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Möbius molecules and fragile Mott insulators LUKAS MUECHLER, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, JOSEPH MACIEJKO, Department of Physics, University of Alberta, Edmonton, Alberta T6G 2E1, Canada, TITUS NEUPERT, Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA, ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA
— Motivated by the concept of Möbius aromatics in organic chemistry, we extend the recently introduced concept of fragile Mott insulators (FMI) to ring-shaped molecules with repulsive Hubbard interactions threaded by a half-quantum of magnetic flux ($hc/2e$). In this context, a FMI is the insulating ground state of a finite-size molecule that cannot be adiabatically connected to a single Slater determinant, i.e., to a band insulator, provided that time-reversal and lattice translation symmetries are preserved. Based on exact numerical diagonalization for finite Hubbard interaction strength U and existing Bethe-ansatz studies of the one-dimensional Hubbard model in the large-U limit, we establish a duality between Hubbard molecules with $4n$ and $4n+2$ sites, with n integer. A molecule with $4n$ sites is an FMI in the absence of flux but becomes a band insulator in the presence of a half-quantum of flux, while a molecule with $4n+2$ sites is a band insulator in the absence of flux but becomes an FMI in the presence of a half-quantum of flux. Including next-nearest-neighbor-hoppings gives rise to new FMI states that belong to multidimensional irreducible representations of the molecular point group, giving rise to a rich phase diagram.
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