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Calculation of nonzero-temperature Casimir forces in the time domain

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We show how to compute Casimir forces at nonzero temperatures with time-domain electromagnetic simulations, for example, using a finite-difference time-domain (FDTD) method. Compared to our previous zero-temperature time-domain method, only a small modification is required, but we explain that some care is required to properly capture the zero-frequency contribution. We validate the method against analytical and numerical frequency-domain calculations, and show a surprising high-temperature disappearance of a nonmonotonic behavior previously demonstrated in a pistonlike geometry.

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In this paper, we show how to compute nonzero-temperature \((T > 0)\) corrections to Casimir forces via time-domain calculations, generalizing a computational approach based on the finite-difference time-domain (FDTD) method that we previously demonstrated for \(T = 0\) [1,2]. New computational methods for Casimir interactions [3–8] have become important in order to model nonplanar micromechanical systems where unusual Casimir effects have been predicted, and there has been increasing interest in \(T > 0\) corrections [9–19], especially in recently identified systems where these effects are non-trivial in the time domain because of the singularity of the zero-frequency contribution, and we show that a naive approach leads to incorrect results. We validate using both a one-dimensional (1D) system where analytical solutions are available and also a two-dimensional (2D) piston-like geometry [3,21] where we compare to a frequency-domain numerical method. In the piston, we observe an interesting effect in which a nonmonotonic phenomenon previously identified at \(T = 0\) disappears for a sufficiently large \(T\).

The Casimir force arises from fluctuations at all frequencies \(\omega\), and the \(T = 0\) force can be expressed as an integral \(F(0) = \int_0^\infty f(\xi) d\xi\) over Wick-rotated imaginary frequencies \(\omega = i\xi\) [20]. At \(T > 0\), this integral becomes a sum over "Matsubara frequencies" \(\xi_n = n\pi\omega_T\) for integers \(n\), where \(\omega_T = 2k_BT/h\) and \(k_B\) is Boltzmann’s constant [20]:

\[
F(T) = \pi\omega_T \left[ \frac{f(0^+)}{2} + \sum_{n=1}^{\infty} f(n\pi\omega_T) \right].
\]  

Equation (1) corresponds to a trapezoidal-rule approximation of the \(T = 0\) integral [8]. At room temperature, \(\xi = \pi\omega_T\) corresponds to a \("wavelength"\) \(2\pi/\xi = 7\ \mu\text{m}\), much larger than most experimental separations, so usually \(T > 0\) corrections are negligible [20]. However, experiments are pushing toward \(> 1-\mu\text{m}\) separations in attempts to measure this phenomenon [17,18], recently culminating in an experiment at several \(\mu\text{m}\) that appears to clearly observe the \(T > 0\) corrections [19]. In addition, we have recently predicted much larger \(T\) corrections with certain materials and geometries [12].

Many of the recent techniques to compute Casimir forces in arbitrary geometries can be related to mature computational methods from classical electromagnetism (EM) [8]. One method is to use the fluctuation-dissipation theorem, by which the mean-square electric and magnetic fields \((E^2)\) and \((H^2)\) can be computed from classical Green’s functions [20], and the mean stress tensor can be computed and integrated to obtain the force [1–3]. In particular, at each \(\omega\), the correlation function \((E^2)\) is

\[
\langle E_j(x)E_k(x') \rangle_\omega = -\frac{k}{\pi} \Im \left[ \omega^2 \tilde{G}^E_{jk}(\omega;x;x') \right] \coth \left( \frac{\omega}{\omega_T} \right),
\]  

where \(\tilde{G}^E_{jk}(\omega;x;x') = (G^E_{jk})_0\) is the classical dyadic "photon" Green’s function, proportional to the electric field in the \(j\) direction at \(x\) due to an electric-dipole current in the \(k\) direction at \(x'\), and solves

\[
(\nabla \times \mu(\omega,x)^{-1} \nabla \times -\omega^2 \epsilon(\omega,x))G^E_{jk}(\omega,x,x') = \delta^3(x-x')\delta_k,
\]  

where \(\epsilon\) is the electric permittivity tensor, \(\mu\) is the magnetic permeability tensor, and \(\delta_k\) is a unit vector in direction \(k\). The magnetic-field correlation \((H^2)\) has a similar form [1,2]. Note that the temperature dependence appears as a coth factor (from a Bose-Einstein distribution). If this is Wick rotated to imaginary frequency \(\omega = i\xi\), the poles in the coth function give the sum (1) over Matsubara frequencies [22]. In our EM simulation, what is actually computed is the electric or magnetic field in response to an electric or magnetic dipole current, respectively. This is related to \(G_{ij}\) by

\[
E_{jk}(\omega,x,x') = -i\omega\tilde{G}^E_{jk}(\omega,x,x'),
\]  

where \(E_{jk}(\omega,x,x')\) denotes the electric field response in the \(j\)th direction due to a dipole current source \(J(\omega,x,x') = \delta(x-x')\delta_k\) [1].

This equation can be solved for each point on a surface to integrate the stress tensor, and for each frequency to integrate the contributions of fluctuations at all frequencies. Instead of computing each \(\omega\) separately, one can use a pulse source in...
time, whose Fourier transform contains all frequencies. As derived elsewhere [1,2], this corresponds to a sequence of time-domain simulations, where pulses of current are injected and some function $\Gamma(t)$ of the resulting fields (corresponding to the stress tensor) is integrated in time, multiplied by an appropriate weighting factor $g(t)$. We perform these simulations using the standard FDTD technique [23], which discretizes space and time on a uniform grid. In frequency domain, Wick rotation to complex $\omega$ is crucial to obtain a tractable frequency integral [3,8], and the analog in time domain is important to obtain rapidly decaying fields (hence short simulations) [1,2].

In time domain, one must implement complex $\omega$ indirectly: Because $\omega$ only appears explicitly with $e$ in Eq. (3), converting $\omega$ to the complex contour $\omega(\xi) \equiv \xi \sqrt{1 + \frac{i\omega}{\xi}}$ is equivalent to operating at a real frequency $\xi$ with an artificial conductivity $\epsilon(\mathbf{r}) \rightarrow \epsilon(\mathbf{r})(1 + \frac{1}{\xi})$ [1,2]. (One cannot use purely imaginary frequencies $\omega = i\xi$ in time domain, because the corresponding material $\epsilon \rightarrow -\epsilon$ has exponentially growing solutions in time [1].) Thus, by adding an artificial conductivity everywhere, and including a corresponding Jacobian factor in $g(t)$, one obtains the same (physical) force result in a much shorter time (with the fields decaying exponentially due to the conductivity). (Note that the resulting “time” is not physical time but is instead a mathematical construction equivalent to a frequency-domain calculation for equilibrium or quasi-static problems.)

Now, we introduce the basic idea of how $T > 0$ is incorporated in the time domain, and explain where the difficulty arises. The standard $T > 0$ analysis of Eq. (1) is expressed in frequency domain, so we start there by exploiting the fact that the time-domain approach is derived from a Fourier transform of a frequency-domain approach. In particular, $g(t)$ is the Fourier transform of a weighting factor $g[\omega(\xi)]$ [1,2]. At real $\omega$, the effect of $T > 0$ is to include an additional factor $\coth \left( \frac{i\omega}{\omega_T} \right)$ in the $\omega(\xi)$ integral from Eq. (2). So, a naive approach is to replace $g[\omega(\xi)]$ with

$$g[\omega(\xi)] \rightarrow g[\omega(\xi)] \coth \left( \frac{\omega(\xi)}{\omega_T} \right).$$

using the $g[\omega(\xi)]$ expression for $T = 0$ from [1], and then Fourier transform this to yield $g(t)$. However, there is an obvious problem with this approach: The $1/\omega$ singularity in $\coth \left( \frac{i\omega}{\omega_T} \right)$ means that Eq. (5) is not locally integrable around $\xi = 0$, and therefore its Fourier transform is not well defined. If we naively ignore this problem, and compute the Fourier transform via a discrete Fourier transform, simply assigning an arbitrary finite value for the $\xi = 0$ term, this unsurprisingly gives an incorrect force for $T > 0$ compared to the analytical Lifshitz formula for the case of parallel perfect-metal plates in one dimension [24], as shown in Fig. 1 (green dashed line).

Instead, a natural solution is to handle $\omega \neq 0$ by the coth factor as in Eq. (5), but to subtract the $\omega = 0$ pole and handle this contribution separately. We will extract the correct $\omega = 0$ contribution from the frequency-domain expression Eq. (1), convert it to time domain, and add it back in as a manual correction to $g(t)$. In particular, the $\coth \left( \frac{i\omega}{\omega_T} \right)$ function has poles at $\omega = n\pi\omega_T$ for integers $n$. When the $\omega$ integral is
with \( \omega^2 \varepsilon(\mathbf{r}) \rightarrow \xi^2 (1 + \frac{\mu}{\xi}) \varepsilon(\mathbf{r}) \), but what we actually want is 
\(-i\omega \tilde{G}_{ij}(\omega)|_{\xi=0}(\xi) = -i\omega(\xi) \tilde{G}_{ij}(\xi)\). Therefore, the correct \( \omega = 0 \) contribution is given by
\[
\lim_{\omega \to 0^+} \Gamma^E_F(\omega) = \lim_{\xi \to 0^+} \frac{\omega(\xi)}{\xi} \Gamma^E_F(\xi).
\] (10)

Combined with \( \omega(\xi)k_B T \) factor from Eq. (9), this gives an \( n = 0 \) contribution of \( \Gamma_{|\xi=0|} \) multiplied by 
\(-\omega(\xi)^2 k_B T/\xi|_{\xi=0^+} = \sigma k_B T \). This \( \omega = 0 \) term corresponds to a simple expression in the time domain, since \( \Gamma_{|\xi=0|} \) is simply the time integral of \( \Gamma(t) \) and the coefficient \( \sigma k_B T \) is merely a constant. Therefore, while we originally integrated \( g_{n=0}(t)\tilde{\Gamma}(t) \) to obtain the \( n > 0 \) contributions, the \( n = 0 \) contribution is included if we instead integrate
\[
\left[ g_{n=0}(t) + \sigma k_B T \right] \tilde{\Gamma}(t).
\] (11)

The term \( \left[ g_{n=0}(t) + \sigma k_B T \right] \) generalizes the original \( g(t) \) function from [1] to any \( T \geq 0 \).

We check Eq. (11) for the 1D parallel plate case in Fig. 1 against the analytical Lifshitz formula [25]. As noted above, the \( g_{n=0} \) term (6) correctly gives the \( n > 0 \) terms, and we also see that the \( \sigma k_B T \) term gives the correct \( n = 0 \) contribution, and hence the total force is correct.

As another check, we consider a more complicated pistonlike geometry [3], shown schematically in the inset of Fig. 2. Two square rods lie between two sidewalls, which we solve here for the 2D case of \( z \)-invariant fluctuations. At \( T = 0 \), such geometries exhibit an interesting nonmonotonic variation of the force between the two blocks as a function of sidewall separation \( d \) [3,21], which does not arise in the simple pairwise-interaction heuristic picture of the Casimir force. This can be seen in the solid lines of Fig. 2, where the nonmonotonicity arises from a competition between forces from transverse-electric (TE, \( E \) in-plane) and transverse-magnetic (TM, \( E \) out-of-plane) polarizations [26], which can be explained by a method-of-images argument [21]. In Fig. 2, the solid lines are computed by a \( T = 0 \) frequency-domain boundary-element method (BEM) [7], whereas the circles are computed by the \( T = 0 \) FDTD method [1,2], and both methods agree. We also compute the force at \( T = 1 \times \pi \chi h/k_B a \) where the \( \xi = 0^+ \) term dominates. We see that the FDTD method with the \( T > 0 \) modification Eq. (11) (diamonds) agrees with the frequency-domain BEM results (dashed lines), where the latter simply use the Matsubara sum (1) to handle \( T > 0 \).

Interestingly, Fig. 2 shows that the nonmonotonic effect disappears for \( T = 1 \times \pi \chi h/k_B a \), despite the fact that the method-of-images argument of [21] ostensibly applies to the \( \xi = 0^+ \) quasistatic limit (which dominates at large \( T \)) as well as to \( \xi > 0 \). The argument used the fact that TM fluctuations can be described by a scalar field with Dirichlet boundary conditions (vanishing at the metal), and in this case the sidewalls introduce opposite-sign mirror sources that reduce the interaction as \( d \) decreases; in contrast, TE corresponds to a Neumann scalar field (vanishing slope), which requires same-sign mirror sources that increase the interaction [21]. In Fig. 2, however, while the \( T = 1 \times \pi \chi h/k_B a \) TM force still decreases as \( d \) decreases, the TE force no longer increases for decreasing \( d \) at \( T = 1 \times \pi \chi h/k_B a \). The problem is that the image-source argument most directly applies to \( z \)-directed dipole sources in the scalar-field picture—electric \( J^E \) currents for TM and magnetic \( J^H \) currents for TE—while the situation for in-plane sources (corresponding to derivative of the scalar field from dipolelike sources) is more complicated [27]. For a sufficiently large \( T \) dominated by the \( \xi = 0^+ \) contribution (as here), we find numerically that the \( J^H \) sources no longer contribute to the force as \( \xi \rightarrow 0^+ \). Intuitively, as \( \xi \rightarrow 0^+ \) a magnetic dipole produces nearly constant (wavelength \( \rightarrow \infty \)) field, which satisfies the Neumann conditions and hence is not affected by geometry. Instead, numerical calculations show that the TE \( \xi = 0^+ \) contribution is dominated by \( J^E \) sources and the corresponding electric stress-tensor terms, which turn out to slightly decrease in strength as \( d \) decreases. (A related effect is that, for small \( d \), it can be observed in Fig. 2 that the \( T = 1 \) force is actually smaller than the \( T = 0 \) force, again due to the suppression of the TE contribution. Since the force diverges as \( T \rightarrow \infty \), this means that the force changes nonmonotonically with \( T \) at small \( d \); a similar nonmonotonic temperature dependence was previously observed for Dirichlet scalar-field fluctuations in a sphere-plate geometry [15].)

In contrast, if we consider the three-dimensional constant cross-section problem with \( z \)-dependent fluctuations, corresponding to integrating \( e^{ikz}\) fluctuations over \( k_z \) [20]; then we find that the nonmonotonic effect is preserved at all \( T \). This is easily explained by the fact that, for perfect metals, \( k_z \neq 0 \) is mathematically equivalent to a problem at \( k_z = 0 \) and \( \xi \rightarrow \sqrt{\xi^2 + k_z^2} \) [3,28], and so the \( n = 0 \) Matsubara term still contains contributions equivalent to \( \xi > 0 \) in which the \( J^H \) mirror argument applies and the situation is similar to \( T = 0 \). In any case, this 2D disappearance of nonmonotonicity seems unlikely to be experimentally relevant, because we find that it only occurs for \( T \geq 0.7 \times \pi \chi h/k_B a \), which for \( a = 1 \mu m \) corresponds to \( T \geq 5000 \ K \).

Thus, a simple (but not too simple) modification to our previous time-domain method allows off-the-shelf FDTD
software to easily calculate Casimir forces at nonzero temperatures. Although the disappearance of nonmonotonicity employed here as a test case appears unrealistic, recent predictions of other realistic geometry and material effects [12], combined with the fact that temperature effects in complex geometries are almost unexplored at present, lead us to hope that future work will reveal further surprising temperature effects that are observable in micromechanical systems. Although various authors have debated which model $\varepsilon(\omega)$ most accurately reflects experiments [10,11,17–19], computational methods such as the one here are independent of such debates, since any desired material can be inserted in the computation (using standard techniques to express material dispersion in FDTD [23]). For example, although the perfect metals used in our examples are obviously an artificial material, it has been argued that if the perfect metal is viewed as the limit of a Drude model then the $n = 0$ contribution should be omitted [10] for the TM mode (using our TE/TM convention)—in our computational method, this is accomplished simply by dropping the second term from Eq. (11) during the TM calculation (and it turns out that nonmonotonicity still disappears in a similar manner).

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