Spectral Measure Computations for Composite Materials

N. B. Murphy, E. Cherkaev, C. Hohenegger, and K. M. Golden

Responses to Referee Reviews

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.

   We have included in the revision of the manuscript a detailed discussion regarding our numerical method, including: the specific algorithm used to compute the eigenvalues and eigenvectors underlying the spectral measure, the size of the data sets used to compute statistical quantities, as well as details regarding the computation of the spectral functions (spectral measure histograms). The computational cost of the simulations was also mentioned, while the simulation time scales were not discussed as they depend strongly on the computer architecture used.

2) The caption of figure 3.6 refers to figures (a), (b), (c) and (d) but figures (c) and (d) are not labeled.

   This typographical error was corrected in the revision of the manuscript.

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.

   Figure 3.6 was changed according to the referee's suggestions.

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.

The authors have chosen not to remove Section 2.3, as it reviews the problem of providing rigorous bounds for the effective transport coefficients of composite media. This is a key application of the analytic continuation method that also illustrates important properties of the associated integral representations and spectral measures. We have clarified in the captions and the body of the revised manuscript that the bounds depend on the values of the local material properties of the composite, such as the constituent conductivities.

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?

   We have discussed in the revision of the manuscript how this deviation from the theoretical prediction, which holds for infinite systems, is a finite system size effect which decreases with increasing system size.

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.

      We have discussed in the revision of the manuscript that the smoothness of the computed spectral functions, underlying the effective resistivity ρ^*, is likely due to a numerical instability in the computations caused by a large condition number of an underlying matrix. We also discussed that the computed spectral functions have a qualitatively correct behavior, which is analogous to the behavior of the spectral functions underlying the effective conductivity σ^*, which were computed in a relatively stable way. We also discussed various consistency checks for the validity of our computations.

      A discussion regarding the relationship between μ and κ is beyond the scope of the present manuscript. The relationship suggested by the formula $\rho^*=1/\sigma^*$ becomes much more complicated for anisotropic random media, for which the formula is no longer valid. This has been a topic of ongoing research.

   b) The authors' discussion of the gap in the spectral function $\kappa(\lambda)$ near $\lambda=1$ 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 grow 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.

In order to reduce the numerical instability associated with this computation, as mentioned above, in the revision of the manuscript we display new spectral functions that were computed using a reduced system size. The new figure illustrates the gap behavior more clearly.

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 $p < p_c$.

We have clarified this in the revision of the manuscript by adding a discussion of Lifshitz tails in the measures.