Heat Transfer at the Nanoscale by Quantum Mechanics

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Abstract Classically, heat is transferred by convection, radiation, and conduction. But at the nanoscale, classical heat transfer is restricted by quantum mechanics (QM) to vanishing specific heat. The QM restriction may be understood from the Einstein-Hopf relation for the harmonic oscillator that shows the average Planck of energy of an atom at temperature is dispersed with wavelength. At room temperature, the thermal kT energy of the oscillator rapidly vanishes below wavelengths of 50 microns, and therefore submicron nanostructures lack heat capacity because their size excludes all thermal wavelengths beyond about 1 micron. Here k is Boltzmann's constant and T absolute temperature. Equivalently, the specific heat of nanostructures vanishes. What this means is any kind of electromagnetic (EM) energy absorbed by the nanostructure cannot be conserved by an increase in temperature.

Today, the heat transfer of nanostructures which are unambiguously not periodic persists on the erroneous assumption of macroscopic specific heat. In effect, the invalid Dulong-Petit law of constant specific heat with temperature has been extended to constancy of specific heat with size. Molecular dynamics (MD) simulations of nanostructures are proudly displayed on the belief they provide precise atomistic explanations of conduction heat transfer when in fact they are not valid because the simulations are performed on the assumption the atoms have kT energy. Perhaps researchers have forgotten the very early MD simulations of bulk liquid properties by Metropolis and Teller who invoked periodic boundary conditions to allow the kT energy of the atoms to be included in submicron computational boxes.

In this paper, heat transfer at the nanoscale explicitly assumes the material of the nanostructure has vanishing specific heat. Both the Debye model of specific heat based on phonon vibrations in a lattice and Einstein's specific heat model of independent vibrations of the atoms as harmonic oscillators are only applicable to macroscopic structures under slow heat transfer. To allow nanostructures to promptly transfer heat in the solid state, heat transfer by QED induced radiation is proposed. Here QED stands for quantum electrodynamics. Unlike thermal radiation given by the Stefan-Boltzmann law, QED radiation is non-thermal. Nanostructures usually absorb low frequency EM energy in the far infrared (FIR) from diverse sources including: lasers, solar and supernovae photons, molecular collisions, frictional rubbing, and Joule heat. By their size, nanostructures have EM confinement frequencies higher than the FIR, typically beyond the ultraviolet (UV). Lacking specific heat, nanostructures may only conserve any absorbed FIR energy by QED induced frequency up-conversion to non-thermal radiation at the UV levels of EM confinement. QED radiation is prompt and renders as inconsequential the far slower heat transfer embodied by Debye's phonons and Einstein's atomic vibrations. The EM confinement is quasi-bound leaking the QED induced radiation at UV levels to the surroundings. In effect, nanostructures act as frequency up-conversion devices converting FIR energy to higher frequency EM radiation that is absorbed in the macroscopic surroundings. Only then is any EM energy absorbed by the nanostructure dissipated by classical heat transfer. To illustrate QED induced radiation, typical applications are discussed including nanofluids and thin films.