MAR14-2013-020190

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

DFT calculations with the exact functional[1]

KIERON BURKE, Department of Physics and of Chemistry, University of California, Irvine, California 92697 USA

I will discuss several works in which we calculate the exact exchange-correlation functional of density functional theory, mostly using the density-matrix renormalization group method invented by Steve White, our collaborator. We demonstrate that a Mott-Hubard insulator is a band metal [1]. We also perform Kohn-Sham DFT calculations with the exact functional and prove that a simple algoritm always converges [2]. But we find convergence becomes harder as correlations get stronger. An example from transport through molecular wires may also be discussed [3].

[1] Lucas O. Wagner, E. M. Stoudenmire, Kieron Burke, Steven R. White, Phys. Rev. Lett. 111, 093003 (2013).
[2] E.M. Stoudenmire, Lucas O. Wagner, Steven R. White, Kieron Burke, Phys. Rev. Lett. 109, 056402 (2012).
[3] J.P. Bergfield, Z.-F. Liu, Kieron Burke, C.A. Stafford, Phys. Rev. Lett. 108, 066801 (2012)

[1]Work supported by DOE grant DE-SC008696.