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Generalized non-equilibrium vertex correction method in coherent medium theory for quantum transport simulation of disordered nanoelectronics[1] JIAWEI YAN, YOUQI KE, School of Physical Science and Technology, ShanghaiTech University — In realistic nanoelectronics, disordered impurities/defects are inevitable and play important roles in electron transport. However, due to the lack of effective quantum transport method, the important effects of disorders remain poorly understood. Here, we report a generalized non-equilibrium vertex correction (NVC) method with coherent potential approximation to treat the disorder effects in quantum transport simulation. With this generalized NVC method, any averaged product of two single-particle Greens functions can be obtained by solving a set of simple linear equations. As a result, the averaged non-equilibrium density matrix and various important transport properties, including averaged current, disordered induced current fluctuation and the averaged shot noise, can all be efficiently computed in a unified scheme. Moreover, a generalized form of conditionally averaged non-equilibrium Green's function is derived to incorporate with density functional theory to enable first-principles simulation. We prove the non-equilibrium coherent potential equals the non-equilibrium vertex correction. Our approach provides a unified, efficient and self-consistent method for simulating non-equilibrium quantum transport through disorder nanoelectronics.

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Jiawei Yan
School of Physical Science and Technology, ShanghaiTech University

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