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Hubbard pair cluster in the external fields. Studies of the chemical potential

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Abstract

The chemical potential of the two-site Hubbard cluster (pair) embedded in the external electric and magnetic fields is studied by exact diagonalization of the Hamiltonian. The formalism of the grand canonical ensemble is adopted. The influence of temperature, Hubbard on-site Coulombic energy U , and electron concentration on the chemical potential is investigated and illustrated in figures. In particular, a discontinuous behaviour of the chemical potential (or electron concentration) in the ground state is discussed.

Keywords: Hubbard model, dimer, pair cluster, chemical potential, exact diagonalization, grand canonical ensemble

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1. Introduction

The Hubbard model [1–4] has been comprehensively studied over the last decades [5–63]. Its applicability involves, for example, the description of metal-insulator transition, ferromagnetism of itinerant electrons, studies of high-temperature superconductors, optical lattices and finite graphene samples. In spite of intensive efforts, so far the exact solution has been obtained only in 1D case [13, 46], including the solution for the case of Hubbard model in external magnetic field [47, 48]. As far as 2D systems are concerned, the Mermin-Wagner theorem about the

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