Spontaneously broken particle-hole symmetry on the Lieb lattice

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We study spinless fermions with nearest-neighbor repulsive interactions ($t - V$ model) on the two-dimensional three-band Lieb lattice. At half-filling, the electronic band structure consists of a flat band at zero energy and a single cone with linear dispersion. The flat band is expected to be instable upon inclusion of electronic correlations, to avoid the violation of the third law of thermodynamics. A natural candidate is charge density wave ordering. However, due to the three-orbital unit cell, commensurate charge ordering implies an imbalance of electron and hole densities and therefore doping away from half-filling, Our numerical results show that below a finite-temperature Ising transition, a charge density wave with one electron and two holes per unit cell and its partner under particle-hole transformation are spontaneously generated. Our calculations are based on recent advances in auxiliary-field and continuous-time quantum Monte Carlo simulations that allow sign-free simulations of spinless fermions at half-filling. In this context, it is interesting to note that spontaneous particle-hole symmetry breaking allows us to access levels of finite doping, without introducing a sign problem.