

**Soliton dynamics in a formamide stack using a Taylor-series expansion for the potential surface. I. Exact equations of motion; dispersion energy.** Foerner, Wolfgang

**Abstract**

The exact equations of motion for a stacked system are derived and their properties are discussed. Results of numerical simulations of soliton dynamics are presented and compared with the previously published ones using an approx. treatment. Qual. and quant. differences are found. The intermol. dispersion energy is included via London's formula into the model of solitary waves in stacked systems. It is shown that 1st-neighbor terms are of sufficient accuracy. The explicit London formula is fitted by a 6th-order Taylor series. The qual. properties of solitary waves are not changed too much upon inclusion of dispersion energy. Quant. changes in velocity, kinetic energy, and effective mass of the waves are found.