Spectral densities of one-dimensional Pauli conductor obtained via exact diagonalization technique

O. Vorobyov and R. Stetsiv

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: vorobyov@icmp.lviv.ua

The systems with proton (ionic) conductivity are a subject of many experimental and theoretical studies in recent years. The special attention is paid to superionic (superprotonic) conductors that exhibit transitions to high-temperature superionic phases that are accompanied the redistribution of protons in plains or chains of ionic groups connected by hydrogen bonds. We investigate the energy spectrum of one-dimensional ionic and protonic conductors described by Pauli statistics taking into account ion (proton) transfer as well as the short-range non-local correlation between particles. Both commutator and anticomutator Green's functions constructed of Pauli creation and annihilation operators are calculated using exact diagonalization technique on the basis of states of finite ionic (protonic) chains with periodic boundary conditions. The frequency and temperature dependences of one-particle density of states is calculated. The possibility of metal-insulator like transition with change of temperature is discussed. In the limit of vanishing correlation strength the results are compared with the ones obtained with fermionization procedure [1] while for different correlation strengths the results are compared with the ones obtained with exact diagonalization technique for similar systems described with Fermi statistics [2].

1. I.V. Stasyuk, I.R. Dulepa, Condens. Matter Phys, 2007, **10**, 2(50), p. 259–268.
2. I.V. Stasyuk, O.A. Vorobyov, Ferroelectrics, 2008, **376**, 1, p. 64–73.