

Simple QED: The Absorption in Raman Scattering?

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Simple QED is a nanoscale heat transfer process that in nanoparticles (NPs) conserves absorbed heat with the emission of EM radiation. Incident light having a wavelength greater than the NP diameter imparts an inwardly disposed spherical Poynting vector of heat that concentrates momentum at the NP surface. Sub-surface penetration requires thermal conduction, but cannot proceed as the Planck law precludes temperature changes in the NP. Instead, the momentum at the NP surface heat acts as the EM confinement to constrain the heat to half-wavelength EM waves equal to the NP diameter. Once the momentum of the simple QED radiation exceeds the momentum of the incident light, the NP emits the standing EM radiation to the surroundings at a frequency depending on the NP diameter, a process similar to absorption in Raman scattering.

INTRODUCTION

Classical physics allows the atom to have heat capacity at the nanoscale, the conservation of heat proceeding by a concomitant change in atom temperature. However, heat transfer at the nanoscale is controlled by the Planck law [1] of quantum mechanics (QM) differing significantly from that of classical physics. Indeed, the Planck law denies the atoms in nanostructures the heat capacity to conserve heat by a change in temperature. Over the past decades, nanotechnology has generally ignored the Planck law and continued to use classical physics to explain nanoscale phenomenon, the consequence of which is an uncountable number of meaningless papers in the literature.

In this regard, the Planck law denies atoms in nanostructures the heat capacity to change temperature upon the absorption of heat - a difficult notion to accept because of our prior training in classical physics. Research in nanoscale heat transfer [2-4] has advanced over the past decades, and a large number of interesting phenomena have been reported. But despite the advances in nanotechnology, there are still challenges existing in understanding the mechanism of nanoscale thermal transport. Perhaps, researchers have not appreciated the significant difference between classical physics and the Planck law with regard to the heat capacity of the atom without which nanoscale heat transfer cannot proceed.

Heat transfer without changes in temperature precludes the Fourier law of heat conduction commonly used in nanoscale heat transfer. Similarly, the Stefan-Boltzmann law for radiative heat transfer depending on temperature is not applicable to nanostructures. Although valid at the macroscale, the Fourier law and Stefan-Boltzmann equation are invalid at the nanoscale. Moreover, Molecular Dynamics (MD) simulations [5] based on classical physics thought to provide an understanding of the atomic response to thermal disturbances assume atoms in nanostructures have temperature. An alternative is to formulate nanoscale heat transfer based on the Planck law itself. In this paper, one such theory called simple QED is presented.

SIMPLE QED METHOD

Simple QED is a method of nanoscale heat transfer analysis that conserves heat with EM radiation instead of temperature. QED stands for quantum electrodynamics, a complex theory based on *virtual* photons advanced by Feynman [6] and others. In contrast, simple QED is a far simpler theory based on the Planck law that only requires the heat capacity of the atoms in nanostructures to vanish allowing conservation to proceed by the creation of *real* photons comprising EM waves that stand within and across the nanostructure. Like electron quantum states standing across orbitals, simple QED quantum states are based on the dimension of the nanostructure over which the EM waves stand.

Of relevance to this light-scattering conference, simple QED is similar to Surface Enhanced Raman Spectroscopy (SERS). Unlike elastic Mie theory, SERS is inelastic as excitation laser light is not only scattered from molecules adsorbed to nanostructure surfaces, but also absorbed in both the molecules and the nanostructure as heat, neither of which by the Planck law increase in temperature.

Instead, simple QED converts: (a) the heat in molecules to EM radiation at the frequencies of the molecular quantum states, and (b) the heat in the nanostructures to size dependent quantum states of the nanostructure. Typically, the size dependent states are beyond the UV and excite lower states by fluorescing down to UV levels to excite NP plasmon resonances in the IR and VIS.

In this regard, the Planck energy E produced in heating the NP assumes the time τ for light to travel at velocity c/n across and back the NP corrected for the index n of refraction is $\tau = 2d/(c/n)$. Hence, $E = h/\tau = hc/2nd$, where h is Planck's constant. For an 80 nm NP with $n = 1.3$, $\tau \sim 0.7$ fs.

The Planck law at 300 K is illustrated in Fig. 1(a). By classical physics, the kT heat capacity of the atom is independent of the EM confinement wavelength λ , where k is the Boltzmann constant and T absolute temperature. QM differs as the heat capacity of the atom decreases under EM confinement $\lambda < 200$ microns, and at the nanoscale for $\lambda < 100$ nm, the kT heat capacity may be said to vanish.

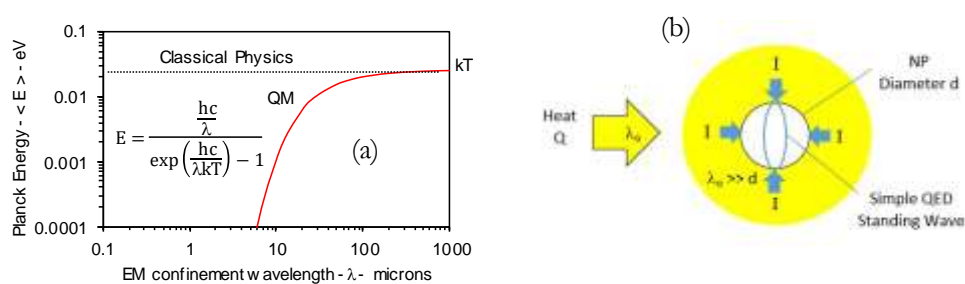


Figure 1. (a) Planck law at 300 K (b) EM heat Q absorption in NP

Laser light or thermal heat flux Q on a NP of diameter d is illustrated in Fig. 1(b). The EM radiation of the laser light is assumed to have wavelengths $\lambda_0 \gg d$ which effectively immerses the NP in EM radiation. Heat usually not thought to have wavelength is included here as laser light in the FIR.

EM confinement of simple QED radiation is required and is proposed as the momentum I of the heat flux Q . Simple QED is the consequence of the Planck law denying NP atoms the heat capacity to allow temperature changes to conserve heat which means the heat flux Q cannot penetrate and concentrates in the NP surface, the momentum I of which providing the EM confinement. Conservation of the heat flux Q in the NP can only proceed by creating simple QED radiation in the manner of non-thermal EM waves transiting across and back the NP diameter.

The heat flux Q is characterized by the Poynting vector $S = Q/c$. For a NP of diameter d having volume $V = \pi d^3/6$, the energy U absorbed by the NP is, $U = V \cdot S = \pi d^3 \cdot S/6$ and carries momentum $I = U/c = \pi d^3 \cdot Q/6c^2$. The number N of standing simple QED photon created having Planck energy E is, $N = U/E$, where $E = hc/2nd$. Here, the units are: $Q \sim W/m^2$, $S \sim J/m^3$, $V \sim m^3$, $U \sim J$, $E \sim J$, and $I \sim N \cdot s \sim Kg \cdot m/s$.

The EM confinement required to convert the energy U under the half-wave constraint $\lambda/2 = d$ into simple QED radiation is the inward spherical momentum $I = U/c$ shown as blue arrows in Fig. 1(b). During EM confinement, the momentum I of the heat Q is greater than the momentum I_P of N photons standing in the NP, $I > N \cdot I_P$, where $I_P = N \cdot h/2nd$. Over a brief EM confinement time, the number N of simple QED photons increases until $N \cdot I_P > I$ whereupon, a burst of simple QED radiation is emitted to the surroundings. Under heat flux Q from CW laser light, discrete bursts of simple QED radiation may not be observed as the creation time is very rapid, say < 1 fs. Perhaps, simple QED has always unknowingly been observed in Raman scattering.

APPLICATION

SERS provides enhanced Raman signals from molecules which have been attached to NPs. Both EM and chemical mechanisms are thought [7] to explain SERS. Unlike elastic Mie theory, SERS is inelastic as excitation laser light is not only scattered from molecules adsorbed to nanostructure surfaces, but also may change in frequency or wavelength. Simple QED in SERS is illustrated in Fig. 2.

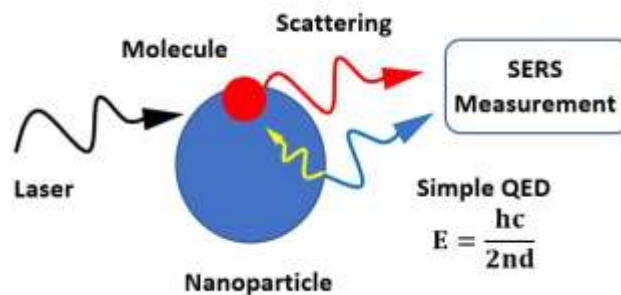


Figure 2. Simple QED in SERS with NPs

A laser is shown to irradiate a molecule (red) adsorbed to a NP (blue) and is scattered (red) and collected by the SERS measurement. However, the laser light is also absorbed by the NP and emits simple QED radiation (blue) which are collected with scattered light (red). But the NP also excites (yellow) quantum states of the molecule that are also collected by the SERS measurement. Typically, the size dependent simple QED states are beyond the UV and excite

lower states by fluorescing down to VIS levels to excite NP plasmon resonances. The myriad of EM variations in a SERS measurement is complex and cannot be attributed to any single mechanism. Simple QED is yet another EM mechanism that complicates SERS.

CONCLUSIONS

Simple QED heat transfer in NPs is similar to inelastic Raman scattering with absorption allowing the emission frequency to increase or decrease depending on size dependent quantum states of the NP.

Classical physics cannot explain simple QED radiation. Indeed, a UVC photon having a Planck energy $E = 4.88$ eV requires a temperature $T = 2E/3k \sim 37,000$ K which cannot occur. QM differs as UVC photons are readily created in NPs at 300 K.

References

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