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DFT treatment of transport through Anderson junction: exact results and approximations[1]

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Since the pioneering break-junction experiments of Reed and Tour measuring the conductance of dithiolated benzene between gold leads, many researchers in physics and chemistry have been calculating conductance for such systems using density functional theory (DFT). Off resonance, the predicted current is often 10-100 times larger than that measured. This error is often ascribed to the application of ground-state DFT to a non-equilibrium problem. I will argue that, in fact, this is largely due to errors in the density functional approximations in popular use, rather than necessarily errors in the methodology. A stark illustration of this principle is the ability of DFT to reproduce the exact transmission through an Anderson junction at zero-temperature and weak bias, including the Kondo plateau, but only if the exact ground-state density functional is used. In fact, this case can be used to reverse-engineer the exact functional for this problem. Popular approximations can also be tested, including both smooth and discontinuous functionals of the density, as well as symmetry-broken approaches.

[1] Kondo effect given exactly by density functional theory, J. P. Bergfield, Z. Liu, K. Burke, and C. A. Stafford, arXiv:1106.3104;
[2] Broadening of the Derivative Discontinuity in Density Functional Theory, F. Evers, and P. Schmitteckert, arXiv:1106.3658;
[3] DFT-based transport calculations, Friedel's sum rule and the Kondo effect, P. Tröster, P. Schmitteckert, and F. Evers, arXiv:1106.3669;
[4] Towards a description of the Kondo effect using time-dependent density functional theory, G. Stefanucci, and S. Kurth, arXiv:1106.3728.

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