Spectral Measure Computations for Composite Materials

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Referee report

The analytic continuation method (ACM) is a powerful mathematical tool in understanding the relationship between microstructure and properties of composite materials. The key element of this paper is Theorem 2.1 which extends the ACM representation for infinite lattice and continuum systems to finite lattice settings. It provides a solid theoretical basis for previous computational work on finite lattices and enables the authors to develop a rigorous computational method for calculating the spectral representation of a finite lattice model. This numerical method is a significant improvement on previous numerical work, particularly the applicability of the method to three dimensional systems. These results (Theorem 2.1, the numerical method, and the 3D calculations) are a significant contribution to the field and should motivate further research in this area. I highly recommend publication although a have some suggestions and a few questions.

Suggested changes

1) The computational method and the numerical calculations are a major contribution of this paper but there are very few details of the numerical method. Providing more information would increase the impact of the paper amongst computational physicists and materials scientists. In particular, it would be helpful if the authors identified the algorithm they used to calculate the spectral measure. It was unclear to the reviewer whether the authors calculated every eigenvalue and then binned them to obtain the spectral measure histograms or whether they used an algorithm that computes the number of eigenvalues in a particular range. Some information about how the algorithm execution time scales with N (the dimension of the matrix M) and information about the binning of the eigenvalues such as how many elements there are in the histogram representations of μ and κ would also be useful. If the authors do not want to include this in the main body of the paper it could be included in an appendix.
2) The caption of figure 3.6 refers to figures (a), (b), (c) and (d) but figures (c) and (d) are not labeled.
3) In figure 3.6 the authors should just plot the actual data without "connecting the dots." With the connecting lines the figure showing the endpoint masses for the 2D random resistor network suggests a significant endpoint mass for $0.3 < p < 0.5$. In fact (within the limits of finite size effects) the end point masses should be zero for all $p < p_c = 0.5$ and if the endpoint mass were calculated just below p_c (say $p=0.48$) it would probably be appear to be zero on this figure. The same comment also applies to the figure for the endpoint masses in the 3D system.
4) To save space, section 2.3 could be eliminated. None of the theory developed in in this section is specific to the finite lattice problem: all the analysis seems to be valid for both the infinite system and the finite system and the results are all available in previous work on the infinite system. If section 2.3 is eliminated figures 3.1(d), 3.2(c), 3.3(c) and figure 3.5 could be

eliminated. If these figures are not eliminated the paper would be easier to read if the figure captions made it clear that the bounds are specific to a model with the material parameters of sea ice and brine.

Questions

1) In Figure 3.3(b) for the locally isotropic lattice there seems to be an anomalously large difference between the theory and the numerical calculation in the neighborhood of $\lambda = 0.2$. Do the authors have any explanation for this "bump" in the numerical curve?
2) The results for the three dimensional network shown in Figure 3.4 are a significant result of this paper and raise a number of questions.
    a. The authors discuss the relationship between the spectral measures μ and α but it seems there should also be a relationship between μ and κ. Specifically, if you know μ the effective conductivity σ* can be determined. This in turn determines $\rho^*=1/\sigma^*$. Once ρ* is known κ can be determined using the Stieltjes-Perron inversion theorem. Obviously the relationship is complicated but it is surprising that the curve for κ is so smooth. Even at low concentrations κ does not display any of the sharp peaks that are evident in μ at low concentrations. Because these peaks are identified with "lattice animals" it is surprising that they are not present in the in κ which, after all, is describing the same lattice. It would be interesting if the authors could comment on this.
    b. The authors' discussion of the gap in the spectral function κ(λ) near λ=1 does not seem to agree with the curves plotted in figure 3.4 (b). The authors state: "For a volume fraction of p_1=0.001 (not shown) there is a clear gap in the spectral function about $\lambda = 0$ and $\lambda = 1$. The gap near $\lambda = 1$ collapses as $p \rightarrow p_c$." However, in the figure, as p increases from 0.05 to 0.13 to 0.17 to 0.2488 the spectral function seems to shift to the left (away from $\lambda = 1$) and the gap seems to <u>grow</u> as p approaches $p_c = 0.2488$. In fact, at p=0.2488 there appears to be a clear gap in the spectrum near λ=1.
    c. In figure 3.4 (a) there seems to be a dark line along the vertical axis at λ=0 suggesting endpoint masses even for $p < p_c$. Is this a finite size effect? For the infinite system the endpoint mass should be zero for $p < p_c$.

Summary

I highly recommend publication if the authors address the suggested changes and clarify the discussion of figure 3.4(b) (Question 2(b)). It would be interesting if the authors could address some of the other questions.