Abstract Submitted
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Incommensurate quantum-size oscillations in Acene-based molecular wires - effects of quantum-fluctuations[1] FERDINAND EVERS, Institut fr Theoretische Physik, Universitt Regensburg, PETER SCHMITTECKERT, Institut fr Theoretische Physik, Universitt Wrzburg, Germany, RICHARD KORYTAR, Institut fr Theoretische Physik, Universitt Regensburg, Germany, RONNY THOMALE, Institut fr Theoretische Physik, Universitt Wrzburg, Germany — Molecular wires of the acene-family can be viewed as a physical realization of a two-rung ladder Hamiltonian. For acene-ladders, closed-shell ab-initio calculations and elementary zone-folding arguments predict incommensurate gap oscillations as a function of the number of repetitive ring units, N_R, exhibiting a period of about ten rings. Results employing open-shell calculations and a mean-field treatment of interactions suggest anti-ferromagnetic correlations that could potentially open a large gap and wash out the gap oscillations. Within the framework of a Hubbard model with repulsive on-site interaction, U, we employ a Hartree-Fock analysis and the density matrix renormalization group to investigate the interplay of gap oscillations and interactions. We confirm the persistence of incommensurate oscillations in acene-type ladder systems for a significant fraction of parameter space spanned by U and N_R.

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