

Abstract Submitted
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A density functional that works for transport through Anderson junction¹ ZHENFEI LIU, JUSTIN BERGFELD, KIERON BURKE, Departments of Chemistry and Physics, University of California, Irvine, CHARLES STAFFORD, Department of Physics, University of Arizona — Transport through an Anderson junction can be exactly described by density functional theory, at zero temperature and in the linear response regime. Using Bethe ansatz, we calculate the exact Kohn-Sham potential delivering the exact transmission. We propose a simple parametrization for the Kohn-Sham potential, using a known exact condition. Our parametrization faithfully reproduces numerical results, including the gradual development of the derivative discontinuity that is essential in describing Coulomb blockade correctly.

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