} = \int d\vec{r}' \tilde{T}_n^{(j)}(\vec{r}') \vec{E}^{(0)}(\vec{r}') \quad (39)$$

enables one to write

$$\vec{J}^{(j)}(\vec{r}) = \sum_n \vec{t}_n(\vec{r} - \vec{r}_j) \tilde{J}_n^{(j)} \quad (40)$$

We get a physically transparent representation for the self consistent current excited inside of ensemble j th particle as expansion along vector basis functions, with expansion coefficients being equal to the quantities (39). These expansion coefficients satisfy the equations' system

$$\tilde{J}_n^{(j)} = \tilde{J}_{(1)n}^{(j)} + \sum_m \sum_{j' \neq j} \langle nj | \tilde{g}^{(0)} | mj' \rangle \tilde{J}_m^{(j')} \quad (41)$$

which is originated from Eqs. (17) system. An inhomogeneous term in the new obtained equations' system RHS is defined by

$$\tilde{J}_{(1)n}^{(j)} = \int d\vec{r}' \tilde{t}_n(\vec{r}' - \vec{r}_j) \vec{E}^{(0)}(\vec{r}') \quad (42)$$

and presents expansion coefficient along vector basis functions of current excited inside single j -th particle.

The matrix of obtained Eqs. (41) system coincides with matrix A_N defined by Eq. (20) and hence this system can be resolved with the help of the resolvent matrix R_N and recursive procedure of preceding section. At the same time, the Eqs. (41) system is interesting itself in special cases of low dimensional ordered arrays of particles.

6. Quasi-separable T-scattering operator for electromagnetic crystal unit cell

In previous Secs.2-5 we considered T-scattering operators in QS approach for single particle as well as coupled particles' ensemble arbitrarily placed without overlapping in free space. The aim of this section is to show that QS approach can be used also at evaluating the homogenized electromagnetic crystal structure effective dielectric permittivity tensor (dyadic).

The way of QS application on this area is opened by the principal observation that above effective dielectric permittivity dyadic is simple expressed via crystal structure unit cell T-scattering operator. The scattering potential $V(\vec{r})$ of crystal structure has periodic property $V(\vec{r}) = V(\vec{r} + \vec{r}_S)$ where $\vec{r}_S = s_1\vec{a}_1 + s_2\vec{a}_2 + s_3\vec{a}_3$ is lattice point, with $\vec{a}_1, \vec{a}_2, \vec{a}_3$ and $S = (s_1, s_2, s_3)$ being the primitive vectors and generic multi-index of integers, respectively. The incident electric field $\vec{E}^0(\vec{r})$ is supposed after [1] to have the Floquet property, i.e., $\vec{E}^0(\vec{r})\exp(i\vec{k}\vec{r}) = \vec{E}_{\vec{k},\omega}^{(0)}(\vec{r})$ is periodic in the crystal, for example, constant vector as we imply in the future. Under this condition a solution to LS equation (1) for the total electric field $\vec{E}(\vec{r})$ has Floquet property also, becoming a Bloch (Floquet) wave field with wave vector \vec{k} [39]. LS equation (1) for the Floquet electric field is transformed [1, 40] to a productive form

$$\vec{E}(\vec{r}) = \vec{E}_{av}(\vec{k}, \omega) \exp(-i\vec{k}\vec{r}) + \int_{\Omega} d\vec{r}' \overline{\overline{G}}_{p0}(\vec{r} - \vec{r}') V(\vec{r}') \vec{E}(\vec{r}') \quad (43)$$

Here the RHS inhomogeneous term represents the averaged over crystal structure unit cell Ω Floquet electric field given by

$$\vec{E}_{av}(\vec{k}, \omega) = \frac{1}{|\Omega|} \int_{\Omega} d\vec{r} \vec{E}(\vec{r}) \exp(i\vec{k}\vec{r}) \quad (44)$$

with $|\Omega|$ denoting the unit cell volume. In Eq.(43) RHS integral term one sees integration over structure unit cell and an electric field reduced lattice dyadic Green function defined [1] as

$$\overline{\overline{G}}_{p0}(\vec{r} - \vec{r}') = \frac{1}{|\Omega|} \sum_{J \neq 0} \overline{\overline{G}}^{(0)}(\vec{k}_J) \exp[i\vec{k}_J(\vec{r} - \vec{r}')] \quad (45)$$

In this definition the multi-index J components must not be all equal to zero simultaneously; the vector $\vec{k}_J = \vec{k}_J^{(0)} - \vec{k}$, where $\vec{k}_J^{(0)} = j_1 \vec{b}_1 + j_2 \vec{b}_2 + j_3 \vec{b}_3$ and $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are reciprocal lattice primitive vectors; $\overline{\overline{G}}^{(0)}(\vec{k}) = (\overline{\overline{I}} - \vec{k} \otimes \vec{k} / k_0^2) / (k_0^2 - k^2)$ denotes the spatial Fourier transform of the electric field dyadic Green function (3) in free space. The averaged electric field (44) satisfies the Dyson equation

$$\vec{E}(\vec{k}, \omega) = \vec{E}_{\vec{k}, \omega}^{(0)} + \overline{\overline{G}}^{(0)}(\vec{k}, \omega) \overline{\overline{M}}(\vec{k}, \omega) \vec{E}(\vec{k}, \omega) \quad (46)$$

The dyadic mass operator $\overline{\overline{M}}(\vec{k}, \omega)$ is related to the effective dielectric permittivity dyadic $\overline{\overline{\epsilon}}_{eff}(\vec{k}, \omega)$ via well known relation (see, e.g., [21]) $\overline{\overline{\epsilon}}_{eff}(\vec{k}, \omega) / \epsilon_0 = \overline{\overline{I}} - \overline{\overline{M}}(\vec{k}, \omega) / k_0^2$.

Return now to transformed LS Eq.(43) for Floquet electric field and write its solution similar to Eq. (4) in a form

$$\vec{E}(\vec{r}) = \vec{E}_{inc}(\vec{r}) + \int_{\Omega} d\vec{r}' \int_{\Omega} d\vec{r}'' \overline{\overline{G}}_{p0}(\vec{r} - \vec{r}') \overline{\overline{T}}(\vec{r}', \vec{r}'') \vec{E}_{in}(\vec{r}'') \quad (47)$$

where we denote $\vec{E}_{ia}(\vec{r}) = \vec{E}_{av}(\vec{k}, \omega) \exp(-i\vec{k}\vec{r})$. The dyadic $\overline{\overline{T}}(\vec{r}', \vec{r}'')$ in the Eq. (47) RHS has physical sense of the crystal structure unit cell T-scattering operator. Comparison Eqs. (43) and (47) leads to LS integral equation for unit cell T-scattering operator

$$\overline{\overline{T}}(\vec{r}, \vec{r}') = V(\vec{r}) \overline{\overline{I}} \delta(\vec{r} - \vec{r}') + V(\vec{r}) \int_{\Omega} d\vec{r}'' \overline{\overline{G}}_{p0}(\vec{r} - \vec{r}'') \overline{\overline{T}}(\vec{r}'', \vec{r}') \quad (48)$$

that is obtained also from LS integral equation (5) for single particle in free space T-scattering operator by formal replacing the electric field dyadic Green function in free space to electric field reduced lattice dyadic Green function.

Now we are ready to resolve the main problem of this section, concerning the application of crystal structure unit cell T-scattering operator for structure effective dielectric permittivity dyadic evaluation. The problem is resolved with the aid of identity for dyadic mass operator $\overline{\overline{M}}(\vec{k}, \omega)$ in a form

$$\overline{\overline{M}}(\vec{k}, \omega) \vec{E}_{av}(\vec{k}, \omega) = \frac{1}{|\Omega|} \int_{\Omega} d\vec{r} V(\vec{r}) \vec{E}(\vec{r}) \exp(i\vec{k}\vec{r}) \quad (49)$$

This identity, being actually definition for structure effective dielectric permittivity dyadic, jointly with Eqs.(47) and (48) lead to desired result

$$\overline{\overline{M}}(\vec{k}, \omega) = \frac{1}{|\Omega|} \int_{\Omega} d\vec{r} \int_{\Omega} d\vec{r}' \exp[i\vec{k}(\vec{r} - \vec{r}')] \overline{\overline{T}}(\vec{r}, \vec{r}') \quad (50)$$

The got result shows that dyadic mass operator can be written as double Fourier transform over crystal structure unit cell from the unit cell dyadic T-scattering operator.

Side by side with the unit cell T-scattering operator satisfied the LS Eqs. (48) we introduce T-scattering operator of a virtual unit cell in free space satisfied LS Eqs. (5), solution to which we denote $\overline{\overline{T}}^{(0)}(r, r')$. One can exclude scattering potential of unit cell from LS Eqs. (48) RHS, via replacing its by T-scattering operator of unit cell

in free space. After that one gets a LS equation for crystal structure unit cell T-scattering operator in transformed form

$$\bar{\bar{T}}(\vec{r}, \vec{r}') = \bar{\bar{T}}^{(0)}(\vec{r}, \vec{r}') + \int_{\Omega} d\vec{r}'' \int_{\Omega} d\vec{r}''' \bar{\bar{G}}_{\text{int}}(\vec{r}'' - \vec{r}''') \bar{\bar{T}}(\vec{r}''', \vec{r}') \quad (51)$$

where $\bar{\bar{G}}_{\text{int}}(\vec{r} - \vec{r}') = \bar{\bar{G}}_{p0}(\vec{r} - \vec{r}') - \bar{\bar{G}}^{(0)}(\vec{r} - \vec{r}')$ denotes [1] electric field lattice dyadic Green function interaction part defined as difference between electric field reduced lattice dyadic Green function (45) and electric field dyadic Green function in free space (3). QS solution to transformed LS Eqs. (51) we seek in a form

$$\bar{\bar{T}}(\vec{r}, \vec{r}') = \sum_{njmj'} \langle nj | \chi^{-1} | mj' \rangle \vec{t}(\vec{r} - \vec{r}_j) \otimes \vec{t}(\vec{r}' - \vec{r}_{j'}) \quad (52)$$

with inversion to an unknown generating matrix χ . Direct substituting representations (24) for $\bar{\bar{T}}^{(0)}(r, r')$ and (52) into transformed LS Eqs.(51) determines the seeking generating matrix as difference of two matrices

$$\langle nj | \chi | mj' \rangle = \langle nj | \chi_N^{(0)} | mj' \rangle - \langle nj | g | mj' \rangle \quad (53)$$

first of which coincides with inversion to matrix in Eqs. (22) LHS and second is given by

$$\langle nj | g | mj' \rangle = \int_{\Omega} d\vec{r} \int_{\Omega} d\vec{r}' \vec{t}_n(\vec{r} - r_j) \bar{\bar{G}}_{\text{int}}(\vec{r} - \vec{r}') \vec{t}_m(\vec{r}' - r_{j'}) \quad (54)$$

and describes coupling between particles of a unit cell via crystal structure. The obtained exact expression (50) for mass operator in terms of unit cell T-scattering operator and QS representation (52) for this unit cell T-scattering operator enable one to evaluate contribution effects of coupling between unit cell particles into crystal structure effective dielectric permittivity tensor, without relating a priory to Clausius-Mossotti homogenization formula.

7. Quasi-separable T-scattering operator applications

In this section we consider several applications of QS technique for T-scattering operator. First of all one should show how this technique gives classical Mie result on plane wave scattering by homogeneous dielectric sphere.

7.1. Plane wave scattering from and transmitting into spherical particle

Apply the QS T-scattering operator (13) to the case of homogeneous spherical particle of radius r_0 in free space. We choose a vector expansion functions' basis $\vec{t}_n(\vec{r})$ in the form of infinite set of regular at the origin spherical vector wave functions [41,42,43] denoted in spherical coordinates r, θ, ϕ as $\vec{M}_{e(o)mn}(k)$ and $\vec{N}_{e(o)mn}(k)$. In these denotations indices e and o mean even and odd spherical harmonics with respect to latitude angle ϕ , respectively, and indices mn number spherical harmonics with respect to azimuth angle θ and ϕ again. Argument k denotes wave number inside the spherical particle, $k = (\omega/c)\hat{\epsilon}^{1/2}$. Introducing a multi-index $\hat{p} = \vec{M}_{e(o)mn}(k)$ or $\vec{N}_{e(o)mn}(k)$ we write below $\vec{t}_{\hat{p}}(\vec{r})$ or $\vec{t}_{\hat{q}}(\vec{r})$. Note that these vector expansions' functions satisfy the solenoidal restriction in the last Eq.(6) automatically due to definition of vector spherical wave functions.

We need evaluating the generating matrix (10). To this end one can previously make a productive identical transformation of coupling matrix (11), using differential wave equations for electric field dyadic Green function Eq. (3) in free space and for spherical vector wave functions and applying then vector Green theorem [41]. The described transformation of coupling matrix (11) permits one to rewrite the generating matrix (10) as follows

$$\chi_{\hat{p}\hat{q}}^{(0)} = -\frac{1}{k_0^2 - k^2} \int_{\Omega} d\vec{r} \int_{\Sigma} d\Sigma' \vec{v}(\vec{r}') \left[\vec{p}(\vec{r}') \times \nabla' \times \vec{t}_{\hat{q}}(\vec{r}') - \vec{t}_{\hat{q}}(\vec{r}') \times \nabla' \times \vec{p}(\vec{r}') \right] \quad (55)$$

where a vector $\vec{p}(\vec{r}') = \overline{\overline{G}}^{(0)}(\vec{r}' - \vec{r}) \vec{t}_{\hat{p}}(\vec{r})$. The out and inner integrations in the rewritten generating matrix expression RHS are performed along the spherical

particle volume Ω and surface Σ , respectively, with $d\vec{r}$ being volume element and $d\Sigma'$ and $\vec{v}(\vec{r}')$ being surface element and unit normal to surface element.

The detailed integrations in the Eq. (55) RHS is not difficult in the main and gives the diagonal generating matrix $\chi_{\hat{p}\hat{q}}^{(0)} = \chi_{\hat{p}}^{(0)} \delta_{\hat{p}\hat{q}}$ after that the QS T-scattering operator (13) takes a form

$$\begin{aligned} \bar{\bar{T}}^{(0)}(\vec{r}, \vec{r}') = & \sum_{mn} \frac{1}{\chi_{Me(o)mn}^{(0)}} \vec{M}_{e(o)mn}(k) \otimes \vec{M}'_{e(o)mn}(k) \\ & + \sum_{mn} \frac{1}{\chi_{Ne(o)mn}^{(0)}} \vec{N}_{e(o)mn}(k) \otimes \vec{N}'_{e(o)mn}(k) \end{aligned} \quad (56)$$

where the primed spherical vector wave functions are related to primed spherical coordinates r', θ', ϕ' . The elements $\chi_{\hat{p}}^{(0)}$ of diagonal generating matrix (55) are presented in terms of Mie scattering coefficients and special bilinear (k_0, k) -functionals of spherical vector wave functions on spherical particle volume (see Appendix A).

Let the incident on spherical particle electric field has form [43] of transversal plane wave

$$\vec{E}^{(0)}(\vec{r}) = \sum_{n=1}^{\infty} E_n \left[\vec{M}_{o1n}(k_0) - i \vec{N}_{e1n}(k_0) \right] \quad (57)$$

with denoting $E_n = i E^{(0)} (2n+1)/n(n+1)$. The electric field $\vec{E}_{ins}(\vec{r})$ transmitted inside spherical particle is evaluated with the aid of general Eqs.(6) and expression (56) for QS T- scattering operator of spherical particle. The evaluation result is as follows

$$\vec{E}_{ins}(\vec{r}) = \sum_{n=1}^{\infty} E_n \left[c_n \vec{M}_{o1n}(k_0) - i d_n \vec{N}_{e1n}(k_0) \right] \quad (58)$$

where transmitting coefficients c_n and d_n coincide with usual for Mie theory (see Ref. 43, page 128). The electric field $\vec{E}_{sc}(\vec{r})$ scattered by spherical particle is

evaluated automatically with the aid of LS equation (1) for total electric field, provided one knows the electric field transmitted inside the particle. The result is as follows

$$\vec{E}_{sc}(\vec{r}) = \sum_{n=1}^{\infty} E_n \left[-b_n \vec{M}_{o1n}(k_0) + i a_n \vec{N}_{e1n}(k_0) \right] \quad (59)$$

where scattering coefficients a_n and b_n coincide with usual for Mie theory (see Ref. 43, pages 129 and 130).

7.2. Pre-Haar basis of vector functions defined on particle finite elements

Having applied the QS T-scattering operator (13) for homogeneous spherical particle in the preceding subsection, we chose a vector expansion functions' basis $\vec{t}_n(\vec{r})$ in the form of infinite set of spherical vector wave functions defined over whole particle volume Ω . Consider now another choosing for vector expansion functions' basis consisting the functions defined on finite elements of particle volume in spirit of general finite element method [33]. Such choosing may be useful in the case of particle with complicate shape and leads to QS approximation of particle scattering potential operator when LS equation for T-scattering operator is resolved exactly.

Subdivide the particle volume Ω into set of not overlapping subdomains Ω_n ; $n = 1, 2, 3, \dots$, so that $\Omega = \bigcup_n \Omega_n$ and $\Omega_n \cap \Omega_m = 0$ as $n \neq m$. Define the orthogonal and normalized set of functions

$$t_n(\vec{r}) = \frac{H(\vec{r} \in \Omega_n)}{\sqrt{|\Omega_n|}}; \quad \int d\vec{r} t_n(\vec{r}) t_m(\vec{r}) = \delta_{nm} \quad (60)$$

where $H(\vec{r} \in \Omega_n)$ is a subdomain Ω_n characteristic function equal to unite as point \vec{r} belongs to the subdomain and equal to zero if point not belong the subdomain. The set of functions in Eqs. (60), which can be used as first step on the way to construct

the Haar bases [34], we conditionally call as pre-Haar basis. This basis creates the piecewise constant functions defined on the particle volume as

$$f(\vec{r}) = \sum_n f_n t_n(\vec{r}) = \sum_n f(\Omega_n) H(\vec{r} \in \Omega_n) \quad (61)$$

with $f(\Omega_n)$ denoting the function $f(\vec{r})$ averaged over subdomain Ω_n according to

$$f(\Omega_n) = \frac{1}{|\Omega_n|} \int_{\Omega_n} d\vec{r} f(\vec{r}) \quad (62)$$

On set of functions (61) an analog of Dirac delta-function has a form

$$D(\vec{r}, \vec{r}') = \sum_n t_n(\vec{r}) t_n(\vec{r}'); \quad \int d\vec{r}' D(\vec{r}, \vec{r}') f(\vec{r}') = f(\vec{r}) \quad (63)$$

Turn now to LS integral Eqs (5) for T-scattering operator. Its RHS inhomogeneous term has a factor $V(\vec{r}) \delta(\vec{r} - \vec{r}')$ with particle scattering potential $V(\vec{r})$. We replace this factor approximately as

$$V(\vec{r}) \delta(\vec{r} - \vec{r}') \approx V(\vec{r}) D(\vec{r}, \vec{r}') = \sum_n V(\Omega_n) t_n(\vec{r}) t_n(\vec{r}') \equiv V(\vec{r}, \vec{r}') \quad (64)$$

and obtain QS particle scalar scattering potential $V(\vec{r}, \vec{r}')$ operator. Going to get QS particle dyadic scattering potential $\bar{\bar{V}}(\vec{r}, \vec{r}')$ operator, we generalize the basis of scalar functions $t_n(\vec{r})$ in Eqs. (60) to basis of vector functions

$$\vec{t}_{np}(\vec{r}) = t_n(\vec{r}) \hat{e}_p \quad (65)$$

Here \hat{e}_p denotes a three-valued vector function of integer index $p = 1, 2, 3$, equal to unit vectors $\hat{x}, \hat{y}, \hat{z}$ along the $x_1 = x, x_2 = y, x_3 = z$ axes of the Cartesian coordinate system, respectively. Using identity $\sum_p \hat{e}_p \otimes \hat{e}_p = \bar{\bar{I}}$ we find similarly with

Eqs.(64) an approximation

$$V(\vec{r}) \delta(\vec{r} - \vec{r}') \bar{\bar{I}} \approx V(\vec{r}) D(\vec{r}, \vec{r}') \bar{\bar{I}} = \sum_{np} V(\Omega_n) \vec{t}_{np}(\vec{r}) \otimes \vec{t}_{np}(\vec{r}') \equiv \bar{\bar{V}}(\vec{r}, \vec{r}') \quad (66)$$

that is really QS particle dyadic scattering potential $\overline{\overline{V}}(\vec{r}, \vec{r}')$ operator. The LS Eqs. (5) for T-scattering operator with QS scattering potential operator (66) is resolved exactly as follows

$$\overline{\overline{T}}(\vec{r}, \vec{r}') = \sum_{np, mq} \langle np | \chi^{-1} | mq \rangle \vec{t}_{np}(\vec{r}) \otimes \vec{t}_{mq}(\vec{r}') \quad (67)$$

with generating matrix

$$\langle np | \chi | mq \rangle = \frac{1}{V(\Omega_n)} \langle np | I | mq \rangle - \langle np | g^{(0)} | mq \rangle \quad (68)$$

where the second matrix element in the RHS describing wave coupling between the particle elements is defined as in Eq. (11), i.e.

$$\langle np | g^{(0)} | mq \rangle = \int d\vec{r} \int d\vec{r}' \vec{t}_{np}(\vec{r}) \overline{\overline{G}}^{(0)}(\vec{r} - \vec{r}') \vec{t}_{mq}(\vec{r}') \quad (69)$$

The unit matrix $\langle nj | I | mj' \rangle$ is the same with one before Eq.(20).

There is a formal difference between the first terms in the RHS of Eqs. (10) and (68). In details the first term in the Eq. (10) RHS should seen in the case of basis vector functions (65) as

$$\int d\vec{r} \frac{1}{V(\vec{r})} \vec{t}_{np}(\vec{r}) \vec{t}_{mq}(\vec{r}) = \int_{\Omega_n} d\vec{r} \frac{1}{V(\vec{r})} \langle np | I | mq \rangle \quad (70)$$

The integral in the RHS of this equation tends to the quantity $1/V(\Omega_n)$ in the RHS first term of Eq.(68) in the limit of infinitesimally small subdomains of the particle volume, i.e. when $|\Omega_m| \rightarrow 0$ and mentioned formal difference is dissipated.

The vector expansions' functions (65) satisfy with corresponding accuracy to solenoidal restriction in the last Eq.(6) as is shown in Appendix B. It would be interesting also to compare the pre-Haar basis functions in Eqs.(60) and (65) with

position of the electric and magnetic field vector components about a cubic unit cell of the Yee space lattice [44] in computational electrodynamics of the finite-difference time-domain method [45]. But such comparison is out of our paper aim.

7.3. Artificial double diamagnetic-paramagnetic narrow peak in metamaterial with unit cell of coupled plasmonic particles

In Ref.[21] the Dyson equation technique for averaged wave electric field over statistical ensemble of random discrete media was used to evaluate the medium effective dielectric permittivity with spatial dispersion and then via Lindhard rule [46] the corresponding effective magnetic permeability. In details, the effective diamagnetic property was demonstrated in limit of independent strongly reflected nonmagnetic small spherical particles, which possessing individual high dielectric permittivity or conductivity. The physical base for effective magnetic permeability appearance consisted in circular currents created inside a single particle via magnetic dipole scattering.

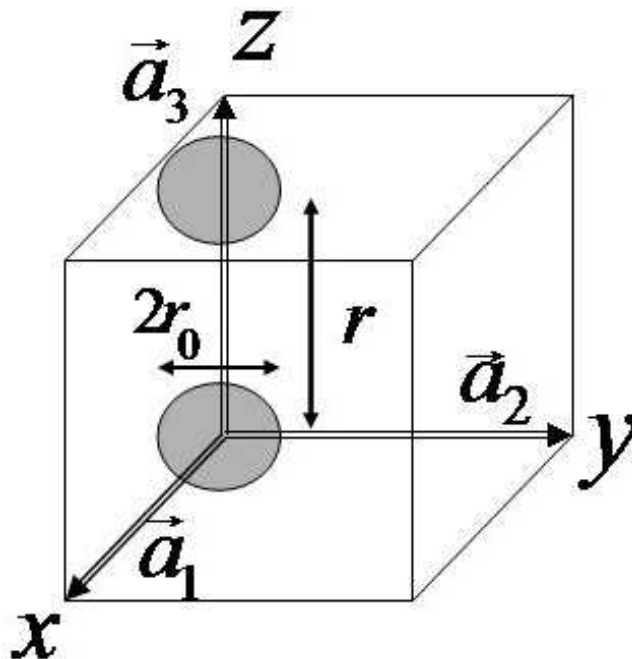


Figure1. A sketch to illustrate an unit cell in a 3D crystal structure (xyz is the Cartesian coordinate system, $\vec{a}_{1,2,3}$ are primitive vectors) with two small coupled plasmonic spherical particles ($2r_0$ and r is a diameter and distance between particles, respectively).

Now we are going to apply the Dyson Eq.(46) for averaged over electromagnetic crystal structure unit cell wave electric field to evaluate the structure effective dielectric permittivity and then via Linhard rule again the corresponding effective magnetic permeability. In particular, we intend to demonstrate a specific parametric resonance effect as narrow in frequency band double diamagnetic-paramagnetic peak caused by space-grope resonance effect [5,6] between unit cell coupled small plasmonic spherical particles. The physical base for double diamagnetic-paramagnetic peak appearance consists in circular currents around coupled particles (see Fig.1) via electric dipole scattering by a single particle.

We start with generalized [1] on the anisotropic case the Linhard rule for effective magnetic permeability dyadic $\bar{\bar{\mu}}_{eff}(\vec{k}, \omega)$ evaluation, which in our denotations and geometry on Fig.1 has for the component $(\mu_{eff})_{yy} \equiv \mu_{yy}$ a form

$$M_{xx}(k_z, \omega) - M_{xx}(k_z = 0, \omega) = \left(\frac{1}{\mu_{yy}} - 1 \right) k_z^2 \quad (71)$$

The dyadic mass operator is given by exact formula (50), with unit cell T-scattering operator double Fourier transform being in the RHS. As our investigation has shown, the space-grope resonance effect between unit cell coupled small plasmonic spherical particles can be considered in tight binding approximation, when direct wave coupling between unit cell particles is substantially greater their coupling via crystal structure. The unit cell T-scattering operator satisfies the transformed LS Eq. (51) and can be approximated in the tight binding limit by the first term of this equation RHS that is by T-scattering operator of unit cell in free space $\bar{\bar{T}}^{(0)}(\vec{r}, \vec{r}')$. But T-scattering operator of two coupled electric dipole scatterers is evaluated in Ref. [6] and is written out, actually, as QS T-scattering operator (24) for two coupled particles, with inverse generating matrix and vector expansion functions being defined as

$$\begin{aligned} \langle nj | \chi_2^{(0)-1} | mj' \rangle = & \hat{e}_n \left[a_t \bar{P}^t(\vec{s}) + a_l \bar{P}^l(\vec{s}) \right] \hat{e}_m \left(\delta_{j1} \delta_{j'1} + \delta_{j2} \delta_{j'2} \right) \\ & + \hat{e}_n \left[b_t \bar{P}^t(\vec{s}) + b_l \bar{P}^l(\vec{s}) \right] \hat{e}_m (1 - \delta_{jj'}) \end{aligned} \quad (72)$$

and $\vec{t}_n^{el}(\vec{r})$ in Eq.(A9). We denote here $a_{t,l} = 1/[1 - (f^{t,l})^2]$ and $b_{t,l} = f^{t,l} a_{t,l}$. The dyadics $\bar{P}^t(\vec{s}) = \bar{I} - \vec{s} \otimes \vec{s}$ and $\bar{P}^l(\vec{s}) = \vec{s} \otimes \vec{s}$ are, respectively, transversal and longitudinal projectors on unit vector $\vec{s} = \vec{r}/r$ along vector \vec{r} connecting two coupled particles inside unit cell. The quantities $f^{t,l} = -4\pi k_0^2 \eta G_0^{t,l}(r)$ where transversal and longitudinal components $G_0^{t,l}(r)$ of the electric field dyadic Green function (3) in free space are defined by the following identity and have the values

$$\bar{G}^{(0)}(\vec{r}) = G_0^t(r) \bar{P}^t(\vec{s}) + G_0^l(r) \bar{P}^l(\vec{s}) \quad (73)$$

where

$$G_0^t(r) = \left(1 + \frac{i}{k_0 r} - \frac{1}{k_0^2 r^2} \right) G_0(r), \quad G_0^l(r) = \left(-\frac{2i}{k_0 r} + \frac{2}{k_0^2 r^2} \right) G_0(r)$$

The electric susceptibility η of small spherical particle with radius r_0 and dielectric permittivity $\hat{\epsilon}_1$ is given according Ref. [43] by $\eta = r_0^3 (\hat{\epsilon}_1 - \epsilon_0) / (\hat{\epsilon}_1 + 2)$. Substituting the inverse generating matrix (72) and vector expansion functions (A9) into QS T-scattering operator (24) and the last into formula (50) for mass operator results in

$$\bar{M}(\vec{k}, \omega) = -\frac{4\pi k_0^2 \eta}{|\Omega|} \sum_{n,m=1}^3 \sum_{j,j'=1}^2 \langle nj | \chi_2^{(0)-1} | mj' \rangle \exp[i\vec{k}(\vec{r}_j - \vec{r}_{j'})] \hat{e}_n \otimes \hat{e}_m \quad (74)$$

Substituting the obtained dyadic mass operator (74) into Linhard rule (71) gives the expression for inverse effective magnetic permeability component evaluation

$$\frac{1}{\mu_{yy}} = 1 + \frac{4\pi\eta}{|\Omega|} \frac{f^t}{1 - (f^t)^2} (k_0 r)^2 \quad (75)$$

We apply this expression to study the space-grope resonance effect on effective magnetic permeability. According to Ref. [5,6], the space-grope resonance is characterized by condition $f^t \rightarrow 1$ that can give in general for resonance distant r_{res} between small spherical particles a value close and even smaller their diameter $2r_0$, provided that unit cell dimensions being smaller the wavelength in free space. In the case of plasmonic particles, whose dielectric permittivity $\hat{\epsilon}_1 \rightarrow -2$, the resonance distant between particles can be more their diameter and in vicinity of space grope resonance the expression (75) for effective magnetic permeability is rewritten as

$$\mu_{yy} = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 - 2\omega_p \Delta\omega} \quad (76)$$

We denote here ω_p the plasmonic resonance frequency related to particle dielectric permittivity by identity $\hat{\epsilon}_1/\epsilon_0 = 1 - 3\omega_p^2/\omega^2$. A quantity $\Delta\omega$ measures a difference between the plasmonic resonance frequency and a space group resonance frequency and is defined according to

$$\frac{\Delta\omega}{\omega_p} = 3\pi \frac{|\Omega_r|}{|\Omega|} \frac{r_0}{r} \left(\frac{\omega_p}{c} r_0 \right)^2 \quad (77)$$

where $|\Omega_r| = 4\pi r^3/3$ is volume of a sphere with radius equal to distance between two particles in the unit cell. Fig.2 demonstrates the resonance dependence (76) in the form of diamagnetic-paramagnetic narrow peak near plasmonic resonance frequency. The parameters values are taken close to ones in Ref. [48] $r_0/\lambda_p = 1/100$, $r_0/r = 1/10$, $\Delta\omega/\omega_p = 1/1000$, $|\Omega_r|/|\Omega| = 1/2$.

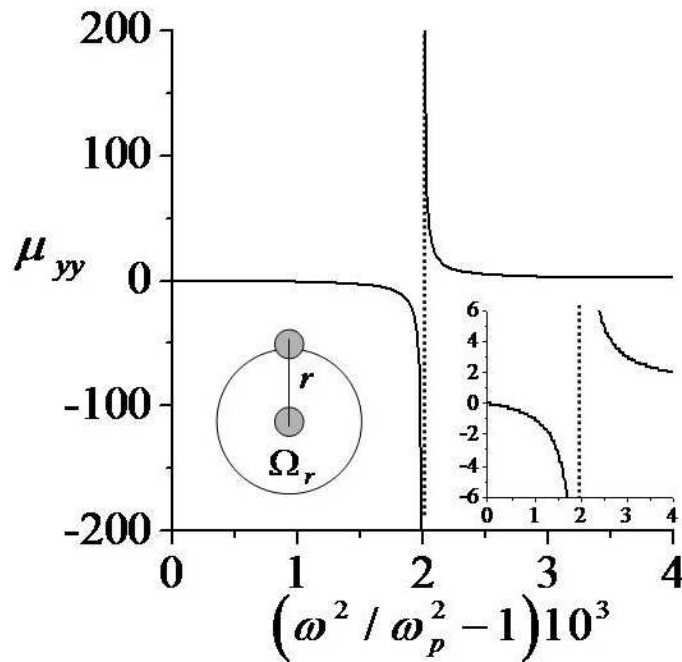


Figure 2. Calculated effective magnetic permeability (76) versus the normalized frequency of electromagnetic wave near plasmonic resonance frequency ω_p (vertical dotted line is given as a reference for eyes). The right inset presents diamagnetic peak in more details. The left inset illustrates the quantity Ω_r (see Eq.(77)).

7.4. Simple low dimensional ordered periodic and linear arrays of particles with coupling matrix of specific properties

As was noticed in Sec.5, the Eqs.(41) system for self consistent currents excited inside coupled particles can be peculiarly interesting in special cases of low dimensional ordered arrays of particles. Let us consider some such cases when the transformed particles' coupling matrix $\langle nj | \tilde{g}^{(0)} | mj' \rangle$ gets property of stochastic matrix or Jacobi's matrix for arrays in the form of periodic polygon chain or a strait linear chain, respectively.

7.4.1. Periodic arrays of particles with coupling matrix of stochastic property

Note that inverse generating matrix (72) of two small coupling spherical particles can be obtained from general formula (22) for inverse generating matrix of coupling arbitrarily particles ensemble if one takes the small spherical particle single T-scattering operator (13) in approximation (A9) of electric dipole single scattering

when the generating matrix (10) of single particle becomes unit one $\langle n | \chi_1^{(0)} | m \rangle = \delta_{nm}$. In this electrical dipole approximation Eqs.(41) system for expansion coefficients $\tilde{J}_z^{(1,2)}$ along vector expansion functions (A9) of self consistent longitudinal currents $J_z^{(1,2)}(\vec{r})$ excited inside two coupled small spherical particles drawn on Fig.1 and considered now in free space takes a form

$$\begin{aligned} \tilde{J}_z^{(1)} - p_{zz} \tilde{J}_z^{(2)} &= \tilde{J}_{(1)z}^{(1)}; & \tilde{J}_{(1)z}^{(1,2)} &= (-4\pi k_0^2 \eta)^{1/2} E_z^{(0)}(\vec{r}_{1,2}) \\ -p_{zz} \tilde{J}_z^{(1)} + \tilde{J}_z^{(2)} &= \tilde{J}_{(1)z}^{(2)} \end{aligned} \quad (78)$$

The longitudinal component $p_{zz} = \langle z1 | \tilde{g}^{(0)} | z2 \rangle$ of transformed two small spherical particles' coupling matrix is given by

$$p_{zz} = -4\pi k_0^2 \eta G^{(0)l}(r) \approx 2 \frac{\eta}{r^3}; \quad k_0 r \rightarrow 0 \quad (79)$$

The matrix of obtained Eqs.(78) system obeys a property of stochastic matrix that is its both rows have the same sum of their elements $1 - p_{zz} \equiv \lambda_1$. Though the true stochastic matrix [35] has positive elements, the mentioned stochastic property of Eqs.(78) system matrix enables one to find its eigenmode, which we call conditionally stochastic one

$$(v_z^{(1)}, v_z^{(2)}) = (1, 1) \quad (80)$$

As one can see, the found stochastic eigenmode (80), corresponding to eigenvalue λ_1 , describes the excited longitudinal currents in both coupling small spherical particles oriented in the same direction of propagation. The matrix of Eqs.(78) system has also another eigenmode (overtone) corresponding to eigenvalue $\lambda_2 = 1 + p_{zz}$ and getting a form

$$(w_z^{(1)}, w_z^{(2)}) = (1, -1) \quad (81)$$

and describing the excited longitudinal currents in both coupling small spherical particles in the opposite directions of propagations. The both found eigenmodes (80)

and (81) can be created at special choice of incident electric field. Resolving Eqs.(78) system gives

$$(\tilde{J}_z^{(1)}, \tilde{J}_z^{(2)}) = \frac{\tilde{J}_{(1)z}^{(1)}}{\lambda_1} (1, 1); \tilde{J}_{(1)z}^{(1)} = \tilde{J}_{(1)z}^{(2)} \quad (82)$$

and

$$(\tilde{J}_z^{(1)}, \tilde{J}_z^{(2)}) = \frac{\tilde{J}_{(1)z}^{(1)}}{\lambda_2} (1, -1); \tilde{J}_{(1)z}^{(1)} = -\tilde{J}_{(1)z}^{(2)} \quad (83)$$

Thus, the stochastic mode (80) and overtone (81) are created by incident electric field excited currents of the same direction and opposite directions inside single particles, respectively.

Consider some details in frequency dependence of eigenvalues λ_1 and λ_2 for stochastic and overtone eigenmodes supposing two small spherical particles to be plasmonic ones. Substituting the electric susceptibility η from Subs.7.3 into particles' coupling matrix longitudinal component (79) leads to following formula for overtone inverse eigenvalue

$$\frac{1}{\lambda_2} = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 - 2\omega_p (\Delta\omega)_2}; \quad \frac{(\Delta\omega)_2}{\omega_p} = \frac{r_0^3}{r^3} \quad (84)$$

and similar formula for stochastic mode inverse eigenvalue that is obtained by replacing $(\Delta\omega)_2 \rightarrow -(\Delta\omega)_2$ in Eq.(84) RHS. Comparison shows that formula (84) for overtone inverse eigenvalue is different from the formula (76) for effective magnetic permeability only in definition of its plasmonic resonance $(\Delta\omega)_2$ width. Physically such close connection between formulas (76) and (84) means that effective magnetic permeability in metamaterial with unit cell of coupled plasmonic particles is coursed by circular currents around coupled particles, as was mentioned above, that corresponds to currents excited inside coupled particles according Eq.(83).This physical reason is illustrated on Fig.3.

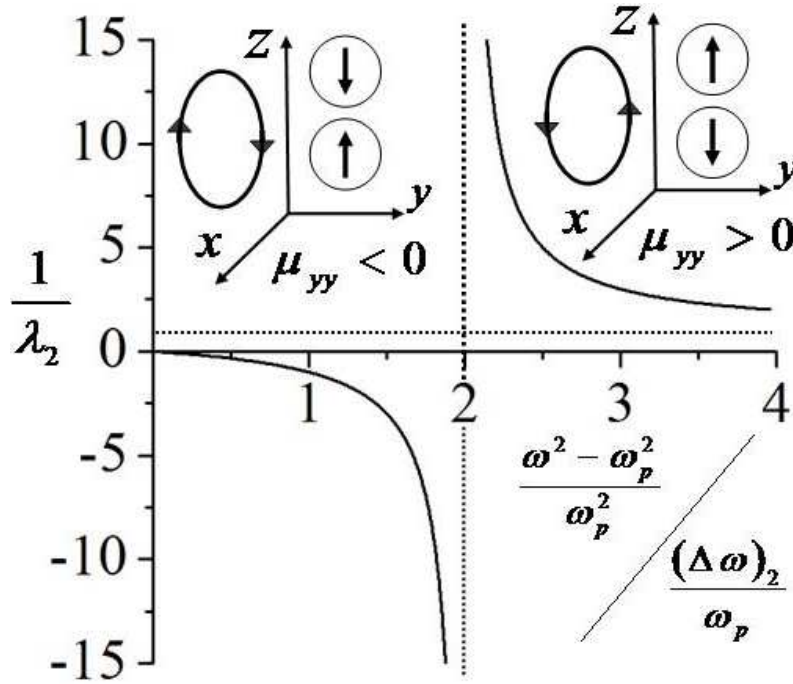


Figure 3. Illustration to correspondence between circular currents around two coupled plasmonic particles and currents excited inside these particles according to Eq.(83), in the cases of positive $\mu_{yy} > 0$ and negative $\mu_{yy} < 0$ effective magnetic permeability component. Dotted lines are given as a reference for eyes.

Returning to the start of this Subs. 7.4.1 we would recognize that did not consider a periodic array of particles yet, though having revealed an interesting stochastic property of two particles' coupling matrix. In order to generalize this stochastic property on the case of a periodic array of particles one could study an ensemble of small spherical particles placed along parallel cylindrical domains when cylinders themselves centered at the corners of N sided equilateral polygon as in Fig.4. Nevertheless we prefer to consider here more simpler model of N coupled parallel wire vibrator–dipoles turned to half wavelength.

7.4.1.1. N coupled parallel wire vibrator–dipoles tuned to half wavelength

We consider an ensemble of N coupled parallel thin wire vibrator-dipoles of length $2h$ each tuned to half wavelength in free space $2h = \lambda / 2$, $k_0 = 2\pi / \lambda$ and centered at the corners of N sided equilateral polygon (Fig.4). The polygon plane

coincides with the xy plane and the wire vibrator-dipoles are oriented along the z axis of the Cartesian coordinate system.

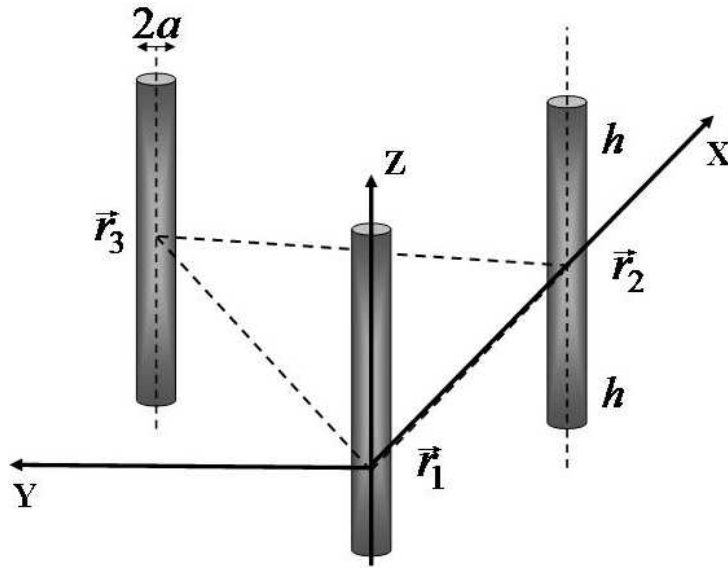


Figure 4. Schematic showing of coupled parallel wire (diameter $2a$) half wavelength $2h = \lambda / 2$ vibrator-dipoles which are extended along the z axis of the Cartesian coordinate system xyz and whose centre positions in the xy plane are defined by radius vectors \vec{r}_i , $i = 1, 2, 3, \dots$.

QS T-scattering operator of single wire vibrator-dipole turned to half wavelength is given according to [15, 48] by Eq. (13), with generating matrix and vector expansion functions being defined approximately as

$$\begin{aligned} \langle n | \chi_1^{(0)} | m \rangle &= \delta_{n1} \delta_{m1}, \quad \vec{t}_n(\vec{r}) = \delta_{n1} \hat{z} \delta(x) \delta(y) t(z); \\ t(z) &= \left(-\frac{1}{Z'_1} \right)^{1/2} \psi_1(z), \quad \psi_1(z) = \cos(\pi z / 2h) \end{aligned} \quad (85)$$

In these equations $\psi_1(z)$ describes harmonics of current distribution, accurate with an amplitude, along the single wire vibrator-dipole excited by incident electric field and Z'_1 is evaluated via double integral

$$Z'_1 = \int_{-h}^h dz \int_{-h}^h dz' \psi_1(z) \hat{z} \overline{\overline{G}}^{(0)}(z - z') \hat{z} \psi_1(z') \quad (86)$$

and related to single wire vibrator-dipole input impedance [15] Z_1 by $Z_1 = (i4\pi\omega/c^2)Z'_1$. The formulas (85) are obtained in approximation of “big logarithm” $|\ln(k_0a)| \gg 1$, with a being the cylindrical vibrator radius. Substituting Eqs. (85) into Eqs. (18) and (19) results in

$$\langle nj | \tilde{g}^{(0)} | mj' \rangle = \delta_{nl} \delta_{ml} g_{11}^{(0)}(\vec{r}_j, \vec{r}_{j'}),$$

$$g_{11}^{(0)}(\vec{r}, \vec{r}') = -\frac{1}{Z'_1} \int_{-h}^h dz \int_{-h}^h dz' \psi_1(z) \hat{z} \bar{G}^{(0)}(\vec{r}_\perp - \vec{r}'_\perp, z - z') \hat{z} \psi_1(z') \equiv a_{12}(|\vec{r}_\perp - \vec{r}'_\perp|) \quad (87)$$

where index \perp notes a projection on the x, y plane. The dimensionless quantity $a_{12}(b)$ was introduced in Ref. [15] as specific coupling factor of two vibrator-dipoles with distant b between them (see Fig. 5).

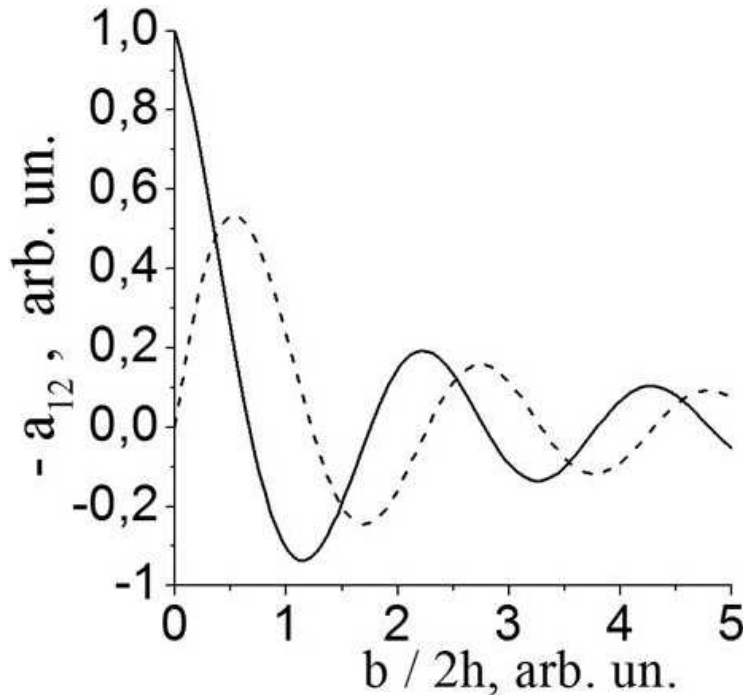


Figure 5. Calculated dependence (87) of the real (solid line) and imaginary (dashed line) parts of the specific coupling factor $-a_{12}$ of two half wavelength $2h = \lambda_1 / 2$ vibrator - dipoles versus normalized distance $b/2h$ between vibrator-dipoles.

As one sees from this figure the coupling factor $a_{12} \rightarrow -1$ as $b/2h \rightarrow 0$ that agrees the Eq.(86) and Eq.(87) second. The more exact asymptotics for coupling factor at small distances $b/2h \rightarrow 0$ between vibrator-dipoles has a form

$$a_{12} \approx -1 - i\pi \frac{b}{h} \frac{k_0}{\omega \epsilon_0} \frac{1}{Z_1}, \quad \frac{\omega \epsilon_0}{k_0} Z_1 = Di(2\pi) - i Si(2\pi) \quad (88)$$

Here $Si(x)$ is the integral sine [49] and regular function $Di(x)$ relates to the integral cosine $Ci(x)$ and Euler constant $C \approx 0.5772$ by $Di(x) = \ln x + C - Ci(x)$.

With expression (87) for transformed particles' coupling matrix the Eqs.(41) system for expansion coefficients $\tilde{J}_z^{(1,2)}$ along vector expansion functions (85) of self consistent longitudinal currents $J_z^{(1,2)}(\vec{r})$ excited inside two coupled parallel thin wire vibrator-dipoles turned to half wavelength takes a form

$$\begin{aligned} \tilde{J}_z^{(1)} - a_{12} \tilde{J}_z^{(2)} &= \tilde{J}_{(1)z}^{(1)}, & \tilde{J}_{(1)z}^{(1,2)} &= \int_{-h}^h dz t(z) E_z^{(0)}(\vec{r}_{\perp 1,2}, z) \\ -a_{12} \tilde{J}_z^{(1)} + \tilde{J}_z^{(2)} &= \tilde{J}_{(1)z}^{(2)} \end{aligned} \quad (89)$$

being similar to Eqs.(78) system in the case of two coupled small spherical particles. The matrix of obtained Eqs.(89) system obeys a property of stochastic matrix and has two eigenmodes, stochastic of type (80) with eigenvalue $\lambda_1 = 1 - a_{12}$ and overtone of type (81) with eigenvalue $\lambda_2 = 1 + a_{12}$. At creating these eigenmodes by special choice of incident electric field, as in Eqs.(82) and (83), the amplitudes of stochastic and overtone eigenmodes $1/\lambda_1$ and $1/\lambda_2$ tend to finite limit and infinity, respectively, as distance between two coupled parallel thin wire vibrator-dipoles becomes too small

$$\frac{1}{\lambda_1} \rightarrow \frac{1}{2}, \quad \frac{1}{\lambda_2} \rightarrow \frac{1.4 + 2.4i}{\pi} \frac{h}{b}, \quad \frac{b}{2h} \rightarrow 0 \quad (90)$$

These limits means that at close spacing two coupled parallel thin wire vibrator-dipoles the overtone eigenmode with opposite excited currents direction of propagations is created more preferably compared to stochastic eigenmode with the same excited currents directions of propagations.

Consider now three coupled parallel thin wire vibrator-dipoles centered at the corners of equilateral triangle (Fig.4). In this case Eqs.(41) system for expansion

coefficients $\tilde{J}_z^{(1,2,3)}$ along vector expansion functions (85) of self consistent longitudinal currents $J_z^{(1,2,3)}(\vec{r})$ excited inside three coupled parallel thin wire vibrator-dipoles, with accounting symmetry relations $a_{12} = a_{23} = a_{31}$, takes a form

$$\begin{aligned} \tilde{J}_z^{(1)} - a_{12}\tilde{J}_z^{(2)} - a_{12}\tilde{J}_z^{(3)} &= \tilde{J}_{(1)z}^{(1)}, & \tilde{J}_{(1)z}^{(1,2,3)} &= \int_{-h}^h dz t(z) E_z^{(0)}(\vec{r}_{\perp 1,2,3}, z) \\ -a_{12}\tilde{J}_z^{(1)} + \tilde{J}_z^{(2)} - a_{12}\tilde{J}_z^{(3)} &= \tilde{J}_{(1)z}^{(2)} \\ -a_{12}\tilde{J}_z^{(1)} - a_{12}\tilde{J}_z^{(2)} + \tilde{J}_z^{(3)} &= \tilde{J}_{(1)z}^{(3)} \end{aligned} \quad (91)$$

The matrix of this system obeys a property of stochastic matrix and has two eigenvalues $\lambda_1 = 1 - 2a_{12}$ with stochastic eigenmode

$$(v_z^{(1)}, v_z^{(2)}, v_z^{(3)}) = (1, 1, 1) \quad (92)$$

and degenerated $\lambda_2 = \lambda_3 = 1 + a_{12}$ with two linearly independent overtone eigenmodes written for example as

$$(w_z^{(1)}, w_z^{(2)}, w_z^{(3)}) = (1, -1/2, -1/2); (-1/2, 1, -1/2) \quad (93)$$

The eigenmodes (92) and (93) can be created at special choice of incident electric field. Resolving Eqs.(91) system gives

$$(\tilde{J}_z^{(1)}, \tilde{J}_z^{(2)}, \tilde{J}_z^{(3)}) = \frac{\tilde{J}_{(1)z}^{(1)}}{\lambda_1} (1, 1, 1); \quad \tilde{J}_{(1)z}^{(1)} = \tilde{J}_{(1)z}^{(2)} = \tilde{J}_{(1)z}^{(3)} \quad (94)$$

and

$$(\tilde{J}_z^{(1)}, \tilde{J}_z^{(2)}, \tilde{J}_z^{(3)}) = \frac{\tilde{J}_{(1)z}^{(1)}}{\lambda_2} (1, -1/2, -1/2), \quad \tilde{J}_{(1)z}^{(2)} = \tilde{J}_{(1)z}^{(3)} = -\frac{1}{2} \tilde{J}_{(1)z}^{(1)} \quad (95)$$

The amplitudes of stochastic and overtone eigenmodes $1/\lambda_1$ and $1/\lambda_2$ tend to finite limit and infinity, respectively, as distances between three coupled parallel thin wire vibrator-dipoles become too small, with $1/\lambda_1 \rightarrow 1/3$ and $1/\lambda_2$ going to infinity as in Eq.(90). These limits means that at close spacing three coupled parallel thin wire vibrator-dipoles the overtone eigenmodes with not the same excited currents direction

of propagations are created more preferably compared to stochastic eigenmode with the same excited currents directions of propagations in all three wire vibrator-dipoles.

7.4.2. Linear array of parallel wire vibrator–dipoles with coupling matrix of Jacobi’s property

Consider again the ensemble of N coupled parallel thin wire vibrator-dipoles of length $2h$ each turned to half wavelength and centered now along a strait line coincided with the X axis and oriented along the Z axis of the Cartesian coordinate system (Fig.4). We are interesting in extinction rate of currents’ exciting along wire vibrator-dipoles when this exciting is transfered from the first vibrator-dipole to one with the number N .

The Eqs.(41) system for expansion coefficients $\tilde{J}_z^{(j)}$ along vector expansion functions (85) of self consistent longitudinal currents $J_z^{(j)}(\vec{r})$ excited inside linear array of N coupled parallel thin wire vibrator-dipoles we are writing in a form

$$\sum_{j'=1}^N A_{Njj'} \tilde{J}_z^{(j')} = \tilde{J}_{(1)z}^{(j)}, \quad A_{Njj'} = \delta_{jj'} - a_{jj'} \quad (96)$$

where a specific coupling factor $a_{jj'}$ of two vibrator-dipoles with numbers j and j' is defined by Eq.(87) again. Our task consists in evaluating the expansion coefficient $\tilde{J}_z^{(N)}$ of current excited inside the vibrator-dipole with number N , provided the incident electric field excites the current inside the fist single vibrator-dipole only $\tilde{J}_{(1)z}^{(1)} \neq 0$ and $\tilde{J}_{(1)z}^{(j)} = 0, j > 1$.

To simplify the problem we use a closest neighbour interaction approach putting $a_{jj'} \approx 0$ as $|j - j'| > 1$ and making the matrix $A_{Njj'}$ of Jacobi’s property one (Jacobi’s approximation). Under this simplification our problem is resolved by formula

$$\tilde{J}_z^{(N)} = \frac{a_{12}^{N-1}}{\det A_N} \tilde{J}_{(1)z}^{(1)} \quad (97)$$

Determinant of matrix A_N is evaluated with the aid of recurrent relation

$$\det A_N = \det A_{N-1} - a_{12}^2 \det A_{N-2} \quad (98)$$

For rough estimations one can use an asymptotic solution to this recurrent relation in the form

$$\det A_N = 1 - (N - 1) a_{12}^2 + O(a_{12}^4) \quad (99)$$

The numerical evaluation results of current exciting inside vibrator-dipole with number N relatively to exciting the first vibrator dipole $\tilde{J}_z^{(N)} / \tilde{J}_{(1)z}^{(1)}$ is depicted in Fig.6.

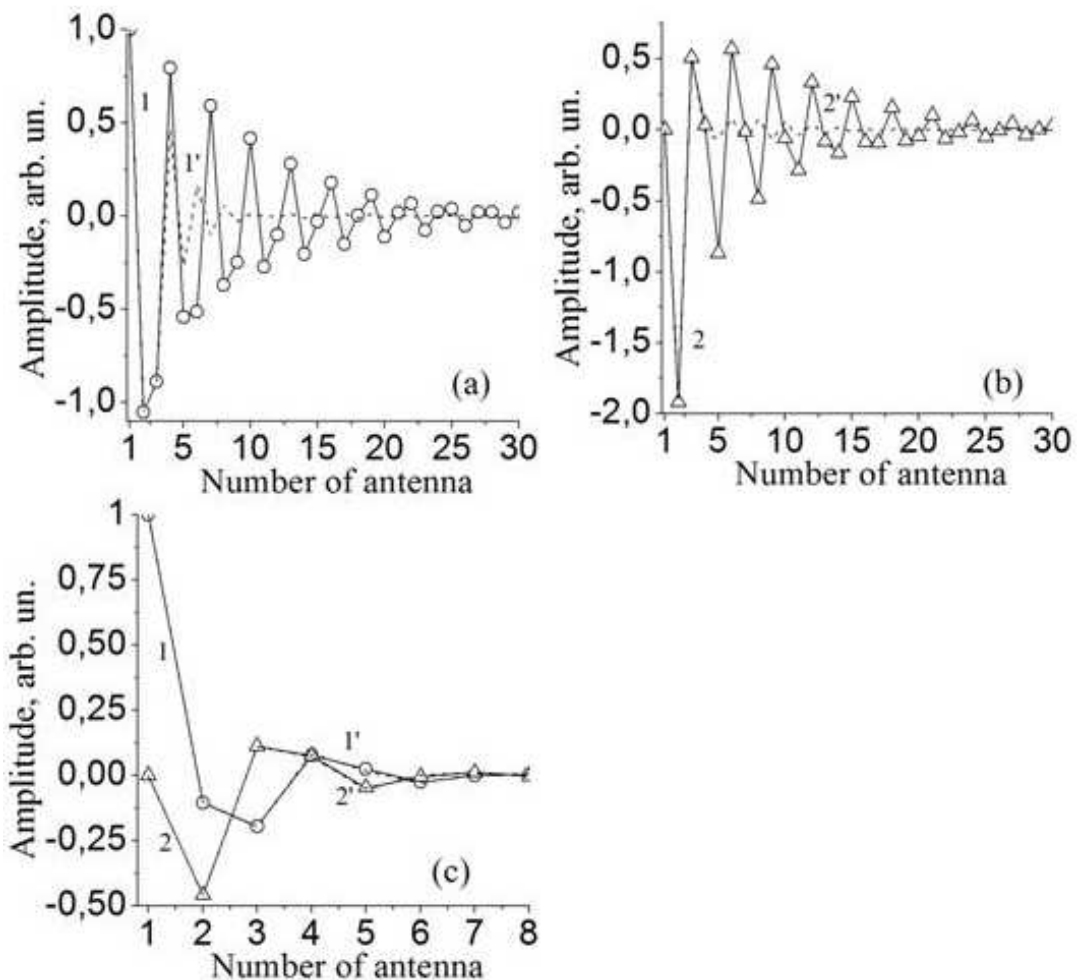


Fig.6. Relative current $\tilde{J}_z^{(N)} / \tilde{J}_{(1)z}^{(1)}$ (Eqs.97) exciting inside N th vibrator

dipole real (curve 1 with circles) and imaginary (curve 2 with triangles) parts dependence on N at $b/2h = 0.1$ (panels (a) and (b)) and 0.5 (panel (c)).

Touch lines 1' and 2' are obtained with the aid of asymptotics (99).

According to these figures the current exciting is transferred from the first vibrator-dipole to one with the number N along straight line of vibrator-dipoles with substantial oscillation in dependence on N and experienced extinction at $N \approx 10$ on level 0.25, with normalized distance between next vibrator-dipoles being $b/2h = 0.1$. The asymptotics (99) gives for curves on Fig.6(a,b) not enough in accuracy approximation yet. This accuracy is enough for curves on Fig.6(c) where spacing between next vibrator dipoles becomes bigger $b/2h = 0.5$ and current exciting is transferred along straight line of vibrator-dipoles to $N \approx 3$ only.

7.4.2.1. Standing and propagating waves of currents' exciting along linear array of vibrator-dipoles and particles at all

According to Fig.6 the currents' exciting is transferred from the first vibrator-dipole to the N th one along straight line of vibrator-dipoles with substantial oscillations in dependence on N . The physical reason for these oscillations consists in specific property of Eqs.(96) system matrix A_N in Jacobi's approximation. Namely, the middle $N-2$ rows of this matrix have sum of their elements equal to $1-2a_{12}$ whereas the first and N -th rows have sum of their elements equal to $1-a_{12}$. Because of that the first and N -th equations of system (96) play role of specific boundary conditions for the rest middle $N-2$ equations and solution to the Eqs.(96) system becomes similar to elastic string oscillations [36], being rather standing wave of currents' exciting along linear array of vibrator-dipoles than propagating wave. Nevertheless in the middle part of a long array the solution under study is approximately a propagating wave. Next we give analytic confirmation for predicted physical feature of Eqs.(96) system solution.

Recurrent relation (98) for determinant of Eqs.(96) system matrix in Jacobi's approximation enables one to get solution to this system analytically, provided the incident electric field excites the current inside the first single vibrator-dipole only (see some details to solution in Appendix C)

$$\tilde{J}_z^{(j)} = (-1)^{j+1} 2 \cos \vartheta \frac{\sin(N+1-j)\vartheta}{\sin(N+1)\vartheta} \tilde{J}_{(1)z}^{(1)}, \quad \cos \vartheta = -\frac{1}{2a_{12}} \quad (100)$$

The second Eq.(100) is dispersion equation for the complex variable $\vartheta = \vartheta' + i\vartheta''$. In the middle part of a long linear array of vibrator-dipoles, when $N \rightarrow \infty$ and vibrator position number j is fixed, Eq.(100) gives asymptotically

$$\tilde{J}_z^{(j)} \rightarrow -2 \cos \vartheta \exp(ibjk) \tilde{J}_{(z1)}^{(1)}, \quad k = \frac{\pi - \vartheta'}{b} \quad (101)$$

where $\vartheta'' > 0$ and k is a wave number. Having known the wave number, one can evaluate as usually [41] corresponding phase velocity v_{ph} and group velocity v_g putting

$$v_{ph} = \frac{\omega}{k}, \quad v_g = \frac{d\omega}{dk}, \quad \frac{1}{v_g} = \frac{1}{v_{ph}} - \frac{\omega}{v_{ph}^2} \frac{dv_{ph}}{d\omega} \quad (102)$$

The frequency dependence of wave number is obtained by solution of dispersion Eq.(100). Being complicate in general, this dispersion equation is simple resolved analytically in physically interesting case of $|a'_{12}| > 1/2$ and $a''_{12} = 0$ when wave number takes a form

$$k = \frac{1}{b} \arccos \frac{1}{2|a'_{12}|}, \quad \vartheta'' = 0 \quad (103)$$

Apply the obtained form (103) for dispersion equation to the limit of small distances between linear array vibrator-dipoles tuned to half wavelength when according Eq.(88) the coupling factor a_{12} approximates to minus one and wave phase velocity in Eq.(102) due to Eq.(103) is given by

$$\frac{v_{ph}}{c_0} \rightarrow \frac{3}{\pi} k_0 b \ll 1 \quad (104)$$

where c_0 denotes the light speed in free space. To evaluate the group velocity one needs considering the case of weakly detuned vibrator-dipoles, which length is lightly different from half wavelength and vibrator-dipole input impedance Z_1 is defined according to [48] via relations

$$\begin{aligned} \frac{\omega \mathcal{E}_0}{k_0} Z_1 &= Di(2\pi) - i 2\pi \ln \left(\frac{1}{k_0 a} \right) \frac{\omega - \omega_R}{\omega_T}, \\ \frac{\omega_R}{\omega_T} &= 1 - \frac{Si(2\pi)}{2\pi \ln(1/k_0 a)}, \quad \omega_T = c_0 \frac{\pi}{2h} \end{aligned} \quad (105)$$

As one can verify at resonance frequency $\omega = \omega_R$ the input impedance becomes pure real and at tuned frequency $\omega = \omega_T$ the input impedance value is consistent with Eq.(88). Substituting now the weakly detuned vibrator-dipole impedance (105) into expression for a_{12} in Eq.(88) and the last into Eq.(102) with accounting Eq.(103) gives for group velocity at resonance frequency a value

$$\frac{v_g}{c_0} \rightarrow - \frac{\sqrt{3} Di^2(2\pi)}{4 \ln(1/k_0 a)} \quad (106)$$

The obtained value shows that group velocity of currents' exciting propagation between close packed resonance vibrator-dipoles is negative in sign and small in magnitude compared with light speed in vacuum.

Return to analytic solution (100) to Eq.(96) system. Bearing in mind definition (101) for wave number, this solution describes rather standing wave of currents' exciting along linear array of vibrator-dipoles than propagating wave, though asymptotics (101) for the middle part of a long linear array of vibrator-dipoles when $N \rightarrow \infty$ and j is fixed describes propagating wave. Consider now a limit for the right end part of the long linear array $N = j \rightarrow \infty$ corresponding to solution in Eq.(97). Asymptotics of analytic solution (100) for the right end describes a standing

wave, with exponentially decreasing amplitude as $\exp(-N|\vartheta''|)$ in accordance to Fig. 6(c). Especially interesting from physical point of view to note a special case $\vartheta'' = 0$, which realized for dispersion equation (103) and when above amplitude exponentially decreasing effect is canceled. In this case the asymptotics for expansion coefficient (97) of current excited inside the vibrator-dipole with number N takes a form

$$\tilde{J}_z^{(N)} \rightarrow 2 \cos \vartheta' \left[\exp(i 2\vartheta') \exp(i N(\pi + \vartheta')) - \exp(i N(\pi - \vartheta')) \right] \tilde{J}_{(1)z}^{(1)} \quad (107)$$

This asymptotics substantially oscillates in dependence on N as was noticed on the Fig.6.

8. Conclusion

In this work, we have presented obtained for the first time analytic solution to fundamental in electromagnetic wave multiple scattering theory Lippmann-Schwinger (LS) integral equation for T-scattering operator of electric wave field by dielectric and conducting nonmagnetic particle of arbitrary size and shape. The solution is derived with the aid of a chosen vector expansion functions' basis and written as sum of separable scattering operators weighted by inverse of a generating matrix and named quasi-separable (QS) T-scattering operator. The QS solution to LS equation is generalized for ensemble of coupled particles in free space as well as for coupled particles inside unit cell of electromagnetic crystal. An equations' system for self consistent currents excited inside coupled particles was derived also in QS form.

In the case of a single spherical particle we have verified that vector expansion functions' basis chosen as vector spherical wave functions the QS T-scattering operator gives the Mie solution for incident transverse plane wave scattered from particle and transmitted inside particle. The elements of diagonal generating matrix are presented for this case in terms of Mie scattering coefficients and special bilinear functionals of spherical vector wave functions on spherical particle volume. We considered also a principally another choosing the vector expansion functions'

defined on finite elements of particle volume and named conditionally pre-Haar basis. It was shown that such “basis”, even including finite number of expansions’ functions, leads to QS simplified scattering potential operator and automatically to a corresponding exact solution to LS equation, which tends to solution of LS equation with actual, not simplified scattering potential operator when number expansions’ function of pre-Haar basis becomes infinite.

Mentioned above equations’ system for self consistent currents excited inside coupled particles can be resolved in general case with the aid of recursive procedure, which is appeared at a particle attachment in spirit of invariant imbedding method. But for some interesting special cases this system is resolved via simple methods analytically. On this way were considered such phenomena as artificial double diamagnetic-paramagnetic narrow peak in metamaterial with unit cell of coupled plasmonic particles; creation for eigenmodes with overtones in periodic arrays of particles with coupling matrix of stochastic property; extinction rate for transfer of currents’ exciting in linear array of particles with coupling matrix of Jacobi’s property and standing and propagation wave phenomenon for such transfer.

APENDIX A. Diagonal generating matrix (55) in terms of Mie scattering coefficients and bilinear (k_0, k) -functional of spherical vector wave functions

Let us denote (k_0, k) a bilinear functional of spherical vector wave functions on spherical particle volume Ω defined by

$$\begin{aligned} & \left[\vec{M}_{e(o)mn}(k_0), \vec{M}_{e(o)mn}(k) \right] \\ & \equiv \int_{\Omega} d\vec{r} \left(\vec{M}_{e(o)mn}(k_0) \vec{M}_{e(o)mn}(k) \right) \\ & = \kappa_{mn} \frac{1}{k_0 k (k_0^2 - k^2)} \times \left[k \psi_n(k_0 r_0) \psi_n'(k r_0) - k_0 \psi_n(k r_0) \psi_n'(k_0 r_0) \right] \end{aligned} \tag{A1}$$

and similarly

$$\begin{aligned}
 & \left[\vec{N}_{e(o)mn}(k_0), \vec{N}_{e(o)mn}(k) \right] \\
 & \equiv \int_{\Omega} d\vec{r} \left(\vec{N}_{e(o)mn}(k_0) \vec{N}_{e(o)mn}(k) \right) \\
 & = \kappa_{mn} \frac{1}{k_0 k (k_0^2 - k^2)} \times [k_0 \psi_n(k_0 r_0) \psi'_n(k r_0) - k \psi_n(k r_0) \psi'_n(k_0 r_0)]
 \end{aligned} \tag{A2}$$

Here an auxiliary matrix is used

$$\kappa_{mn} = 2\pi(1 + \delta_{m0}) \frac{n(n+1)(n+m)!}{2n+1(n-m)!} \tag{A3}$$

and $\psi_n(\rho)$ is Riccati-Bessel function (see [43], page 129). The basic result of this Appendix A consists in the following formulas for diagonal generating matrix (55) elements

$$\begin{aligned}
 \frac{ik_0}{\chi_{Me(o)mn}^{(0)}} &= \frac{\kappa_{mn} b_n}{\left[\vec{M}_{e(o)mn}(k_0), \vec{M}_{e(o)mn}(k) \right]^2}, \\
 \frac{ik_0}{\chi_{Ne(o)mn}^{(0)}} &= \frac{\kappa_{mn} a_n}{\left[\vec{N}_{e(o)mn}(k_0), \vec{N}_{e(o)mn}(k) \right]^2}
 \end{aligned} \tag{A4}$$

There are also simple relations between Mie scattering and transmission coefficients

$$\begin{aligned}
 \frac{b_n}{c_n} &= ik_0 \frac{k_0^2 - k^2}{\kappa_{1n}} \left[\vec{M}_{e(o)1n}(k_0), \vec{M}_{e(o)1n}(k) \right], \\
 \frac{a_n}{d_n} &= ik_0 \frac{k_0^2 - k^2}{\kappa_{1n}} \left[\vec{N}_{e(o)1n}(k_0), \vec{N}_{e(o)1n}(k) \right]
 \end{aligned} \tag{A5}$$

that can help to understand the derivation of Eqs.(58) and(59) with the aid of QS T-scattering operator (56).

In electric and magnetic dipole approximation the QS T-scattering operator (56) becomes equal to a sum

$$\overline{\overline{T}}(\vec{r}, \vec{r}') \cong \overline{\overline{T}}^{el}(\vec{r}, \vec{r}') + \overline{\overline{T}}^{mag}(\vec{r}, \vec{r}') \tag{A6}$$

where the RHS first “electric” and second “magnetic” terms are created by Eq.(56) second and first terms, respectively, taken in approximation $n = 1$, $m = 0, 1$. For the case of small spherical particle $k_0 r_0 \ll 1$, $kr_0 \ll 1$ we find

$$\begin{aligned} \bar{\bar{T}}^{el}(\vec{r}, \vec{r}') &\cong -4\pi k_0^2 \eta \delta(\vec{r}) \delta(\vec{r}') \bar{\bar{I}}, \\ \bar{\bar{T}}^{mag}(\vec{r}, \vec{r}') &\cong -4\pi \mu (\nabla \times) \otimes (\nabla' \times) \delta(\vec{r}) \delta(\vec{r}') \bar{\bar{I}} \end{aligned} \quad (A7)$$

with $\eta = (3i/2k_0^3)a_1$ and $\mu = (3i/2k_0^3)b_1$ being the spherical particle electric and magnetic susceptibilities, respectively.

In the first formula (A7) for QS T-scattering electric dipole approximation a Dirac delta-function is appeared, actually, as expression

$$\delta(\vec{r}) \cong \frac{H(\vec{r} \subset \Omega)}{|\Omega|} \quad (A8)$$

and similarly when argument \vec{r} is replaced to \vec{r}' , in accordance with Dirac delta-function analog definition in Eqs.(63) by considering functions defined on particle finite elements. Formulas (A7) were obtained in ref.[17] via the Hertz’s vector of electric dipole and magnetic dipole scattering study. One can rewrite the electric and magnetic dipole approximations (A7) for T-scattering operator in QS form (13) as

$$\begin{aligned} \bar{\bar{T}}^{el} &= \sum_{n=1}^3 \vec{t}_n^{el}(\vec{r}) \otimes \vec{t}_n^{el}(\vec{r}'); \bar{\bar{T}}^{mag} = \sum_{n=1}^3 \vec{t}_n^{mag}(\vec{r}) \otimes \vec{t}_n^{mag}(\vec{r}') \\ \vec{t}_n^{el}(\vec{r}) &= (-4\pi k_0^2 \eta)^{1/2} \hat{e}_n \delta(\vec{r}); \vec{t}_n^{mag}(\vec{r}) = (-4\pi \mu)^{1/2} \nabla \times \hat{e}_n \delta(\vec{r}) \end{aligned} \quad (A9)$$

where unit vectors \hat{e}_n are defined in subsection 7.2. Note that electric dipole vector expansion function $\vec{t}_n^{el}(\vec{r})$ in Eq.(A9) with analog Dirac delta-function (A8) satisfies automatically the solenoidal restriction in the last Eq.(6) for points laying strictly inside spherical particle domain. With accounting points on spherical particle surface or in the case of true Dirac delta-function the solenoidal restriction on electric dipole vector expansion function is verified with the aid of generalized function theory (see next Appendix B). Magnetic dipole vector expansion function in Eq.(A9) satisfies the solenoidal restriction automatically.

APENDIX B. Solenoidal restriction on finite element vector expansions' functions (65)

Let us verify that vector expansions' functions (65) defined on finite elements of particle volume satisfy with corresponding accuracy to solenoidal restriction in the last Eq. (6) in weak sense of theory of generalized functions [51]. For points lying strictly inside particle volume domain the solenoidal restriction is satisfied exactly. Take divergence of a vector function (65) and integrate this differential operation with product by a test smooth function $\varphi(\vec{r})$ of compact support. We obtain

$$\int d\vec{r} \varphi(\vec{r}) \nabla \vec{t}_{np}(\vec{r}) = - \int d\vec{r} \frac{\partial \varphi(\vec{r})}{\partial x_p} t_n(\vec{r}) \quad (\text{B1})$$

We suppose for simplicity that all subdomains Ω_n have form of cubes with their edges being parallel to the axes of the Cartesian coordinate system. Denoting $\varphi(x_p; \Omega_{p\perp})$ the test function averaged over cube 2D section $\Omega_{p\perp}$ perpendicular to x_p axis one can transform

$$\int d\vec{r} \varphi(\vec{r}) \nabla \vec{t}_{np}(\vec{r}) = -\sqrt{|\Omega_n|} \frac{1}{a} \left[\varphi(x_{np} + \frac{a}{2}; \Omega_{np\perp}) - \varphi(x_{np} - \frac{a}{2}; \Omega_{np\perp}) \right] \quad (\text{B2})$$

where x_{np} is subdomain centre coordinate and a denotes the cube edge length, with $|\Omega_n| = a^3$. In the limit of $a \rightarrow 0$ Eq.(B2) RHS tends to zero as $-a^{3/2} \partial \varphi(x_{np}; \Omega_{np\perp})$.

APENDIX C. Analytic solution to Eqs.(96) system in Jacobis' approximation

Turn to recurrent relation (98) for Eqs.(96) system matrix determinant. One can directly verify the following solution to this recurrent relation

$$\det A_N = \frac{\sin(N+1)\vartheta}{2^N (\cos \vartheta)^N \sin \vartheta} \quad (\text{C1})$$

Solution in Eq.(100) to Eqs.(96) system is written out first as

$$\tilde{J}_z^{(j)} = (-1)^{j+1} (-a_{12})^{j-1} \frac{\det A_{N-j}}{\det A_N} \tilde{J}_{(1)z}^{(1)} \quad (C2)$$

that is verified directly again. Transformation of solution (C2) to the form in Eq.(100) is performed using Eq.(C1).

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