

Thermalization in a quantum Fermi-Pasta-Ulam-Tsingou problem

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We investigate thermalization in a quantum Fermi - Pasta - Ulam - Tsingou problem for anharmonic vibrations in atomic chains applying semi-quantitative analysis of resonant interactions complemented by exact numerical studies. We estimate the energy at transition from the localized low-energy phase to the chaotic high-energy phase. The transition energy is inversely proportional to the number of atoms in the classical regime and reaches a plateau in the quantum regime. Systems with free or fixed ends boundary conditions reach the chaotic regime at lower energies than the periodic systems. We discuss the applications of the theory to realistic molecules and their spectral properties.

Topics

Session A. Physics of condensed matter and spectroscopy

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