Single-particle spectral density of ionic (proton) Pauli conductor with competitive interactions

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We study the single-particle spectrum and analyze the equilibrium states of proton and ionic conductors using the lattice gas model where particles are described by Pauli statistics. The model takes into account the particle hopping as well as the two-particle short-range and long-range interactions. First, we perform analytical calculations with simplified model using Green's function approach to analyze within the RPA the shape of single-particle spectral density. We are able to conclude whether the system is in the superfluid-like (SF) state, Mott insulator state or charge density wave (CDW) like state by analyzing the specific features of the spectral density (in particular, the presence of negative branch or gap). Next, we perform calculations of spectral densities of the finite clusters with periodic boundary conditions for the cases of both ionic and proton conductor via exact diagonalization technique. According to mentioned above criterion, we analyse the conditions of appearance of the various states of the system at different temperatures (depending on relation between the values of interaction constants and hopping parameter). In CDW-like state the ordering is similar to the one observed in ferroelastic phases of superprotonic conductors. The SF-like state is analogous to superionic phase. The corresponding diagrams of state are discussed.