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Theory of electron hopping through atomic-scale contacts KENJI HIROSE, Fund. Res. Labs., NEC Corp. and CREST, JST, NOBUHIKO KOBAYASHI, Nanotech. Res. Inst., AIST and CREST, JST — With the rapid progress of constructing atomic-scale nanostructure devices, understanding of electron transport between electrodes becomes an important problem. In such systems, the transfer of an electron is achieved *via* tunneling or ballistically through atomic-scale contacts. Here, we consider the junction system with atomic-scale contacts and evaluate the current-voltage characteristics as a function of the distance between electrodes. We use the recursion transfer matrix (RTM) method with plane-wave basis sets to obtain accurate scattering states between electrodes under finite bias voltages. Then we construct the nonequilibrium Green's function (NEGF) to evaluate charge densities and current-voltage characteristics from the obtained scattering states. Based on the density-functional method, we perform self-consistent calculations of the charge density and effective potential for the junctions systems. This method enables us to treat accurate scattering states from tunneling to ballistic transport regimes. As the distance between electrodes becomes large, we find a strong nonlinear behavior in the current-voltage (I-V) characteristics and correspondingly a gap structure appears in conductance. We consider the mechanism to appear such nonlinear behavior in I-V characteristics and compare the experimental observations.

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