Abstract

Bulk Response of Composites from Finite Samples

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Received: Fri, 15 Mar 2002 21:55:48

Due to the long range of the dipolar interaction, boundary effects on the polarization induced on composite media made up of a disordered array of spherical particles remain finite even in the thermodynamic limit. Thus, the numerical calculation of the response of composites has frequently been preformed on infinite systems constructed by repeating periodically replicas of a unit cell with a finite number of particles and using Ewald summation techniques to compute the interactions between particles and their replicas [1]. As this procedure is computationally demanding, the number of particles in the unit cell has necessarily been modest. In this work we propose an alternative procedure. We calculate directly in real space the response of a finite spherical disordered composite sample taking account explicitly of its depolarization. To obtain an accurate result we have to include a relatively large number of particles, but with no replicas and therefore with simpler interactions. Furthermore, we accomplish our calculation in a very efficient way by employing a newly developed multi-resolution hierarchical scheme [2]. We compare our results with the numerical results of Ref. [1] and with those of an analytical theory [3] based on a renormalized polarizability which differs from the response of individual particles due to the fluctuations of the dipolar interactions. We have also extended the renormalized polarizability theory by calculating these fluctuations within our scheme without employing approximate expressions in terms of the two-particle correlation functions [3].

This work was supported by DGAPA-UNAM, CONACYT and CIP-COMEX.

- [1] B. Cichocki and B. U. Felderhof J. Chem. Phys. 90 4960 (1989) 92 6104 (1990).
- [2] G. P. Ortiz and W. L. Mochán, SPIE 4419, 752 (2001) submitted to PRB.
- [3] R. G. Barrera, G. M. Monsivais, and W. L. Mochán. Phys. Rev. B 38, 5371, (1988).

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Filename: Ortiz2 Last document update: Wed Jul 10 08:15:31 MDT 2002