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Order $O(1)$ algorithm for first-principles transient current through open quantum systems KING TAI CHEUNG, ZHIZHOU YU, BIN FU, JIAN WANG, The University of Hong Kong — First principles transient current through molecular devices is known to be extremely time consuming with typical computational complexity T^3N^3 where N and T are the dimension of the scattering system and the number of time steps respectively. Various algorithms have been developed which eventually brings the complexity down to cTN^3, a linear scaling in T, where c is a large coefficient comparable to N. Here we provide an order $O(1)$ algorithm that reduces it further to $c_1N^3 + c_2TN^2$ where c_1 and c_2 are $\sim$50 and 0.1 respectively. Hence for $T < N$, the transient calculation is independent of T, thus order $O(1)$ is achieved. To make this happening four important ingredients are essential: (1). availability of exact solution based on non-equilibrium Green's function (NEGF) that goes beyond wideband limit; (2). the use of complex absorbing potential (CAP) so that all the pole of Green's function can be found; (3). the exact solution is separable between real space and time domain; (4). the exploit of Vandermonde matrix further reduces the scaling of TN^2 to $TlnTN$ for $T > N$. Benchmark calculation has been done on graphene nanoribbons using Tight-binding (TB) Hamiltonian with a huge speed up factor of $100T$, confirmed the $O(1)$ scaling.

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