

Abstract Submitted
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Projection operators - non-equilibrium Green functions approach to quantum transport MAICOL OCHOA, MICHAEL GALPERIN, UC San Diego, MARK RATNER, Northwestern University — We consider projection operator approach to non-equilibrium Green function equation-of-motion (PO-NEGF EOM) method. The technique resolves problem of arbitrariness in truncation of an infinite chain of EOMs, and prevents violation of symmetry relations resulting from the truncation. The approach, originally developed by Tserkovnikov [Theor. Math. Phys. **118**, 85 (1999)] for equilibrium systems, is reformulated to be applicable to time-dependent non-equilibrium situations. We derived canonical form of EOMs, thus explicitly demonstrating a proper introduction of the non-equilibrium atomic limit in junction problems. A simple practical scheme applicable to quantum transport simulations is formulated. We perform numerical simulations within simple models, and compare results of the approach to other techniques, and where available also to exact results.

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