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Coexistence and competition of on-site and intersite Coulomb interactions in Mott-molecular-dimers ALBERTO ARRUDA, RAFFAEL JULIANO, THIAGO WERLANG, LUIS CRACO, Instituto de Física - Universidade Federal de Mato Grosso — Recent findings of Mott-Hubbard physics in ultracold atoms trapped in periodic potentials have reinvigorated the search for quantum simulators of fermionic and bosonic Hubbard-like models. With this in mind, we performed a systematic study of a two-site realization of the Hubbard model, i.e, in a regime where this model can exactly treated. Particularly, we reveal the interplay between on-site (U) and intersite (V) Coulomb interactions in the extended two-site Hubbard model. Due to its atomic-like form quantum correlations intrinsic to Mott-molecular-dimers are exactly computed. Our results for physical quantities such as double occupancy and specific heat are consistent with those obtained for the one-band Hubbard model, suggesting that a two-site dimer model is able to capture the essential thermodynamic properties of strongly interacting electron systems. It is shown that intersite Coulomb interactions promotes the formation of doublons, which compete with the spin-singlet state induced by the on-site Coulomb repulsion. Our results are expected to be relevant for understanding electronic and thermodynamical properties of interacting electrons in strongly coupled magnetic atoms.

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