Many-body radiative heat transfer theory

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In this Letter a N-body theory for the radiative heat exchange in thermally non equilibrated discrete systems of finite size objects is presented. We report strong exaltation effects of heat flux which can be explained only by taking into account the presence of many body interactions. Our theory extends the standard Polder and van Hove stochastic formalism used to evaluate heat exchanges between two objects isolated from their environment to a collection of objects in mutual interaction. It gives a natural theoretical framework to investigate the photon heat transport properties of complex systems at mesoscopic scale.

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The photon heat tunneling between two bodies has attracted much attention in the last decades since it has been predicted that the heat flux (HF) can exceed, at nanoscale, the far field limit set by Planck's black body law by several orders of magnitude [1, 2]. This discovery has opened the way to promising technologies for energy conversion and data storage as for example the near-field thermophotovoltaics [3, 4] and the plasmon assisted nanophotolitography [5]. This dramatic increase is generally speaking due to the contribution of evanescent modes, which are not accounted for in the Stefan-Boltzmann law and become only important if the distance between the objects is smaller than the thermal wavelength [6]. The detailed mechanisms which lead to such an enhancement are nowadays for a number of geometries and materials well understood [6–22] and recent experiments [23–27] have confirmed all theoretical predictions both qualitatively and quantitatively.

However, some questions of fundamental importance remain unsolved in complex mesoscopic systems. Indeed, so far, only the HF between two objects [6–9] out of equillibrium has been considered, but how does the heat transport for a collection of individual objects in mutual interaction look like? The collective effects in such many particle systems has not been explored yet, although it is of prime importance for understanding the different heat propagation regimes in disordered systems, determining the thermal percolation tresholds in random nanocomposites structures and studying thermal effects due to the presence of localized modes in such systems.

Inside a discrete system of bodies maintained at different temperatures the local thermal fluctuations give rise to oscillations of partial charges which, in turn, radiate their own time dependent electric field in the surrounding medium. These thermally generated fields interact with the nearby bodies and modify through different cross interactions all these primary fields to generate secondary fields which in turn affect the radiated fields and so on. Generally speaking, this problem belongs to the vast category of many-body problems which constitute the theoretical framework of numerous branches of physics (celestial mechanics, condensed matter physics, atomic physics, quantum chemistry). A general theoretical framework to treat the many-body problem of non-radiative photon heat transport does not vet exist. In this Letter we introduce a self-consistent theory to describe heat transfers inside thermally non equilibrated discrete systems. After deriving the HF exchanged between two individual objects in mutual interaction inside a N-body system, we investigate the thermal conductance between a couple of particles versus the position of a third object inside a three body system. We highlight some emergent phenomena which specifically result from many-body interactions. In addition, we will show that for systems with at least three objects at different temperatures one can actively control the heat flow in nanoscale junctions, i.e., one has a thermal heat transfer transistor.

To start, let us consider a discrete set of N objects located at positions r_i and maintained at different temperatures T_i with i = 1, ..., N. Suppose that the size of these objects is small enough compared with the smallest thermal wavelength $\lambda_{T_i} = c\hbar/(k_{\rm B}T_i)$ so that all individual objects can be modeled to simple radiating electrical dipoles. For metals one has also to include the magnetic dipole moments due to the induction of eddy currents [10]. Such an extension of our approach is straightforward so that for convenience we will consider electric dipoles only. The Fourier component of the electric field at the frequency ω (with the convention $\hat{f}(t) = \int \frac{d\omega}{2\pi} f(\omega) e^{-i\omega t}$) generated at the position r_i by the fluctuating part $\mathbf{p}_j^{\rm fluc}$ of electric dipole moment of the particle j which is located at r_j reads

$$\mathbf{E}_{ij} = \omega^2 \mu_0 \mathbf{G}^{ij} \mathbf{p}_j^{\text{fluc}},\tag{1}$$

with μ_0 the vacuum permeability and $\mathbb{G}^{ij} \equiv \mathbb{G}(\mathbf{r}_i, \mathbf{r}_j; \omega)$ the dyadic Green tensor (i.e. the propagator) between the particles *i* and *j* inside the set of N particles. On the other hand, by suming the contribution of fields radiated by each particle, the dipolar moment induced by the total field on the *i*-th particle is given by

$$\mathbf{p}_i^{\text{ind}} = \varepsilon_0 \alpha_i \sum_{j \neq i} \mathbf{E}_{ij}, \qquad (2)$$

where α_i is the particle's polarizability and ε_0 is the vacuum permittivity. Then, the power dissipated inside the particle *i* at a given frequency ω by the fluctuating field \mathbf{E}_{ij} generated by the particle *j* can be calculated from the work of the fluctuating electromagnetic field on the charge carriers as

$$\mathcal{P}_{j \to i,\omega} = 2 \operatorname{Re} \langle -i\omega \mathbf{p}_i^{\operatorname{ind}}(\omega) \cdot \mathbf{E}_{ij}^* \rangle, \qquad (3)$$

where the brackets represent the ensemble average. Using relations (1) and (2) between the dipole moments and the fluctuation dissipation theorem, i.e. $\langle p_{j,\alpha}^* p_{i,\beta} \rangle = 2\frac{\epsilon_0}{\omega} \text{Im}(\alpha_j) \Theta(\omega, T_j) \delta_{\alpha\beta} \delta_i j$ we find after a straightforward calculation that

$$\mathcal{P}_{j \to i} = 3 \int_0^\infty \frac{\mathrm{d}\omega}{2\pi} \,\Theta(\omega, T_j) \mathcal{T}_{i,j}(\omega) \tag{4}$$

introducing the transmission coefficient (TC)

$$\mathcal{T}_{i,j}(\omega) = \frac{4}{3} \frac{\omega^4}{c^4} \operatorname{Im}(\alpha_i) \operatorname{Im}(\alpha_j) \operatorname{Tr}\left[\mathbb{G}^{ij} \mathbb{G}^{ij\dagger}\right].$$
(5)

In order to present the HF in an obvious Landauer-like manner [29, 30] we rewrite the HF in terms of the conductance $G_{i,j} = \partial \mathcal{P}_{j \to i} / \partial T_j$ so that $\mathcal{P}_{j \to i} = G_{i,j} \Delta T$. Then we find

$$\mathcal{P}_{j \to i} = 3 \left(\frac{\pi^2 k_{\rm B} T}{3h} \right) \overline{\mathcal{T}}_{i,j} \Delta T \tag{6}$$

where $\overline{\mathcal{T}}_{i,j} = \int \mathrm{d}x f(x) \mathcal{T}_{i,j}(x) / (\pi^2/3)$ is the mean TC [29] with $f(x) = x^2 \exp(-x)/(\exp(x) - 1)^2$. This expression generalizes the Meir-Wingreen Landauer type formula [31] for photon HF in N-body systems. In the case of two particles (N = 2) one can easily show that $\mathcal{T}_{i,j}(\omega,d) \in [0,1]$ and therefore $\overline{\mathcal{T}}_{i,j} \in [0,1]$ as well. Hence the conductance between two dipoles is limited by 3 times the quantum of thermal conductance $\pi^2 k_{\rm B} T/(3h)$ [32]. In other words, only three channels contribute to the HF between two dipoles namely the channels due to the coupling of the three components $p_{j,\alpha}$ with the same three components $p_{j,\alpha}$ (i.e. same polarization). Of course, by adding further particles this limit cannot be exceeded, whereas the HF can be increased or decreased with respect to the case of two particles. Nevertheless, the number of channels increases if electric multipoles [33, 34] as well as the magnetic moments [10] come into play.

Now, for calculating the Green's function (GF) for a system of N particles we use the set of 3N self-consistent equations [36]

$$\mathbf{E}_{ij} = \mu_0 \omega^2 \mathbf{G}_0^{ij} \mathbf{p}_{j\neq i}^{\text{fluc}} + \frac{\omega^2}{c^2} \sum_{k\neq i} \mathbf{G}_0^{ik} \alpha_k \mathbf{E}_{kj}$$
(7)

for i = 1, ..., N with the free space GF $\mathbb{G}_{0}^{ij} = \frac{\exp(ikr_{ij})}{4\pi r_{ij}} \left[\left(1 + \frac{ikr_{ij}-1}{k^2 r_{ij}^2} \right) \mathbb{1} + \frac{3-3ikr_{ij}-k^2 r_{ij}^2}{k^2 r_{ij}^2} \widehat{\mathbf{r}}_{ij} \otimes \widehat{\mathbf{r}}_{ij} \right]$ the vacuum GF defined with the unit vector $\widehat{\mathbf{r}}_{ij} \equiv \mathbf{r}_{ij}/r_{ij}$, \mathbf{r}_{ij} being the vector linking the center of dipoles i and j, while $r_{ij} = |\mathbf{r}_{ij}|$ and $\mathbb{1}$ stands for the unit dyadic tensor. Inserting relation (1) into this sytem leads to the GF

$$\begin{pmatrix} \mathbb{G}^{1k} \\ \vdots \\ \mathbb{G}^{Nk} \end{pmatrix} = \left[\mathbb{1} - \mathcal{A}_0\right]^{-1} \begin{pmatrix} \mathbb{G}_0^{1k} \\ \vdots \\ \mathbb{G}_0^{(k-1)k} \\ 0 \\ \mathbb{G}_0^{(k+1)k} \\ \vdots \\ \mathbb{G}_0^{Nk} \end{pmatrix}$$
(8)

for k = 1, ..., N with

$$\mathcal{A}_{0} = \frac{\omega^{2}}{c^{2}} \begin{pmatrix} 0 & \mathbb{G}_{0}^{12}\alpha_{2} & \cdots & \mathbb{G}_{0}^{1N}\alpha_{N} \\ \mathbb{G}_{0}^{21}\alpha_{1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbb{G}_{0}^{(N-1)N}\alpha_{N} \\ \mathbb{G}_{0}^{N1}\alpha_{1} & \cdots & \mathbb{G}_{0}^{N(N-1)}\alpha_{N-1} & 0 \end{pmatrix}$$
(9)

With these relations and Eq. (4) at hand it is possible to determine the interparticle HF in a system of N particles out of equilibrium.

Let us now apply this theoretical formalism to describe some emerging many-body effects. To this end, we consider the simplest possible configuration where such effects occur that is a triplet of particles. We consider only the interparticle HF between particle 1 and 2 separated by a distance 2l in the presence of the third particle. Here, we assume that $T_1 = 300$ K and $T_2 = T_3 = 0$. The interparticle HF is then given by

$$\varphi_{12}(2l, r_3) = \mathcal{P}_{1\to 2} - \mathcal{P}_{2\to 1} = \mathcal{P}_{1\to 2}.$$
 (10)

In this case, the dyadic GF reads

$$\mathbb{G}^{21} = \mathbb{D}_{213}^{-1} \left[\mathbb{G}_0^{21} + \mathbb{B}^{213} \frac{\omega^2}{c^2} \mathbb{D}_{31}^{-1} \mathbb{G}_0^{31} \right]$$
(11)

with $\mathbb{D}_{213} = \mathbb{D}_{21} - \frac{\omega^4}{c^4} \mathbb{B}^{213} \mathbb{D}_{31}^{-1} \mathbb{B}^{312}$, $\mathbb{D}_{21} = \mathbb{1} - \frac{\omega^4}{c^4} \mathbb{G}_0^{21} \alpha_1 \mathbb{G}_0^{12} \alpha_2$, and $\mathbb{B}^{213} = \mathbb{G}_0^{23} \alpha_3 + \frac{\omega^2}{c^2} \mathbb{G}_0^{21} \alpha_1 \mathbb{G}_0^{13} \alpha_3$. Some numerical results are shown in Fig. 1 and Fig. 2. We plot the resulting interparticle HF ϕ_{12}^* between particle 1 and 2 in the presence of body 3 normalized to the HF for two isolated dipoles. In both Figs. the position of



Figure 1: Normalized HF exchanged between two SiC spherical particles maintained at $T_1 = 300K$ (left particle) and $T_2 = 0$ K (right particle) with respect to the position $r_3 = (x_3, y_3)$ of a third SiC particle of same radius and $T_3 = 0$ K for (a) 2l = 600 nm, and (b) 2l = 800 nm. The HF is normalized by the HF exchanged between two isolated dipoles in the same thermal conditions. The dark zone with a negative HF corresponds to the region which cannot be occupied by the third particle. For the sake of clarity we consider here that all particles are identical (100 nm radius) and their electric polarizability given by the simple Clausius-Mossotti form [28] $\alpha = 4\pi R^3 \frac{\epsilon-1}{\epsilon+2}$, R denoting the particles radius . The dielectric permittivity of particle is described by a Drude-Lorentz model.

the particles for which the interparticle HF is calculated is fixed, but the position of the third particle is changed. It can be seen that for some geometric configurations the HF mediated by the presence of the third particle can be larger than the value we usually measure for two isolated dipoles. In particular, we observe an exaltation of HF of about one order of magnitude when the third particle is located between the two other particles, i.e., when all three particles are aligned. Hence, the HF between two dipoles can dramatically be increased when inserting a third particle in between. Note, that the three body system described above represent a photon heat transistor where the heat HF between two particles can be actively controlled by the presence of a third particle. This could be achieved through classical AFM manipulation techniques.

In order to understand some of the physics behind this enhancement mechanism, we show in Fig. 3 the TC $\mathcal{T}_{2,1}(\omega)$ for two isolated particles and three aligned par-



Figure 2: Normalized HF between two spherical particles of same radius with respect to the position of a third one which is equidistant to both particles $(T_1 = 300K, T_2 = T_3 = 0K)$.

ticles for a frequency range around the surface phonon resonance of the particles and for different interparticle distances. First of all, it can be observed that the TC shows different resonances where it is close to 1. These resonances can be found from the expression for the GF of the N-body system in Eq. (8) by evaluating $det(\mathbb{1}-\mathcal{A}_0) = 0$ where \mathcal{A}_0 is defined in Eq. (9). In fact, for the considered systems of two or three aligned particles one yields three configurational resonances [35]. Two of these resonances are degenerate because of the rotational invariance around the alignement axis (for more details see Ref. [37]). Apart from these configurational resonances we have the surface mode resonance at $\omega = \omega_{sr}$ with $\epsilon(\omega_{sr}) = -2$, which becomes dominant for large distances so that one sees only one resonance in this case. On the other hand, for distances close to the particle radius the multiple interactions become dominant and several resonances show up in the TC. Note, that the dipole model [7, 8] is only valid for l > 2R. Now, from Fig. 3 it is clear that at long separation distances the coupling between two dipoles becomes more efficient in presence of a third mediator than without, so that the HF enhancement can be attributed to a three body effect that is a resonant surface mode coupling mediated by the third particle. Nevertheless, the absolute value for the interparticle HF is still far away from the theoretical upper limit.

In conclusion, we have introduced a theoretical framework to investigate photon heat transport in mesoscopic systems where strong electromagnetic interactions exist. In particular, a Meir-Wingreen-Landauer-type formula for the radiative HF through N-body interacting photon regions has been derived. A detailed study of three body systems has allowed to identify a many body exaltation mechanism of HF due to configurational resonances. This



Figure 3: TC between two spherical SiC particles separated by a distance 2l (top) and between the same particles when a third SiC particle is located on the mass center of this couple (bottom). All particles have the same radius. The vertical dashed lines marks the distance where the particles are touching [38].

effect could be used to improve for example the performance of near-field thermophotovoltaic devices [3, 4], by placing nanoparticles on the surface of photovoltaic cells.

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http://www.aip.org/pubservs/epaps.html.

[38] Here we also show the TC for distances which cannot be achieved in a real situation because in that distance regime one can easily distinguish the different resonances.