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Fluctuating-surface-current formulation of radiative heat transfer for arbitrary geometries

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We describe a fluctuating-surface-current formulation of radiative heat transfer, applicable to arbitrary geometries in both the near and far field, that directly exploits efficient and sophisticated techniques from the boundary-element method. We validate as well as extend previous results for spheres and cylinders, and also compute the heat transfer in a more complicated geometry consisting of two interlocked rings. Finally, we demonstrate how this method can be adapted to compute the spatial distribution of heat flux on the surfaces of the bodies.

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Quantum and thermal fluctuations of charges in otherwise neutral bodies lead to stochastic electromagnetic (EM) fields everywhere in space. In nonequilibrium situations involving bodies at different temperatures, these fields mediate energy exchange from the hotter to the colder bodies, a process known as radiative heat transfer. Although the basic theoretical formalism for studying heat transfer was laid out decades ago,1–10 only recently have experiments reached the precision required to measure them at the microscale,11–15 sparking renewed interest in the study of these interactions in complex geometries that deviate from the simple parallel-plate structures of the past. The near-field regime is particularly interesting, though largely unexplored except in planar structures, due to the contribution of evanescent waves which have been shown to significantly alter and enhance heat transport at submicron separations.9,10

In this Rapid Communication, we propose a formulation of radiative heat transfer for arbitrary geometries based on the well-known surface-integral-equation (SIE) formulation of classical electromagnetism16, which extends our recently developed fluctuating surface-current (FSC) approach to Casimir phenomena17 to the nonequilibrium problem of energy transfer between bodies of unequal temperatures. Unlike previous scattering formulations based on basis expansions of the field unknowns best suited to special18–25 or noninterleaved periodic26,27 geometries, or formulations based on expensive, brute-force time-domain simulations,28 this approach allows direct application of the boundary element method (BEM): a mature and sophisticated SIE formulation of the scattering problem in which the EM fields are determined by the solution of an algebraic equation involving a smaller set of surface unknowns (fictitious surface currents in the surfaces of the objects).16 In what follows, we briefly review the SIE method, derive an FSC equation for the heat transfer between two bodies, and demonstrate its correctness by checking it against (as well as extending) previous results for spheres and cylinders.

The radiative heat transfer between two objects 1 and 2 at local temperatures \( T_1 \) and \( T_2 \) can be written as9,10

\[
H = \int_0^{\infty} d\omega \left[ \Theta(\omega, T_1^2) - \Theta(\omega, T_1^2) \right] \Phi(\omega),
\]

where \( \Theta(\omega, T) = \frac{\omega}{k_B T} \left\{ \exp\left(\frac{\omega}{k_B T}\right) - 1 \right\} \) is the Planck energy per oscillator at temperature \( T \), and \( \Phi \) is an ensemble-averaged flux spectrum into object 2 due to random currents in object 1 (defined more precisely below). The only question is how to compute \( \Phi \), which naively involves a cumbersome number of scattering calculations.

Formulation. We begin by presenting our final result for \( \Phi \), which is derived and validated below. Consider homogeneous objects 1 and 2 separated by a lossless medium 0. Let \( G^r \) denote the \( 6 \times 6 \) Green’s function \( G^r(x,y) = G^r(x-y) \) of the homogeneous medium \( r \) at a given \( \omega \) (known analytically29), relating 6-component electric \( (J) \) and magnetic \( (M) \) currents \( \xi = (J; M) \) \( \{\cdot;\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\...
functions if \( r = 0 \), and
\[
\begin{bmatrix}
W^{11} & W^{12} \\
W^{21} & W^{22}
\end{bmatrix} = \begin{bmatrix}
G^0 & (G^1_0) \\
\hat{G}^0 & G^2
\end{bmatrix}^{-1}
\] (4)
is the SIE matrix inverse, used to solve SIE scattering problems as reviewed below, which relates incident fields to “equivalent” surface currents. In particular, \( W^{21} \) relates incident fields at the surface of object 2 to the equivalent currents at the surface of object 1. Equation (2) is computationally convenient because it only involves standard matrices that arise in BEM calculations,\textsuperscript{16} with no explicit need for evaluation of fields or sources in the volumes, separation of incoming and outgoing waves, integration of Poynting fluxes, or any additional scattering calculations.

In addition to its computational elegance, Eq. (2) algebraically captures crucial physical properties of \( \Phi \). The standard definiteness properties of the Green’s functions (currents do nonnegative work) imply that sym \( G^r \) is negative semidefinite and hence it has a Cholesky factorization \( \text{sym} G^r = −U^r U^r \) where \( U^r \) is upper-triangular. It follows that \( \Phi = \frac{1}{\Phi_1} \text{Tr}[Z^T Z] = \frac{1}{\Phi_1} \|Z\|^2 \), where \( Z = U^r W^{21} U^{12} \) is a weighted Frobenius norm of the interaction matrix \( W^{21} \) and hence \( \Phi \geq 0 \) as required. Furthermore, reciprocity (symmetry of \( \Phi \) under \( 1 \leftrightarrow 2 \) interchange) corresponds to simple symmetries of the matrices. Inspection of \( \Gamma \) shows that \( \Gamma(x,y) = \Gamma^T(x,y)S \), where \( S = S^T = S^{-1} = S^* \) is the matrix that flips the sign of the magnetic components, and it follows from (3) that \( \hat{G}^T = S \hat{G} S \) and \( W^T = S W S \) where \( S = S^T = S^{-1} = S^* \) is the matrix that flips the signs of the magnetic basis coefficients and swaps the coefficients of \( s_n \) and \( \bar{s}_n \). It follows that
\[
\Phi = \frac{1}{2\pi} \text{Tr}[\text{sym} G^r S \text{sym} \hat{G}^1 S] = \frac{1}{2\pi} \text{Tr}[\text{sym} \hat{G}^2 S \text{sym} \hat{G}^1 W],
\] (5)
where the \( S \) factors cancel, leading to the \( 1 \leftrightarrow 2 \) exchange.

\textbf{Derivation.} The key to our derivation of (2) is the SIE formulation of EM scattering,\textsuperscript{16,30} which we briefly review here. Consider the fields \( \phi^+ = \phi^+ + \phi^- \) in each region \( r \), where \( \phi^+ \) is the “incident” field due to sources \( \text{within} \) region \( r \), and \( \phi^- \) is the “scattered” field due to the interface reflections and sources in the other media. The core idea in the SIE formulation is the principle of equivalence,\textsuperscript{30} which states that the scattered field \( \phi^- \) can be expressed as the field of some fictitious electric and magnetic surface currents \( \xi^r \) located on the boundary of region \( r \), acting within an infinite homogeneous medium \( r \). In particular, the field \( \phi^- = 0 \) is \( \phi^0 = \Gamma_0 \xi^1 = (\bar{\xi}^1 + \xi^3) \). Remarkably, the \textit{same} currents with a sign flip describe scattered fields in the interiors of the two objects,\textsuperscript{30} \( \phi^{-r} = -\Gamma_0^* \xi^r \) for \( r = 1,2 \). These currents \( \xi^r \), in turn, are completely determined by the boundary condition of continuous tangential fields \( \phi^{-r} \mid_r = \phi^+ \mid_r \) at the \( r = 1,2 \) interfaces, giving the SIEs \( (\Gamma_0^* + \Gamma_0^* \xi^1 + \Gamma_0^* \xi^3 + \Gamma_0^* \xi^1 - \Gamma_0^* \xi^3) \mid_r = \phi^+ - \Gamma_0 \xi^1 \mid_r \) in terms of the incident fields. To obtain a discrete set of equations, one expands \( \xi^r = \sum_n s^n \xi_{n}^r \) in a basis \( s^n \) as above, and then takes the inner product of both sides of the SIEs with \( s^n \) (a Galerkin discretization) to obtain a matrix “BEM” equation \( W^{-1} x = s \) in terms of exactly the \( W \) matrix from Eq. (4), current coefficients \( x = (x^1, x^2) \), and a right-hand “source” term \( s = (s^1, s^2) \) from the incident fields: \( s_{m}^r = (s_{m}^r, \phi^0 + \phi^-_{0r}) \).

To compute \( \Phi \), we start by considering the flux \( \Phi_2 \) into object 2 due to a single dipole source \( \sigma^1 \) within object 1, so that \( \phi^{1+} = \Gamma_1^* \sigma^1 \) and all other incident fields are zero. This corresponds to a right-hand side \( s = (s^1, 0) \) where \( s_{m}^r = (s_{m}^r, \Gamma_1^* \sigma^1) \) in the BEM equation. \( \Phi_2 \) is the resulting absorbed power in object 2, equal to the net incoming Poynting flux on the surface 2. The Poynting flux can be computed using the fact that \( \xi^r \) is actually equal to the surface-tangential fields: \( \xi^r = (n \times H, -n \times E) \) where \( n \) is the outward unit-normal vector. It follows that the integrated flux is
\[
\Phi_2 = \frac{1}{4} \text{Re} \left[ \int_{\Gamma} (\mathbf{E} \times \mathbf{H}) \cdot \mathbf{n} \right] = \frac{1}{4} \text{Re} (\xi^2 \sigma^2) \quad \text{(equivalent to the power exerted on the surface currents by the total field, with an additional 1/2 factor from a subtlety of evaluating the fields exactly on the surface)}.
\]
Hence,
\[
\Phi_1 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2) \quad \text{and} \quad \Phi_2 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2) \quad \text{and} \quad \Phi_1 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2),
\]
where we used the continuity of \( \phi^0 \) and \( \phi^2 \). Substituting \( \xi^2 = \sum_n x_n s^n \) and recalling the definition (3) of \( G^2 \), we obtain
\[
\Phi_1 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2) \quad \text{and} \quad \Phi_2 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2) \quad \text{and} \quad \Phi_1 = \frac{1}{4} \text{Re} (\xi^2 \sigma^2),
\]
via straightforward algebraic manipulations.

Now, to obtain \( \Phi = \Phi_2 \) we must ensemble-average \( (\cdots) \) over all sources \( \sigma^1 \), and this corresponds to computing the matrix \( C = (s s^*) \), which is only nonzero in its upper-left block \( C^1 = (s^1 s^1) \). Such a Hermitian matrix is completely determined by the values of \( x^1 s^1 (C^1)^T S x^1 \) for all vectors \( x^1 \), where we have inserted the sign-flip matrices \( S \) and the transposition for later convenience, and by study of this expression we will find that \( C^1 \) has a simple physical meaning. To begin with, we write \( \xi^1 = \sum_n x_n s^n \) to obtain
\[
x^1 s^1 (C^1)^T S x^1 = (\langle x^1 s^1 \rangle (S^T \sigma^1)^T \sigma^1) \quad \text{and} \quad \text{where we have integrated over all possible dipole positions.}
\]
The current-current correlation function \( \langle \sigma^1(x) \sigma^1(y) \rangle = \frac{1}{2} \delta (\mathbf{r} - \mathbf{r} \cdot \mathbf{y}) \text{Im} \chi \) is given by the fluctuation-dissipation theorem,\textsuperscript{31} where we have factored out a \( \Theta (\omega, T^1) \) term into Eq. (1) and where \( \text{Im} \chi \) denotes the temperature-independent imaginary part of the \( 6 \times 6 \) material susceptibility (whose diagonal blocks are \( \text{Im} \varepsilon \) and \( \text{Im} \mu \)) related to material absorption (or the conductivity \( \omega \text{Im} \chi \)). This eliminates one of the integrals, leaving
\[
4 \pi \int \xi^1(\mathbf{x})^* (S^T \sigma^1) \text{Im} \chi (\mathbf{y}) \Gamma^1(\mathbf{x}, \mathbf{y}) \, d^2 \mathbf{x} \, d^2 \mathbf{y} \, d^2 \mathbf{x} \, d^2 \mathbf{y} \, d^2 \mathbf{x} \approx \int d^2 \mathbf{x} \Gamma^1(\mathbf{x}, \mathbf{y}) \text{Im} \chi (\mathbf{y}) \xi^1(\mathbf{x}) = S \int d^2 \mathbf{x} \Gamma^1(\mathbf{x}, \mathbf{y}) \xi^1(\mathbf{x}) = S \phi^1,
\]
where \( \phi^1 = \Gamma^1 \cdot \xi^1 \) is the field due to the surface current \( \xi^1 \), and where the commuted \( \mathcal{S} \) can be used to simplify the remaining term \( \xi^1(x)^* \mathcal{S} \mathcal{T}^1(x,y) \mathcal{S} = [\Gamma^1(x,y) \xi^1(x)]^* \), assuming that \( \mathcal{S} \) commutes with \( \Im \chi \) (true unless there is a bi-anisotropic susceptibility, which breaks reciprocity). Finally, we obtain

\[
x^1 \mathcal{S} (\Gamma^1)^T \mathcal{S} x^1 = \frac{4}{\pi} \int d^3y \, \phi^{1*}(\omega \Im \chi) \phi^1.
\]

But \( \frac{1}{2} \phi^{1*}(\omega \Im \chi) \phi^1 = \frac{1}{2} \Re[\phi^{1*}(-i\omega \chi \phi^1)] \) is exactly the time-average power density dissipated in the interior of object 1 by the field \( \phi^1 \) produced by \( \xi^1 \), since \( -i\omega \chi \phi^1 \) is a bound-current density.

Computing the interior dissipated power from an arbitrary surface current is somewhat complicated, but matters here simplify considerably because the \( \mathcal{C} \) matrix is never used by itself—it is only used in the trace expression \( \Phi = -\frac{1}{4} \text{Tr}[\mathcal{C} \mathcal{W}^*(\text{sym} \mathcal{G}^2) \mathcal{W}] = -\frac{1}{4} \text{Tr}[\cdots]^T = -\frac{1}{4} \text{Tr}[\mathcal{S}^T \mathcal{W} \mathcal{S}(\text{sym} \mathcal{G}^2) \mathcal{W}^*], \) by reciprocity as in Eq. (5). From the Cholesky factorization \( \mathcal{G}^2 = -\mathcal{U}^2 \mathcal{U}^2 \), this becomes \( \frac{1}{4} \text{Tr}[\mathcal{X}^* \mathcal{S} \mathcal{C} \mathcal{X}] \), where \( \mathcal{X} = \mathcal{W} \mathcal{G}^{2*} \) are the “currents” due to “sources” represented by the columns of \( \mathcal{U}^2 \), which are all of the form \([0; s^T]\) (corresponding to sources in object 2 only). So, effectively, \( \mathcal{S} (\mathcal{C}^1)^T \mathcal{S} \) is only used to evaluate the power dissipated in object 1 from sources in object 2, and by the same Poynting-theorem reasoning from above, it follows that \( \mathcal{S} (\mathcal{C}^1)^T \mathcal{S} = -\frac{1}{2} \text{sym} \mathcal{G}^1 \). Hence \( \mathcal{C}^1 = -\frac{\omega}{2} \text{sym} \mathcal{G}^1 \mathcal{S} = -\frac{\omega}{2} \text{sym} \mathcal{G}^1 \) by the symmetry of \( \mathcal{G}^1 \), and Eq. (2) follows.

It is also interesting to consider the spatial distribution of the Poynting-flux pattern, which can be obtained easily because, as explained above, \( \frac{1}{2} \Re[\xi^*(x) \phi^1(x)] \) is exactly the inward Poynting flux at a point \( x \) on surface 2. It follows that the mean contribution \( \Phi_n^2 \) of a basis function \( s_n^2 \) to \( \Phi \) is

\[
\Phi_n^2 = \frac{1}{4} \left[ \Re [ s_n^2 W^* e_n^2 s_n^2 \mathcal{G}^2 W s_n ] \right] = \frac{1}{4} \Re [ e_n^2 \mathcal{G}^2 W (s s^*) W^* e_n^2 ] = \frac{1}{2\pi} \Re [ e_n^2 \mathcal{G}^2 W \text{sym} (\mathcal{G}^1) W^* e_n^2 ],
\]

where \( e_n^2 \) is the unit vector corresponding to the \( s_n^2 \) component. This further simplifies to \( \Phi_n^2 = F_{nn}^2 \), where

\[
F^2 = \frac{1}{2\pi} \Re [ \mathcal{G}^2 W \text{sym} (\mathcal{G}^1) W^* ].
\]

Note that \( \Phi = \text{Tr} \Phi^2 \). Similarly, by swapping 1 \( \leftrightarrow 2 \) we obtain a matrix \( F^1 \) such that \( \Phi_n^1 = F_{nn}^1 \) is the contribution of \( s_n^1 \) to the flux on surface 1.

For a single object 1 in medium 0, the *emissivity* of the object is the flux \( \Phi^0 \) of random sources in 1 into 0. Following the derivation above, the flux into 0 is \( -\frac{1}{2} \Re (\xi^1, \phi^0) = -\frac{1}{2} (\xi^1, \Gamma^0 \xi^1) \). The rest of the derivation is essentially unchanged except that \( W = (\mathcal{G}^1 + \mathcal{G}^0)^{-1} \) since there is no second surface. Hence, we obtain

\[
\Phi^0 = \frac{1}{2\pi} \text{Tr}[\text{sym} \mathcal{G}^1 W \text{sym} \mathcal{G}^0 W].
\]

which again is invariant under 1 \( \leftrightarrow 0 \) interchange from the reciprocity relations (Kirchhoff’s law).

**Results.** Figure 1 shows the flux spectra \( \Phi \) of various configurations of isolated and interacting gold cylinders and spheres of radii \( R = 0.2 \mu m \), plotted over a frequency window wide enough to capture the relevant contributions to room-temperature emission. In every case, \( \Phi \) is normalized by the surface area \( A \) of each object to make comparisons easier (at these wavelengths \( \lambda, R \) is several times the skin depth \( \delta = c/\sqrt{\epsilon_0 \sigma} \), which means that most of the radiation is coming from sources near the surface of the objects)\(^{12} \). Our results for isolated and interacting spheres (hollow circles) agree with previous results based on semianalytical formulas\(^{18,32} \) (solid lines). However, we also consider radiation from finite, isolated cylinders (solid circles) of varying aspect ratios \( L/R \), a geometry for which there are currently no semianalytical results except in the special case of infinite cylinders \( L \to \infty \)\(^{32} \) (solid lines). We find that for \( L/R \approx 2 \) (not shown), corresponding to nearly isotropic cylinders, \( \Phi \) is only slightly larger than that of an isolated sphere due to the small but nonnegligible contribution of volume fluctuations to \( \Phi \). As \( L/R \) increases, \( \Phi \) increases over all \( \lambda \) and converges towards the \( L \to \infty \) limit (black solid line) as \( \lambda \to 0 \), albeit slowly. Moreover, \( \Phi_L \gg \Phi_\infty \) at particular wavelengths, a consequence of *geometrical* resonances that are absent in the infinite case—away from these resonances, \( \Phi \) clearly straddles the \( L \to \infty \) result so long as \( \lambda \lesssim L \). In the case of interacting cylinders, \( \Phi \) exhibits significant enhancement at large \( \lambda \) due to near-field effects [Fig. 1 (left inset)], causing the heat transfer rate \( H \to \infty \) with decreasing separation.
A rapid convergent semianalytical formulas of heat transfer in even small surface area and volume, the absolute (unnormalized) $\Phi$ of the isolated ring is $\approx 4.5$ times larger than that of the sphere at the fundamental resonance. The geometrical origin of this resonance enhancement becomes even more apparent upon inspection of the spatial distribution of flux pattern on the surface of the objects, which we compute via Eq. (7) and show as insets in Fig. 2, for both rings and spheres. As expected, at large $\lambda \gg R$, near-field effects dominate and the flux pattern peaks in regions of nearest surfaces. However, for $\lambda \sim R$, the sphere-sphere pattern does not change qualitatively while the ring-ring pattern exhibits resonance patterns characterized by nodes and peaks distributed along the ring. Interestingly, the flux pattern of the first resonance is peaked away from the nearest surfaces. Away from these resonances, the ring emissivity is smaller: For $\lambda \ll R$ (not shown), $\Phi$ is well described by the Stefan-Boltzmann law, and the ratio of their emissivities is given by the ratio of their surface areas $\approx 0.3$. A similar reduction occurs for $\lambda \gg R$ due to the ring’s smaller polarizability.

In conclusion, we presented a short derivation of an FSC approach to nonequilibrium fluctuations based on the SIE framework of classical EM scattering, that allows direct application of sophisticated techniques from classical numerical EM, such as powerful BEM solvers (requiring little if any modifications), to efficiently compute the radiative heat transfer between bodies of arbitrary shape. Although our focus here was on a numerical method for arbitrary geometries, the same formalism can also be applied with a spectral basis to obtain rapidly convergent semianalytical formulas of heat transfer in special high-symmetry geometries, in the spirit of previous work based on the scattering-matrix formalism. A longer and more general derivation of our formulation that subsumes other situations of interest, such as geometries with multiple or nested bodies, along with the aforementioned application of our formulation to high-symmetry situations, will be presented in a subsequent publication. Finally, we believe that it should be possible to employ similar ideas and techniques to study other nonequilibrium phenomena, such as Casimir forces between bodies of unequal temperatures or thermal fluorescence.

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