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**Exact theoretical description of two ultracold atoms in a single site of a 3D optical lattice** ALEJANDRO SAENZ, SERGEY GRISHKEVICH, Humboldt University Berlin, 10117 Berlin (Germany) — Ultracold atoms in optical lattices are exciting systems to study, e.g., phenomena of solid-state physics, since the lattice resembles in some sense the periodicity of a crystal potential. These systems are furthermore supposed to be of great interest for quantum information purposes. We have developed a theoretical approach that allows for an exact numerical description of a pair of ultracold atoms trapped in a three-dimensional optical lattice. This approach includes the possible coupling between center-of-mass and relative motion coordinates in a configuration-interaction (also called exact diagonalization) type of approach. Furthermore, the atoms are allowed to interact by their full inter-atomic interaction potential that is, presently, only limited to be central. With the aid of the newly developed method deviations from the harmonic approximation are discussed. The developed method is also used to model recent experimental data [C. Ospelkaus et al., Phys. Rev. Lett. **97**, 120402 (2006)]. In that experiment heteronuclear molecules were created in an optical lattice and their binding energies were measured close to a Feshbach resonance as a function of the magnetic field and thus of a variable inter-atomic interaction strength.

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