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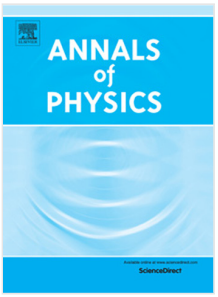

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Scattering matrix of arbitrary tight-binding Hamiltonians

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Abstract
A novel efficient method to calculate the scattering matrix (SM) of arbitrary tight-binding Hamiltonians is proposed, including cases with multiterminal structures. In particular, the SM of two kind of fundamental structures are given, which can be used to obtain the SM of bigger systems iteratively. Also, a procedure to obtain the SM of layer-composed periodic leads is described. This method allows renormalization approaches, which permits computations over macroscopic length systems without introducing additional approximations. Finally, the transmission coefficient of a ring-shaped multiterminal system and the transmission function of a square-lattice nanoribbon with a reduced width region are calculated.

Keywords Scattering Matrix, Scattering Theory, Landauer Conductivity, Tight-binding Hamiltonian

1. Introduction

The conductance is one of the most important properties of a material, which is also very susceptible to quantum effects caused by miniaturization. Theoretically, the conductance (G) for quantum systems in the nanoscale can be calculated from the Landauer formula [1]

$$G = \frac{e^2}{\pi\hbar} T \tag{1}$$

where T is the transmission coefficient for single-channel systems or the transmission function in multi-channel ones [2]. For Layered composed systems, fast techniques to determine the Landauer conductance based on the transfer matrix approach have been widely used [3-8], where the wavefunction behavior is iteratively obtained by means of multiplications of transfer matrixes. However, it is also well known that such multiplications could introduce important numerical instabilities during calculations [9]. To overcome these instabilities, calculations of the scattering matrix (SM) from the transfer matrix [10] or by wave function matching [11] have been proposed. SM of combined systems can then be found by using the Redheffer star product [12]. The SM relates the incoming and outgoing waves of a scattering region and in general also depends on the external systems. This implies the calculation of SM between every different layer interface, which could be computationally expensive. For electromagnetic waves, this issue is solved by separating