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Role of the evanescent states in the elastic quantum transport[1]
ARANTZAZU GARCIA-LEKUE, Chemical Science Division, Lawrence Berkeley
National Laboratory, Berkeley, California 94720, USA, LIN-WANG WANG, Com-
putational Research Division, Lawrence Berkeley National Laboratory, Berkeley,
California 94720, USA — The role of evanescent states is always an issue in elec-
tronic transport, especially when the energy of the propagating electron is close to
a band structure minimum. In this work, we investigate the effects of exact evanes-
cent states on the calculation of the elastic quantum transport through a molecule
connected by two quantum wires, based on the method presented in Ref. [1]. An
exact treatment of evanescent (decaying) states involves the calculation of the com-
plex band structure of the electrodes with imaginary parts of the k vectors. We
have calculated the complex band structure under the plane-wave pseudopotential
approach. The exact evanescent states are used in the transport calculations with
auxiliary boundary condition as described in Ref. [1]. The results are exact numeri-
cal solutions of the scattering states under a plane-wave pseudopotential formalism.

[1] L.W. Wang, Phys. Rev. B. **72**, 045417 (2005).

Arantzazu Garcia-Lekue
Chemical Science Division, Lawrence Berkeley National Laboratory
Berkeley, California 94720, USA

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