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SymGF: A Symbolic Green's Function Derivation Method ZIMIN FENG, Physics Department, McGill University, Montreal, Canada, QINGFENG SUN, Institute of Physics, Chinese Academy of Sciences, Beijing, P. R. China, HONG GUO, Physics Department, McGill University, Montreal, Canada — Keldysh non-equilibrium Green's function (NEGF) formalism is widely used in quantum transport theory. For transport problems involving interacting electrons, it can be a tedious and error prone process to derive the transport formula and various NEGF. We have developed a symbolic method called SymGF, based on Mathematica, for computer aided derivation tasks of NEGF in quantum transport theory. By inputting second quantized Hamiltonian of the transport model, the commutation and truncation rules for the operators and correlators, SymGF automatically derives various NEGF that enters transport formula such as conductance and current-voltage characteristics. SymGF is useful to deal with transport structures having multiple spin-resolved quantum dots with on-site Coulomb repulsion, connected to external non-interacting leads. It achieves overwhelming efficiency compared with manual derivation. We will present several examples of SymGF.

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