Capacitor physics in ultra-near-field heat transfer

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Abstract – Using the nonequilibrium Green’s function (NEGF) formalism, we propose a microscopic theory for near-field radiative heat transfer between charged metal plates focusing on the Coulomb interactions. Tight-binding models for the electrons are coupled to the electric-field continuum through a scalar potential. For a two–quantum-dot model a new length scale emerges below which the heat current exhibits great enhancement. This length scale is related to the physics of parallel plate capacitors. At long distances $d$, the energy flux decreases as $1/d^2$.

The thermal radiation in a cavity can be well described by Planck’s theory of black-body radiation [1] —a great achievement of the twentieth century physics, which started the quantum physics revolution. Two plates at temperatures $T_0$ and $T_1$ will transfer radiative heat at a rate proportional to $T_0^4-T_1^4$ in the black-body limit, following the Stefan-Boltzmann law. In the 1970s both theoretical [2] and experimental [3–5] works have indicated corrections to the far-field prediction when the distances between the plates are comparable to the thermal wavelengths of the electromagnetic fields. Near-field effects can be as large as a thousand fold that of the far-field results [6–8].

Most recently, due to great progress in technology and precision measurements, much closer proximity is possible, on the scale of nanometers, or near contact. The near-field enhancement reported experimentally in refs. [9,10] is consistent with the established theory. However, the result in [11] is much too large to be explained by the existing theories. Are there other mechanisms for the near-field effects?

Polder and van Hove (PvH) [2] were the first to give a quantitative theory of near-field radiation using the Rytov formulation of fluctuating electromagnetic fields [12,13]. The current-current correlation is assumed to follow the equilibrium fluctuation-dissipation theorem. The ensemble averaged value of the Poynting vector is computed from the solution of macroscopic Maxwell equations. In this picture, the near-field contribution is largely due to evanescent modes which are absent in the far field. A quantum electrodynamics treatment with linear media and NEGF reproduces the PvH theory [14].

The large near-field effects have been recently explained by phonon tunneling or surface phonon polaritons [15–17]. In these works, although the Coulomb interaction is dealt with indirectly, it is still treated as dipole-dipole fluctuations in a charge-neutral system. We advocate that charge-charge fluctuations are important features at short distances. The aim of this letter is to propose such a fundamental theory. We begin with a tight-binding model of the electrons, as in a metal, for example, and couple it to the scalar field in a quantized form. While the electrons are on discrete lattices, the electromagnetic field is continuous and permeates the whole space. Due to the scalar-field nature, we need to use Lorentz gauge quantization [18], and then take the limit of the speed of light $c$ going to infinity in order to be consistent with the gauge condition. To demonstrate the basic idea, we define a toy model for a nano-sized capacitor consisting of two quantum dots and a one-dimensional (1D) scalar field, mediating the Coulomb interactions of the charges. The same formulation can be applied to more realistic models, such as two graphene sheets. Figure 1 illustrates the model.

We imagine a nanoscale parallel plate capacitor for which each of the plates can have a charge of $0$ or $-Q$. The plates located at $z=0$ and $d$ are connected to their respective electron baths so that their charges can fluctuate. The baths are a necessary ingredient so that an infinite amount of energy can be transferred from one dot to the other given time. The couplings of the quantum dots with the baths are bilinear in the system and bath fermion operators; their effects are captured by the self-energies of the baths [19]. We ignore the vector potential and consider...
the scalar potential $\phi(z)$ defined for all $z$. For short distances, the scalar potential, giving rise to the Coulomb interaction, is more important [20,21]. The quantum of the scalar potential, giving rise to the Coulomb interaction, is more important [20,21]. The quantum of the scalar photon satisfies the unusual commutation relation, for the Hermitian conjugate of the preceding term. The creation operators, and their Hermitian conjugates are fermionic annihilation and creation operators. The photon field can be expressed as (in the interaction picture)

$$\phi(z,t) = \sum_q \sqrt{\frac{\hbar}{2\omega_q sL}} (a_q e^{i(qz-\omega_q t)} + \text{h.c.}),$$  

where $\omega_q = c|q|$ is the photon dispersion relation, with the wave number $q = 2\pi k/L$, $k$ an integer, $a_q$ the bosonic annihilation operator of a photon of mode $q$, and h.c. stands for the Hermitian conjugate of the preceding term. The scalar photon satisfies the unusual commutation relation, $[a_q, a^\dagger_p] = -\delta_{qp}$. We will take the limits $L \to \infty$ and $e \to \infty$ at the end of calculation. The latter reproduces Poisson’s equation for the field. We should regard this limiting procedure as only a calculational technique; alternative and equivalent methods based on the Joule heating [20] or the Boltzmann equation [23] are also possible.

Our task is to compute the energy current between the dots. From continuity requirements of the field energy, we can establish an expression for the current density operator to be $\epsilon_0 \phi \partial \phi / \partial z$. However, to obtain a correct quantum version of the operator, we need to symmetrize the two factors and also demand anti-normal order [24]\(^1\) (denoted by the bars and colons here):

$$j = \frac{\epsilon_0}{2} \left[ : \frac{\partial \phi}{\partial z} : + : \frac{\partial \phi}{\partial z} : \right].$$  

Anti-normal order dictates that we swap the annihilation operator to the left of the creation operator if that is not already the case. This removes the zero-point motion contribution. We can relate the expectation value of $j$ in a steady state to the Green’s functions of the photons. The end effect of the operator ordering is to take only the positive frequency contribution of the Green’s function (a justification depends on omitting correlations between annihilation-annihilation operators, and similarly creation-creation operators, and it will be presented elsewhere [25]). The average energy current per unit area at location $z$ can be obtained from

$$\langle j(z) \rangle = \epsilon_0 \int_0^\infty \frac{d\omega}{\pi} h\omega \text{Re} \frac{\partial D^\dagger(\omega, z, z')}{\partial z'} \bigg|_{z'=z},$$  

where $D^\dagger(\omega, z, z') = \int_{-\infty}^{+\infty} D^\dagger(z, t; z', 0)e^{i\omega t}dt$ is the frequency domain greater Green’s function for the field $\phi$.

We evoke the machinery of NEGF [26–29] to calculate the required Green’s functions. First, we define the contour-ordered Green’s function as

$$D(z, \tau; z', \tau') = -\frac{i}{\hbar} (T_r \Delta_\phi(z, \tau) \Delta_\phi(z', \tau'))_{\text{noneq}},$$  

where $\tau$ and $\tau'$ are Keldysh contour times, $T_r$ is the contour order operator, and the average is over a nonequilibrium steady state, $\Delta_\phi(z, \tau) = \phi(z, \tau) - \langle \phi(z, \tau) \rangle_{\text{noneq}}$. The operators are in the Heisenberg picture. Transforming into the interaction picture, and using the standard diagrammatic expansion [30], we can summarize the result in a contour-ordered Dyson equation, which can be organized as a pair of equations in real time, the retarded Dyson equation and the Keldysh equation. Due to time translational invariance, the equations become simple in the frequency domain, given as, for the Keldysh equation,

$$D^\dagger(\omega, z, z') = \sum_{j,k=0,1} D^\dagger(\omega, z, z_j) \Pi^\dagger_{jk}(\omega) D^\dagger(\omega, z_k, z'),$$  

where $z_0 = 0$, $z_1 = d$. The retarded Green’s function satisfies

$$D^\dagger(\omega, z, z') = D^\dagger_0(\omega, z, z') + \sum_{j,k=0,1} D^\dagger_0(\omega, z, z_j) \Pi_{jk}(\omega) D^\dagger(\omega, z_k, z'),$$  

where $D^\dagger_0(\omega, z, z') = -e^{i\frac{\pi}{4}i(\omega - \omega')}/(2i\epsilon_0 A\omega/c)$, is the free photon retarded Green’s function. The advanced Green’s function is obtained by symmetry, $D(\omega, z, z') = D^\dagger(\omega, z', z)^*$. We also have the identity $D^\dagger - D^\leq = D^\dagger - D^a$. To make contact with the usual dyadic Green’s function method [8], one can turn the Dyson equation into a differential equation by operating with the inverse of the free Green’s function. However, due to the discrete nature of the problem, $z_i$ takes only a finite set of values. The above equation (9) can be solved directly, by choosing a

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\(^1\)The anti-normal order is because the creation operators annihilate the photon vacuum state, $a_q^\dagger(0) = 0$. 

Fig. 1: (Colour online) Schematic diagram of the 1D quantum-dot model.
finite set of values \{0, d, z, \cdots \}. It becomes a system of linear equations.

In addition to the Green’s functions of the photons, we also need the Green’s functions of the electrons to compute the photon self-energies. A similar Dyson equation for the electrons can be established, with the Green’s function \[ G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle T \sigma_j c_j(\tau) c_k^\dagger(\tau') \rangle \] and electron self-energy \( \Sigma \). The problem is completely specified if these self-energies are known. However, for interacting systems like the electron-photon interaction \( H_{\text{int}} \), no simple closed form is possible (except for the formal Hedin equations [31]). For the two-dot model, we present a calculation with the self-consistent Born approximation (SCBA) [30]. In this framework the photon self-energy due to the electron-photon interactions to the lowest order is essentially a charge-charge correlation, in contour time, as \( (j, k = 0, 1) \)

\[
\Pi_{jk}(\tau, \tau') \approx -\frac{i}{\hbar} \langle T \sigma_j q_j(\tau) q_k(\tau') \rangle_{H_e} = -i\hbar Q^2 G_{jk}(\tau, \tau') G_{kj}(\tau', \tau),
\]

where \( q_j = (-Q)c_j^\dagger c_j \), and the second line is obtained by applying Wick’s theorem. The appearance of the self-energy \( \Pi \) (which is the linear response of the induced charge by the potential) underlines the difference between the present theory and the standard P\( \chi \)H, which relies on the current-current correlation, or frequency-dependent dielectric function. The contour expression can be used to derive the real-time formula [26], e.g., the retarded one in the frequency domain needed for solving the Dyson equation is

\[
\Pi_{jk}(\omega) = -i\hbar Q^2 \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \left[ G_{jk}(E)G_{kj}(E - \hbar\omega) + G_{jk}^\ast(E)G_{kj}^\ast(E - \hbar\omega) \right].
\]

These formulas above are general. Since the electrons cannot jump from the left lead to the right lead, the off-diagonal elements of the self-energies are zero; we only have nonzero diagonal terms \( \Pi_{jj} \). The electron retarded Green’s function is given by \( G_{rj}(E) = 1/(E - v_j - \Sigma_{rj}^\ast(E) - \Sigma_{rj}(E)) \), where the bath contribution to the self-energy is chosen to follow the Lorentz-Drude model [19], \( \Sigma_{rj}(E) = \frac{i}{\hbar} \Gamma_j/(i + E/E_j) \), where \( \Gamma_j \) and \( E_j \) are the bath model constants. The bath self-energy represents the process of an electron going into and out of the bath, causing the electron at the dot to have a finite lifetime. The lesser Green’s function is given by a Keldysh equation, \( G_{\text{l}}^\ast(E) = G_{rj}^\ast(E)(\Sigma_{\text{rj}}^\ast(E) + \Sigma_{\text{lj}}(E))G_{lj}^\ast(E) \). The lesser components of the bath self-energies follow from the fluctuation-dissipation theorem of the electrons, \( \Sigma_{\text{lj}}(E) = -f_j(E)\Sigma_{\text{rj}}^\ast(E) - \Sigma_{\text{lj}}^\ast(E) \), where \( f_j(E) = 1/\exp[(E - \mu_j)/(k_B T_j)] + 1 \) is the Fermi function at temperature \( T_j \) and chemical potential \( \mu_j \). The baths are in respective thermal equilibrium, but not the dots. The nonlinear self-energies (hence the subscript “n”) \( \Sigma_{\text{nlj}}(E) \) of the electrons arising from the Hartree and Fock diagrams under SCBA due to the electron-photon interaction [32,33] are (for dot \( j = 0, 1 \))

\[
\Sigma_{\text{nlj}}^\ast(E) = i\hbar Q^2 \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \left[ 1 + \sum_{k=0}^{2\pi} D^\ast(\omega, z_j, z_j) + \frac{d\omega}{2\pi} \right],
\]

\[
\Sigma_{\text{nlj}}(E) = i\hbar Q^2 \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \left[ D(\omega, z_j, z_j) \right].
\]

The current formula, eq. (6), can be further simplified using the solution of the Dyson equation and then taking the limit \( c \to \infty \), given that

\[
(j)A = \int_{0}^{\infty} \frac{d\omega}{\pi} h\omega |D_{01}|^2 i(\Pi_{11}^\ast \text{Im}\Pi_{00} - \Pi_{00}^\ast \text{Im}\Pi_{11}),
\]

where \( D_{01} = [\Pi_{00}^\ast \Pi_{11} - (\Pi_{00} + \Pi_{11})^{-1}]^{-1} ; C = c_0 A/d \) is the capacitance.

We now discuss the results of the two-dot model. Figure 2(a) shows the heat current density \((j)\) as a function of the two-dot separation \( d \). A key parameter is the area \( A \); we choose it to be close to the experimental values in ref. [11]. The results are insensitive to the onsite potentials \( v_j \) and chemical potentials \( \mu_j \), provided \( \Gamma_j \) is large. We note that the energy current takes an exact scaling form, \( (j)A = F(x), x = A/(Q^2d), \) with the area \( A \), distance \( d \), and charge \( Q \). Further analysis shows that \( F(x) \propto x^2 \) for small \( x \) and it approaches a constant for large \( x \). Under the strong-coupling limit, \( k_B T_j \ll \Gamma_j \), in addition to a \( T_j^4 \) temperature dependence, the current

\[
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\]
parameters) for small \( x \) and 1/(\( A^2 \)) for large \( x \) (here \( \Gamma \approx \max(\Gamma_0, \Gamma_1) \)). The crossover from one type of behavior to the other type of behavior is controlled by \( \Gamma \approx Q^2/(2\mathcal{C}) \). Alternatively, a length scale can be obtained from \( \Delta_0 \), giving \( d = -e_0 A[1/\Pi_{00}(0)+1/\Pi_{11}(0)] \). The current decreases as \( 1/d^2 \) for large \( d \) and saturates at the scale given by \( d \) (about 40 nm with our choice of parameters) for small \( d \).

This phenomenon is different from near-field radiative heat transfer results at a length scale less than \( \hbar c/(k_B T) \) dominated by evanescent modes when the transverse component of the wave vector \( q_\perp > \omega/c \). There are no evanescent modes in our 1D model since \( q_\perp = 0 \) permanently. Besides, fig. 2(a) also shows large values of heat transfer. At the saturation value, the heat current density is approximately \( 9 \times 10^7 \text{W/m}^2 \), which is about a thousand times larger than the black-body (BB) limit of \( 5.6 \times 10^4 \text{W/m}^2 \). This enhancement is at least one order of magnitude larger than a typical PvH theory prediction for metals, which is in the range of hundreds. Compared to a one-dimensional Landauer formula (1D BB) result with perfect transmission, \( i.e., 1.1 \times 10^9 \text{W/m}^2, \) our numbers are about \((1/12)-\)th of that upper limit [34]. Such enhancement is mainly due to transverse confinement (there is only one transmission mode) and the small area \( A \). The temperature dependence of the current density is plotted in fig. 2(b). Asymptotically for large \( T_0 \) fixing \( T_1 \), the Stefan-Boltzmann law gives the fourth power of \( T_0 \) and the 1D BB limit gives a quadratic function of \( T_0 \).

The results presented above are for strong couplings, where \( \Gamma_j \) is comparable to an electron energy scale of order eV. For weak couplings, SCBA convergence is difficult. However, we observe that the physics remains qualitatively the same if we do not do self-consistency. In such a framework, the photon self-energies \( \Pi_0 \) can be approximated by the fluctuation-dissipation theorem, assuming that each dot is in local thermal equilibrium. Within this framework of approximation, we can recover a Caroli/Landauer formula [25].

In summary, we have presented a fundamental theory of near-field heat transfer due to Coulomb interactions of the electrons that applies to distances approaching atomic lattice constants. At ultra-short distances, we should consider charge fluctuations and Coulomb interactions through a scalar field, which is the dominating contribution. PvH and later improvements [2,6] are formulated in a gauge-invariant way, thus the longitudinal Coulomb interaction is also included. Our treatment is beyond the usual assumption of local equilibrium, thus the fluctuation-dissipation theorem is not assumed for the charges. The approach proposed here opens the way for the treatment of other geometries such a surface and a tip. Such calculations could resolve the controversies regarding the recent experiments [11]. Our approach can be interfaced with first-principle calculations, thus enabling more rigorous predictions of near-field properties.

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