Phase diagram and Neel temperature of fermions in a three-dimensional optical lattice

CHARLES MATHY, DAVID HUSE, Princeton University — One of the most exciting prospects in the field of ultracold atoms is the experimental realization of an antiferromagnetic Mott state, in a system of fermions in a three-dimensional optical lattice. Experimentalists are currently wrestling with achieving the requisite ordering temperatures. We address the question of which regions of parameter space one should explore to find the highest Neel temperatures. To this end, we perform Hartree-Fock calculations and map out the magnetic phase diagram of two component fermions in a three-dimensional simple cubic lattice. We find that the superexchange and Neel temperature are maximized in a regime of intermediate coupling, where the system is no longer well described by a one-band Hubbard model. We also perform a perturbative expansion in a Wannier basis, and study the corrections to the Hubbard model in this region. We find that the largest correction is a Hund’s rule ferromagnetic coupling. Finally, our calculations suggest that the Mott plateau would be large in the intermediate coupling regime, and therefore experimentally accessible.

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