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Numerical classical and quantum mechanical simulations of charge density wave models[1] ANDREW BECKWITH, Department of Physics and Texas Center for Superconductivity and Advanced Materials at the University of Houston — First, using a driven harmonic oscillator model by a numerical scheme as initially formulated by Littlewood, we present a computer simulation of charge density waves (CDW); next, we use this simulation to show how the dielectric model presented via this procedure leads to a blow up at the initialization of a threshold field E_T. Finding this approach highly unphysical, we initiated inquiry into alternative models. We investigate how to present the transport problem of CDW quantum mechanically, through a numerical simulation of the massive Schwinger model. We find that this single-chain quantum mechanical simulation used to formulate solutions to CDW transport is insufficient for transport of soliton-antisolitons (S-S') through a pinning gap model of CDW. We show that a model Hamiltonian with Peierls condensation energy used to couple adjacent chains (or transverse wave vectors) permits formation of S-S' that can be used to transport CDW through a potential barrier. This addition of the Peierls condensation energy term is essential for any quantum model of CDW to give a numerical simulation to tunneling behavior.

[1]TcSAM/from dissertation

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