Numerical classical and quantum mechanical simulations of charge density wave models

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

Andrew Beckwith
TcSAM/U. of Houston physics department

Date submitted: 12 Nov 2004