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The Lieb lattice near 1/6 filling RAIMUNDO DOS SANTOS, NATANAEL COSTA, TIAGO MENDES-SANTOS, JOSE LUIZ FERREIRA, THEREZA PAIVA, Universidade Federal do Rio de Janeiro, RICHARD SCALETTAR, University of California - Davis — The interplay between van Hove singularities, nesting, and particle-hole symmetry influences the magnetic and transport properties of interacting electrons in fundamental ways. We consider a Hubbard model for interacting electrons on a Lieb lattice (or CuO_2 lattice) under the following simplifying assumptions: an on-site repulsion $U_d > 0$ is assumed to be effective solely on Cu sites, so that $U_p = 0$; vanishing site energies, $\varepsilon_d = \varepsilon_p = 0$; and hopping is only allowed between Cu and O sites. For the non-interacting case at 1/6 filling (electronic density $\rho = 1/3$), the density of states (DOS) displays a van Hove singularity, and the Fermi surface is nested. In order to probe the interplay between these features, we use Determinant Quantum Monte Carlo simulations and Lanczos diagonalizations (with twisted boundary conditions) to investigate the physical properties at this filling and slightly doped away from it. We identify sharp enhancement of antiferromagnetic correlations on d sites exactly at this filling, due to nesting, and investigate possible Mott insulating behavior with U_d. Further, we examine the behavior of charge correlations, and different pairing susceptibilities in order to probe some enhancement of superconducting correlations.

Raimundo dos Santos
Universidade Federal do Rio de Janeiro

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