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Density Matrix Embedding Theory of Strongly Correlated Models QIAONI CHEN, GERALD KNIZIA, GARNET KIN-LIC CHAN, Princeton University — We apply the recently developed density matrix embedding theory(DMET), to the honeycomb Hubbard model and the cuprate p-d model. DMET is based on the density matrix rather than the Green's function, thus all computations are frequency independent and of much lower cost than in DMFT. In DMET large clusters can be treated with similar accuracy but lower cost than in DMFT. (i) In the honeycomb Hubbard model, QMC calculations suggested a spin-liquid between a metal and insulator, but suffered from potential finite size errors. Using cluster DMET we find only a second-order phase transition near $U = 3.3$ between the metal and insulator, with no spin-liquid. Our thermodynamic data allows direct comparison to QMC calculations, highlighting the finite size errors. (ii) Three band model calculations with large cluster DMFT are infeasible, however cluster DMET calculations are very affordable. Earlier DMFT calculations place the metal-insulator transition at an unphysical d-occupancy. Using cluster DMET treatments, we show that the transition between metal and insulator shifts into the physical regime due to our ability to include large cluster correlations.

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