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Modified Iterated perturbation theory in the strong coupling regime and its application to the 3d FCC lattice[1] LOUIS-FRANÇOIS ARSENAULT, (1) Departement de Physique and RQMP, Universite de Sherbrooke, Sherbrooke, QC, Canada, PATRICK SÉMON, (1), B. SRIRAM SHASTRY, (2) Physics Department, University of California, Santa Cruz, CA 95064, USA, A.-M.S. TREMBLAY, (1,3) Canadian Institute for Advanced Research, Toronto, Ontario, Canada — The Dynamical Mean-Field theory(DMFT) approach to the Hubbard model requires a method to solve the problem of a quantum impurity in a bath of non-interacting electrons. Iterated Perturbation Theory(IPT)[1] has proven its effectiveness as a solver in many cases of interest. Based on general principles and on comparisons with an essentially exact Continuous-Time Quantum Monte Carlo (CTQMC)[2], here we show that the standard implementation of IPT fails when the interaction is much larger than the bandwidth. We propose a slight modification to the IPT algorithm by requiring that double occupancy calculated with IPT gives the correct value. We call this method IPT-D. We show how this approximate impurity solver compares with respect to CTQMC. We consider a face centered cubic lattice(FCC) in 3d for different physical properties. We also use IPT-D to study the thermopower using two recently proposed approximations[3]S^* and S_{Kelvin} that do not require analytical continuation and show how thermopower is essentially the entropy per particle in the incoherent regime but not in the coherent one.[1]H.Kajueter et al. Phys. Rev. Lett. 77, 131(1996)[2]P. Werner, et al. Phys. Rev. Lett. 97, 076405(2006)[3]B.S. Sriram Shastry Rep. Prog. Phys. 72 016501(2009)

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