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Molecular transport in the language of many-body states
MICHAEL GALPERIN, UCSD — Recent advancements in experimental techniques at nanoscale caused a surge in research of transport through molecular junctions. Nonlinearity of current-voltage characteristic at resonance makes this regime particularly important for potential molecular based memory, switchers and logic devices. One of important differences of molecular junctions (compared e.g. to semiconductor QDs) is sensitivity of electronic and vibrational structure of the junction to oxidation/reduction of the molecule. This implies necessity of treating the transport at resonance in the language of molecular states rather than single particle orbitals. The latter are the choice of majority of available ab initio approaches. We consider two possible schemes capable of incorporating isolated molecule (many-body) states as a basis for transport calculations. The schemes utilize Hubbard operators for description of single electron transitions between many-body states and go beyond previously proposed scattering theory and standard quantum master equation approaches.

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