Green's function method and its application to first-principles calculation of electric transport phenomena

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The Green's function method has been widely used in the field of condensed matter theory. In this lecture I explain the basic idea of Green's function method in the first principles electronic structure calculation and its application to electric transport phenomena.

Contrary to its apparent simplicity of the Green's functions method constructed in a finite Hilbert space, the Green's functions actually used in the first principle calculation contain fundamental difficulties arising from their unbound nature (the energy spectrum extends to infinity). This requires very careful treatment of the Green's functions as well as numerical works including computer coding. Despite of these, the Green's function method becomes one of the most powerful methods in the first principles electronic structure calculation.

One of the reasons of the above exists in its computational efficiency. It is fast and compact. Another reason is its wide applicability. For example, the application of the method to disordered systems is straightforward in the framework of the coherent potential approximation. Also, various correlation functions can be calculated without any extra work, which sometimes would require extremely heavy computation.

As examples of the applications of the Green's function method, I will show the results of the first principles calculation of electric transport phenomena, which contain DC conductivity, optical conductivity, X-ray absorption and magnetic circular dichroism, and Seebeck coefficient.