Computing the non-interacting electronic response function using Wannier interpolation: applications to magnons

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Obtaining the non-interacting electronic response function of bulk systems or surfaces is a key step in describing their collective electronic excitations.

Computing this response function from ab initio can be an extremely demanding numerical task because the necessary sum over the first Brillouin zone must be performed on a dense mesh; this is especially true when studying low frequency features.

We propose a novel method for computing the response function which utilizes maximally localized Wannier functions [1,2]. While their construction requires the ab initio eigenvalues and wavefunctions on a relatively coarse reciprocal space "k" mesh, they can be used to interpolate the necessary input to the response calculation on a very dense "k" mesh. The numerical cost of this procedure is but a small fraction of the cost of performing a full non-self consistent ab initio calculation.

In this talk we will also present results when the method is applied to various systems of interest and particularly the computation of magnon dispersions in ferromagnets.

References

[1] Marzari, Nicola and Vanderbilt, David, Phys. Rev. B, **56** (1997) 12847
[2]Souza, Ivo and Marzari, Nicola and Vanderbilt, David, Phys. Rev. B**, 65** (2001) 035109