

STATIONARITY PRINCIPLE FOR NON-EQUILIBRIUM STATES

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Stationary current transport through molecular electronic devices (MEDs) represents a non-equilibrium problem. We develop a pseudo-Hermitian Hamiltonian that yields eigenfunctions describing the non-equilibrium state. A stationarity principle for the pseudo-Hermitian Hamiltonian is constructed that resembles the variational method of conventional Hermitian quantum mechanics. This stationarity principle permits the use of many techniques of conventional electronic structure theory, such as the configuration interaction method. As an application of the stationarity principle, we develop a generalization of Kohn-Sham density functional theory suitable for MEDs.