Non-equilibrium Green's Function

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1. INTRODUCTION

In 1822, the theory of thermal transport in solids began with Fourier's transient heat conduction equation allowing the derivation of temperatures in macroscopic systems. Quantum mechanics (QM) was introduced through the specific heat capacity in combination with phonons as heat carriers by Einstein and Debye [1,2] in 1907 and 1912. Over the past decade, however, the anomalous thermal conductivity found for microscopic systems prompted review of Fourier's equation. The microscopic systems reviewed were 1-D chains of atoms [3] that because of their simplicity would allow our understanding of microscopic thermal conductivity. Contrarily, even in the simplest harmonic chain, classical physics gave anomalous results, at least anomalous with respect to the macroscopic world we know, e.g., the proportionality of heat flux to temperature difference instead of thermal gradient, a disordered chain with fixed boundaries became an insulator, and thermal conductivity increased with the length of the chain.

But is this of concern? Classical physics should give similar results independent of the size of the system, but this was not observed. Instead, unphysical results were found, e.g., the thermal conductivity of a 1-D chain would not be expected to increase with its length. Perhaps, QM would show conductivity of a 1-D chain is independent of its length.

In this regard, the Boltzmann-Peierls equation [4] extended from kinetic theory by treating lattice vibrations as an interacting gas of phonons, even if correct, could not be applied to discrete microscopic systems that lack translational invariance. Density functional theory (DFT) based on QM would be more suitable to analysis by molecular dynamics (MD). However, DFT was only intended [5] for microscopic ensembles of atoms under periodic boundary conditions. Recently, DFT combined with non-equilibrium Green's functions (NEGF) based on phonon interactions and neglecting electron interactions was proposed [6] to describe thermal transport in discrete microscopic systems. The NEGF for thermal transport was thought analogous to that for the more established NEGF for electron transport [7, 8] described and shown [9] in Fig. 1

2. PROBLEM

Electron transport cannot be used as an analog for thermal transport by the NEGF because electron transport is not affected by thermal heat capacity. Of course, electron transport induces Joule heat, but electron transport itself is not restricted in any way by QM. However, QM restricts the heat capacity of microscopic systems thereby significantly affecting thermal transport by phonons as heat carriers. Indeed, it is questionable [10-13] whether thermal transport in microscopic systems exists at all. In fact, QM embodied in the Einstein-Hopf relation for the harmonic oscillator precludes any and all thermal transport in discrete microscopic systems based on their submicron size alone.

Hence, the problem is not one of whether NEGF theory replaces Fourier's equation, but rather to overcome the notion by Einstein and Debye that conduction by phonons that serves well in macroscopic systems may be extended to microscopic systems. Arguments that NEGF theory agrees with experiments [14] should be set aside because the experiments may be explained with other theories. See references in: http://www.nanoqed.org

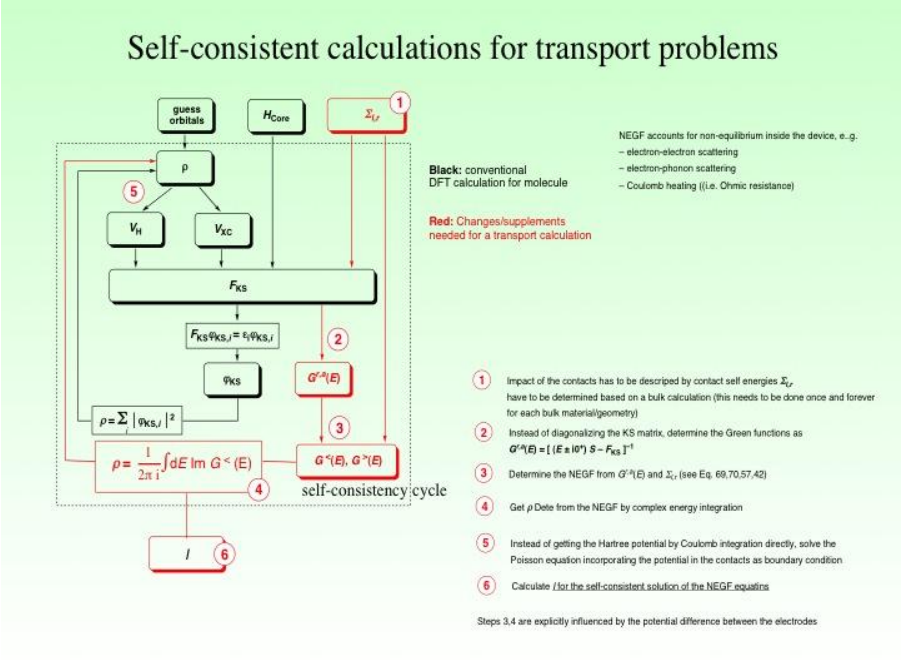

Fig. 1 NEGF for Electron Transport

3. QED INDUCED RADIATION

Classical physics by statistical mechanics cannot be applied to microscopic systems to derive the thermal response because of QM restrictions on heat capacity. Unlike classical physics that allows the atoms in microscopic systems to have heat capacity, QM embodied by the Einstein-Hopf harmonic oscillator requires [13] the heat capacity of microscopic systems to vanish. The difference between classical and QM oscillators is illustrated in Fig. 2.

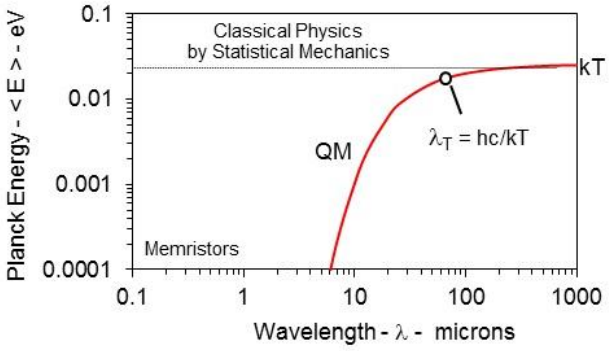

Fig. 2 Classical and QM Oscillators - Heat Capacity at 300 K

Unlike classical oscillators having kT energy at all wavelengths, QM oscillators only allow kT energy for $\lambda > \lambda_T$ and restrict kT for $\lambda < \lambda_T$. Here, k is Boltzmann's constant and T is absolute temperature. At 300 K, $\lambda_T \approx 50$ microns. Fig. 2 shows the specific heat capacity is less than kT for $\lambda < \lambda_T$ with kT energy available only for $\lambda > \lambda_T$. For microscopic systems having $\lambda < 1$ micron, QM by requiring specific heat to vanish precludes any increase in temperature upon the absorption of EM energy. Conservation of the absorbed EM energy (thermal, Joule, lasers) therefore cannot proceed by an increase in temperature. Hence, thermal gradients cannot exist, and therefore thermal conduction simply does not does not occur in microscopic systems.

Lacking heat capacity, QM conserves the absorbed EM energy by the creation of QED radiation *inside* the microscopic system. QED stands for quantum electrodynamics. Creation is prompt with QED inducing the absorbed EM energy to coincide with the total internal reflection (TIR) resonance. The TIR confinement only occurring during EM absorption is a natural consequence of microscopic systems that have a high surface to volume ratio, i.e., the absorbed EM energy is almost totally confined to the surface of the microscopic system. But without heat capacity, there is no increase in temperature, and therefore conservation proceeds by the emission of QED induced radiation.

Similar to creating QED photons of wavelength λ by supplying EM energy to a QM box with sides separated by $\lambda/2$, the absorbed EM energy is frequency up-converted to the characteristic dimension D_C of the microscopic system. The QED photon energy E and frequency f of the TIR confinement are:

$$E = hf \quad f = c/\lambda \quad \lambda = 2nD_C$$

where, h is Planck's constant, c the velocity of light, and n the refractive index of the microscopic system. For thin films and nanowires, the characteristic dimensions D_C are the thickness d and diameter D, respectively.

However, many microscopic systems are not continua such as thin films or nanowires, and may be molecules lacking thickness or diameters. But the molecules have EM spectra, and therefore upon the absorption of EM energy, QED induces the molecule to emit its unique EM spectrum. Consider the absorption of a single VIS photon by a nitrogen molecule. By NEGF, the nitrogen molecule having heat capacity is raised to a high temperature and vaporizes, but this is never observed. By QED, the nitrogen molecule lacking heat capacity is induced to emit QED radiation corresponding to its vibration spectra without any increase in temperature.

4. DISCUSSION

4.1 Thin Films Classically, Joule heat in thin films is conserved by an increase in temperature. But by QM, conservation proceeds by QED induced conversion of absorbed Joule heat to the TIR confinement frequency of the film. QED induced heat transfer [10] for thin films of thickness δ, width W, and length L emitting EM radiation in the absorption of Joule heat in Fig. 3.

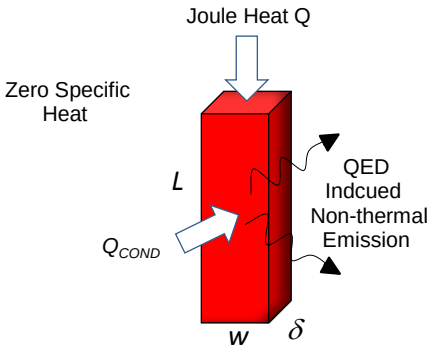

Fig. 3 Thin Film under Joule Heating

Thin films are generally thought to have large reductions in thermal conductivity through the thickness. Experimental conductivity K_{eff} data for thin copper layers is shown in Fig. 4. The input Joule heat Q is conserved by conduction Q_{COND} through the film and Q_{QED} emission from the film surface, the latter currently neglected in the heat balance.

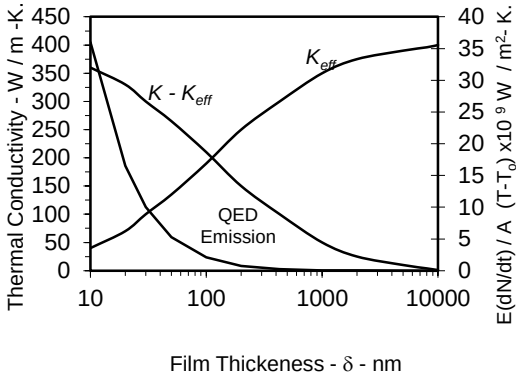

Fig. 4 Thin Film – Data and QED Response

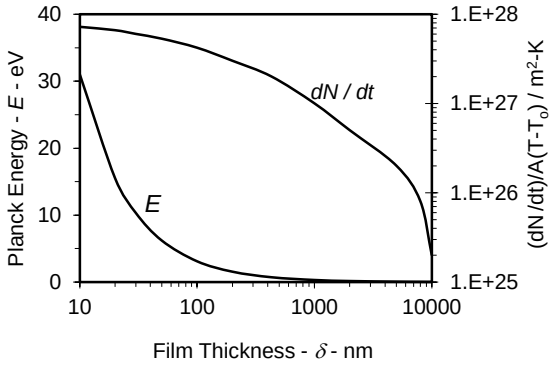

Fig. 5 Thin Film – QED Photon energy and rate

Currently, the Boltzmann Transport Equation (BTE) method excludes the emission of Q_{QED} radiation in conserving the absorbed Joule heat Q_{ABSORB} with conduction Q_{COND} alone. Fig. 4 estimates Q_{QED} by subtracting measured conductivity K_{eff} from bulk K. The QED emission given by the Planck energy E and rate dN/dt of QED photons is given in Fig. 5. Hence, conclusions that the thermal conductivity is reduced from bulk are erroneous because the QED radiation losses are excluded from the heat balance, but if included, the film maintains bulk conductivity.

4.2 Nanofluids Over the past few decades, nanofluids comprising nanoparticles (NPs) in common solvents are generally thought to significantly enhance thermal conductivity. But thermal conductivity determined from the temperature response of a thermocouple near an electrically heated wire generally shows enhancements far greater than that given by Hamilton-Crosser (HC) mixing rules.The HC rules for thermal conductivity were derived by extending Maxwell's treatment of electrical conductivity for macroscopic particles, but still should be valid

for NPs, although some proposals have been made to alter the HC rules for NPs. But this is not necessary if the NPs are enhancing heat transfer of the solvent by a mechanism that is independent of thermal conductivity. A NP exchanging radiation during collisions with solvent molecules is illustrated in Fig. 6.

Classically, solvent molecule collisions increase the NP temperature and are remitted as IR radiation. By QM, the collision energy [11] is reemitted in the VUV and penetrates farther than the IR under classical physics. Hence, heat transfer is enhanced in proportion to the number of NPs without increasing the nanofluid conductivity.

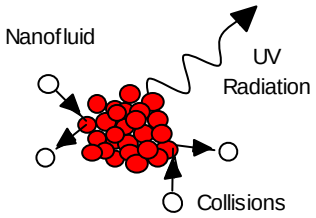

Fig. 6 Nanofluids – NPs emitting UV radiation

4.3 Memristors Memristors are generally thin films and nanowires. Fig. 7 shows thin films having material of thickness d sandwiched between metal electrodes of thickness t and a nanowire of a single material having diameter D and length L. Bias voltage is applied producing current I.

Thin films Nanowires

Fig. 7 Memristors

QED radiation is depicted creating excitons comprising mobile holes and electrons *inside* the memristor that decrease the resistance, but the resistance is promptly recovered in the same cycle as the holes and electrons are destroyed upon being neutralized at the voltage terminals. Simulations [12] of switching at 1 GHz are depicted in Fig. 8.

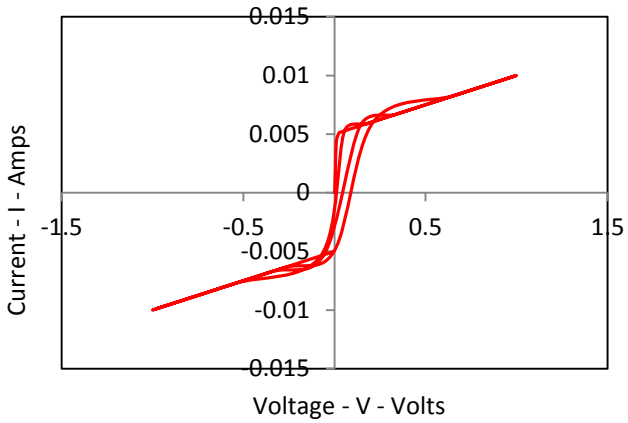

Fig. 8 Memristor I-V Curve – 2 Cycles at 1 GHz
$\mu_E = \mu_H = 500$ cm^2/V-s, P = 10 mW, V= 1V, $R_O = 100\ \Omega$, I = 10 mA
E = 4 eV, A = 200x200 nm^2, d = 50 nm

4.4 Graphene Graphene enhanced thermal management [13] of personal computers (PC) may have been overstated. Classically, almost all of the Joule heat loss from a PC is controlled by natural convection thereby negating any enhanced conductivity provided by graphene. QED differs. A single layer of graphene in intermittent contact with a PC component will not increase in temperature, and instead dissipate heat by emitting QED radiation that is absorbed in the air surroundings. Similarly, graphene nanoribbons dissipate Joule heat without danger of overheating by emitting QED radiation to the surroundings.

CONCLUSIONS

1. DFT in combination with NEGF or any other exotic theory to derive the thermal transport by phonons in microscopic systems is meaningless because conduction is precluded by QM. In contrast, QED avoids conduction by conserving absorbed EM energy by the emission of QED radiation. QM does not produce strange results. Contrarily, QM provides far more reasonable physical interpretations of microscopic systems compared to the unphysical results obtained by classical physics.

2. Phonons are unable to explain electrical charging of microscopic systems for the simple reason that there is no known phonon-electric effect. Only Einstein's photo-electric effect will create charge from photons – not phonons. In microscopic systems, the photons are created naturally by QM and emitted by the microscopic system as QED radiation.

3. Implementation of QED radiation only requires the absorbed EM energy to be partitioned into the emission spectra of the microscopic system, the effect on the surroundings assessed by more conventional heat transfer methods.

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