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Nanoscience & *non-quantum* limitations of classical theories

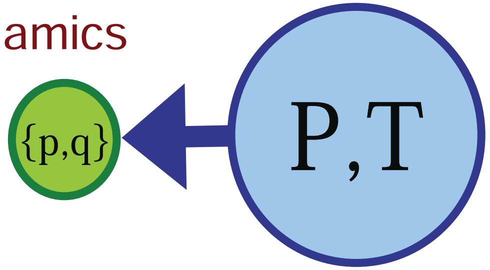
CMTH@ IMPERIAL COLLEGE

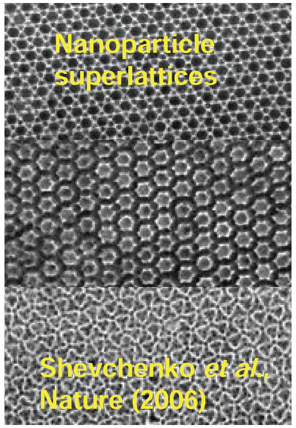
Classical mechanics

- Deterministic & precise
- Mind-boggling for many degrees of freedom

Thermodynamics

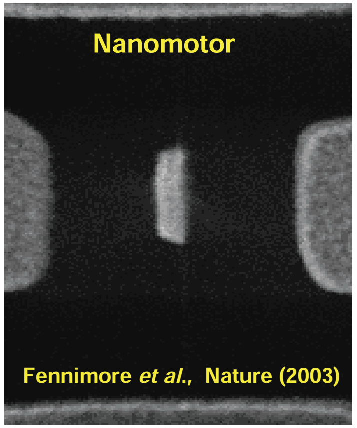
- Simple and precise for many degrees of freedom
- Well-defined probabilities for small subsets {p,q}





Materials

- We can deduce the properties of crystals from those of atoms.
- How do two 5,000-atom nanocrystals interact ?
- What are the properties of ***nanoparticle superlattices*** ?

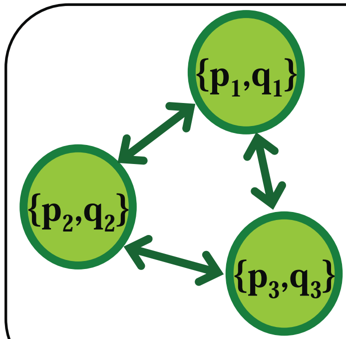


Devices

- > μm scale: predictable mechanical & electronic devices
- < μm scale: unpredictable jiggling of atoms becomes relevant.

Smaller ⇒ Less predictable

…***but how do we quantify this ?***



"Nanothermodynamics" ?

When each component of a nanosystem has

– enough atoms to boggle the mind

– too few atoms to be well described by conventional thermodynamics

how do we understand and characterize it ?

Our task

- Atomistically simulate nanosystems
- Guide & interpret experiments
- Discover new phenomena
- Seek a useful probabilistic theory (without the ergodic theorem)