Probing the ab-initio Fermi surface efficiently using Wannier interpolation

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Modern *Ab-initio* techniques are able to provide an accurate description of the electronic structure for a wide range of materials. However, evaluation of the transport properties of metals requires an extremely detailed, and hence computationally expensive, sampling of the Fermi surface. We show that the electron group velocity and effective mass can be obtained directly from the Wannier representation of a system. This leads to an efficient and precise method for the calculation of transport properties using Wannier interpolation. We will present calculations of the ordinary Hall coefficient for a variety of materials. Calculations were performed using the Wannier90 code[1].

[1] www.wannier.org