Fundamental properties of correlated electrons in nanochains

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We discuss electronic properties of a nanochain within the recently proposed approach [1] combining ***E**xact **D**iagonalization* in the Fock space with an ***Ab I**nitio* calculations (EDABI method). In particular, the microscopic parameters of the second–quantized Hamiltonian are determined and the evolution of the system properties is traced in a systematic manner as a function of the interatomic distance (the lattice parameter, R). Both the many–particle ground state and the dynamical correlation functions are discussed within a single scheme. The principal physical results are: (i) the evolution of the electron momentum distribution and its analysis in terms of the Tomonaga–Luttinger scaling, (ii) the appearance of mixed metallic and insulating features (*partial localization*) for the *half–filled* band case, (iii) the appearence of a universal *renormalized* dispersion relation of electron energy, and (iv) the transformation from a *highly–conducting* nanometalic state to the *charge–ordered* nanoinsulator in the quarter–filled case. The analysis is performed using the adjustable Gaussian $1s$–like basis set composing the Wannier functions, as well as includes the *long–range* Coulomb interaction.

[1] J. Spalek, *et al.* Phys. Rev. B **61**, 15676 (2001); A. Rycerz and J. Spalek, *ibid.* **63**, 073101 (2001); *ibid.* **65**, 035110 (2002).