The Mott-Hubbard transition revisited

Garcia, D.J.,¹ Miranda, E.,¹ Hallberg, Karen,² and Rozenberg, M.J.³

 ¹Instituto de Fisica Gleb Wataghin, Unicamp, CEP 13083-970 Campinas, SP, Brazil
²Instituto Balseiro and Centro Atomico Bariloche, CNEA, (8400) San Carlos de Bariloche, Argentina
³Laboratoire de Physique des Solides, CNRS-UMR8502, Universite de Paris-Sud, Orsay 91405, France and Departamento de Fisica, FCEN, Universidad de Buenos Aires, Ciudad Universitaria, Pabellon 1, Buenos Aires (1428), Argentina.

We study the Hubbard model at half filling and away from particle-hole symmetry using a new numerical method for the solution of the Dynamical Mean Field Theory self-consistent equations. This new technique is based on the accurate calculation of the associated impurity problem using the Density Matrix Renormalization Group technique. The new algorithm makes no a priori approximations and is only limited by the number of sites that can be considered. We obtain accurate estimates of the critical values of the metal-to-insulator and insulator-to-metal transitions and provide evidence of substructure in the Hubbard bands of the correlated metal. In addition, we demonstrate the capabilities of this precise method by obtaining the frequency dependent optical conductivity spectra.