Electron-vibration interactions for AC driven quantum transport

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Molecular junctions, consisting of molecules bonded between macroscopic leads, allow researchers to probe and design charge and energy transport at some of the smallest scales possible, with the promise of device functionalities whose descriptions range from efficient to exotic. Such systems are often manipulated and observed whilst time-dependent lead and gate voltages are applied, with many devices, including pumps and rectifiers, designed with time-dependent, usually alternating, voltages in mind. Given such small scales and the sensitivity of these systems, vibrations can often influence transport properties and contribute significantly to device failure. Naturally, understanding the interplay between time-dependent voltages and vibrations will be an essential part of molecular junction design. Of particular importance is the interplay of periodically driven leads and vibrations of the central region, with research already suggesting the possibility of 'cooling' of vibrations due to the application of driving [1,2], whereas the introduction of phonons within a mean-field approximation saw significant deviations from noninteracting behaviour in a time-scale separation approach [3]. To this end, we make use of nonequilibrium Green's functions in a Floquet setting [4], where electron-phonon coupling is considered within the self-consistent Born approximation. This allows for the calculation of nonequilibrium phonon occupations within the central molecule whilst lead energies are varied periodically. This result extends the of theory used to explain point-contact spectroscopy and inelastic tunnelling spectroscopy to consider alternating drivings, which sees the characteristic signs of inelastic transport gain photon-assisted side-peaks. The presence of photon-assisted transport is also observed within the nonequilibrium phonon occupations. Within a period of driving, phonon occupancy is found to change significantly when driving and vibrational frequencies come into resonance, giving support to the intuition that the system may be more susceptible to failure when driven at resonance.

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[3] T. Honeychurch and D. Kosov, Phys. Rev. B 100, (2019)

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