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The energy spectrum of electromagnetic normal modes in dissipative media: modes between two metal half spaces

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Abstract

The energy spectrum of electromagnetic normal modes plays a central role in the theory of the van der Waals and Casimir interaction. Here we study the modes in connection with the van der Waals interaction between two metal half spaces. Neglecting dissipation leads to distinct normal modes with real-valued frequencies. Including dissipation seems to have the effect that these distinct modes move away from the real axis into the complex frequency plane. The summation of the zero-point energies of these modes render a complex-valued result. Using the contour integration, resulting from the use of the generalized argument principle, gives a real-valued and different result. We resolve this contradiction and show that the spectrum of true normal modes forms a continuum with real frequencies.

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1. Introduction

An alternative to using the full many-particle machinery in calculating the interaction energy in a system is to study the energy shifts of the electromagnetic normal modes of the system [1]. The energy, or frequency, of a normal mode is found as a solution to an equation of the type

$$f(\omega) = 0, \quad (1)$$

the condition for having a mode. The function $f(\omega)$, which involves the dielectric properties of the system, is often obtained as a determinant of a matrix. The solution to equation (1) approaches a pole of the function $f(\omega)$ when the interaction in the system is gradually turned off. When the interaction is turned on the zeros move away from the poles and $\hbar/2$ times

this shift in frequency is the contribution to the interaction energy of this particular mode; the interaction energy is the change in total zero-point energy when the interaction in the system is turned on, i.e., the following sum over zeros and poles of the function $f(\omega)$:

$$E = \frac{\hbar}{2} \sum_i (\omega_{0,i} - \omega_{\infty,i}). \quad (2)$$

The longitudinal bulk modes can be used to find, e.g., the polaron energy in a polar semiconductor or the exchange-correlation energy in a metal, the transverse modes to find the Lamb shift [2], the surface modes to find the van der Waals interaction between objects, and the vacuum modes to find the Casimir [3] interaction.

Using the sum-over-modes approach, or mode-summation method, equation (2), is a very physically transparent approach where the contribution from each mode is visible. Unfortunately, it is sometimes not possible to find an explicit solution to equation (1) and sometimes the poles and zeros form a continuum. In those cases the result may be obtained with the so-called generalized argument principle [1],

$$E = \frac{1}{2\pi i} \oint dz \frac{\hbar}{2} z \frac{d}{dz} \ln f(z), \quad (3)$$

where the integration is performed along a contour including the poles and zeros in the right half of the complex frequency plane. The integration should be performed in the positive sense, i.e. in the counter-clockwise direction. The result in equation (3) is consistent with what one arrives at from many-particle theory where the focus is put on the interacting particles in the system, not the electromagnetic normal modes; there is no explicit reference to zero-point energies. This is demonstrated in detail in [1] in the case of the exchange-correlation energy of a metal. In [4] the van der Waals and Casimir forces between two quantum wells were derived both in terms of the zero-point energy of the normal modes and as the result from correlation energy; both approaches produced the same result. Thus, there are different complementary approaches to the interactions in a system.

In the present work we are concerned with the sum-over-modes approach to the van der Waals interaction between two metal half spaces in the presence of dissipation. Van Kampen *et al* [5] studied the force between two dielectric half spaces separated by a dielectric layer. They applied equations (2) and (3) to the surface modes of the geometry to find the interaction energy and force. They considered non-dissipative materials only with real-valued dielectric functions. In that case there are distinct modes with real-valued frequencies. In the case of dissipative materials the sum-over-modes approach runs into yet another problem. The solution of equation (1) produces complex-valued frequencies or energies, signalling that the normal modes are no longer stable—the modes decay. If this were the case they would no longer be true normal modes. The interaction energy in equation (2) becomes complex valued. Using, instead, equation (3) produces a real-valued interaction energy. This situation has made many researchers confused and led them to believe that there is something fundamentally wrong with the mode-summation method. With the present work we will try to resolve this confusion and show that the result of equation (3) is the correct result in the case of dissipation; the complex-valued result of equation (2) is not correct. In an earlier brief report [6] we have illustrated the problem by considering the longitudinal bulk modes in a metal. In the present work we study the modes associated with the van der Waals interaction between two metal half spaces.

In section 2 we discuss the analytical properties of the dielectric function and show that its zeros and poles are all located at the real frequency axis. In section 3 we apply the different formalisms to the van der Waals interaction between two metal half spaces. We introduce a

modified mode-summation method that works reasonably well in section 4 and finish with a summary and conclusions in section 5.

2. Analytical properties of a dielectric function

In the problem we are addressing we use metals and represent the dielectric function with one of the Drude type,

$$\varepsilon(\omega) = 1 - \omega_{\text{pl}}^2 / \omega(\omega + i\eta). \quad (4)$$

We let the parameter η be a positive real-valued constant; η , which is the result of electron scattering against impurities or other defects, is really ω dependent and complex valued; the approximation we use is good for a metal in the low momentum limit, for frequencies below the plasma frequency, ω_{pl} .

Before we continue let us discuss the general analytical properties of a dielectric function. The physical dielectric function, the one that can be measured in experiments, exists on the real frequency axis only. It is retarded, which means that it obeys causality. In theoretical treatments one obtains a function that is analytical in the whole complex frequency plane except on the real axis, where all the poles are situated. To obtain the retarded version one either shifts all the poles downwards to an infinitesimal distance below the real axis and perform the calculation on the real axis. Alternatively one lets the poles stay put and perform the calculation just above the axis. For the discussion in this work it is better to use this last method. There are other versions of the function, advanced, time-ordered and anti-time-ordered. The time-ordered is often used in many-body calculations since it allows some very useful theorems to be used. With this version one calculates the function just above the positive real axis and below the negative real axis. All different versions are identical everywhere except at the real frequency axis. From now on, if not stated otherwise, when we discuss the dielectric function we mean the function with its poles on the real axis. The function has the properties $\varepsilon(-\omega) = \varepsilon(\omega)$ and $\varepsilon(\omega^*) = \varepsilon(\omega)^*$. From these equations it follows that the relation between the different forms of the function in the lower and upper half planes is $\varepsilon_l(\omega) = \varepsilon_u(\omega^*)^*$. For the full dielectric function with frequency-dependent η these two analytical expressions are the same but not when η is treated as a constant. Then we have $\varepsilon_u(\omega) = 1 - \omega_{\text{pl}}^2 / \omega(\omega + i\eta)$ and $\varepsilon_l(\omega) = 1 - \omega_{\text{pl}}^2 / \omega(\omega - i\eta)$, respectively. In the full treatment we have

$$i\eta(\omega^*) = [i\eta(\omega)]^* = -i[\eta(\omega)]^* = -i\text{Re}[\eta(\omega)] - \text{Im}[\eta(\omega)], \quad (5)$$

and we may identify

$$\text{Re}[\eta(\omega^*)] = -\text{Re}[\eta(\omega)], \quad \text{Im}[\eta(\omega^*)] = \text{Im}[\eta(\omega)]. \quad (6)$$

We see that the dominating real part changes sign when we cross the real axis while the imaginary part does not.

As an illustration, let us look at the expression for the dielectric function of an impure metal in the so-called generalized Drude approach [7]. Let n_i , n , $S(\mathbf{q})$ and $\omega_0(\mathbf{q})$ be the density of impurities, electron density, structure factor for the impurities and impurity potential, respectively. Then the dielectric function in the small momentum limit is

$$\varepsilon(\omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega \left\{ \omega + \frac{n_i}{24\pi e^2 m_e \omega n \Omega} \sum_{\mathbf{q}} S(\mathbf{q}) q^4 |\omega_0(\mathbf{q})|^2 [\varepsilon^{-1}(\mathbf{q}, \omega) - \varepsilon^{-1}(\mathbf{q}, 0)] \right\}}, \quad (7)$$

where Ω is volume of the system. The second term within the parentheses in the denominator is $i\eta$. For a large system the summation over momentum is usually replaced by an integral over

a continuous momentum variable. Let us now keep the discrete summation. The derivation of the dielectric function of the pure metal at finite momentum also contains a discrete summation, now over the electron momentum. The function in the RPA (random phase approximation) is

$$\varepsilon(\mathbf{q}, \omega) = 1 + (v_q/\Omega) \sum_{\mathbf{k}, \sigma} n(\mathbf{k})[1 - n(\mathbf{k} + \mathbf{q})] \times \{[\hbar\omega + (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})]^{-1} - [\hbar\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})]^{-1}\}, \quad (8)$$

where $n(\mathbf{k})$ is the Fermi–Dirac occupation number. We see that if we make the calculation just off the real frequency axis, the imaginary part consists of a sum of δ -functions, infinitesimally spaced when the volume of the system goes to infinity. These form the single particle continuum in the ωq -plane. The real part passes through zero between each neighbouring pair of δ -functions. When the volume goes to infinity one can replace the summation by an integral. The imaginary part then turns into a smooth continuous function and the real part does no longer pass through zero inside the continuum. When one wants to find the zeros and poles of the function $\varepsilon(\omega)$, in equation (7), one should keep the discrete summations everywhere. Then one realizes that this function also has its poles and zeros on the real axis and that they are in the form of a continuum.

If we now instead let all summations turn into integrals the parameter η is a smooth complex-valued function of frequency. However, its real part dominates and is almost constant for frequencies below the plasma frequency. From the expression in equation (7) we can easily verify that the real part of η changes sign when one crosses the real axis. For higher frequencies the contribution to the interaction energy quickly drops off, so equation (4) is good enough for our purpose here.

3. Modes between two metal half spaces

We are interested in the van der Waals interaction between two metal half spaces separated by the distance d . The modes in this system are characterized by the 2D (two-dimensional) wave vector \mathbf{k} . There are several modes for each wave vector. To find the modes of wave vector \mathbf{k} we let $f(\omega)$ in equation (1) be [1]

$$f_{\mathbf{k}}(\omega) = [\varepsilon(\omega) + 1]^2 - e^{-2kd}[\varepsilon(\omega) - 1]^2 = \{[\varepsilon(\omega) + 1] - e^{-kd}[\varepsilon(\omega) - 1]\} \times \{[\varepsilon(\omega) + 1] + e^{-kd}[\varepsilon(\omega) - 1]\} = f_{\mathbf{k}}^1(\omega)f_{\mathbf{k}}^2(\omega). \quad (9)$$

Equation (1) then gives us four zeros, The two in the right half plane are

$$\omega_{\mathbf{k}} = \begin{cases} \omega_{\text{pl}}\sqrt{[1 + \coth(kd/2)]^{-1} - (\eta/2\omega_{\text{pl}})^2} - i\eta/2; & f_{\mathbf{k}}^1(\omega) = 0 \\ \omega_{\text{pl}}\sqrt{[1 + \tanh(kd/2)]^{-1} - (\eta/2\omega_{\text{pl}})^2} - i\eta/2; & f_{\mathbf{k}}^2(\omega) = 0 \end{cases} \quad (10)$$

Thus the zeros are below the real frequency axis. The problem is that the expression in equation (4) for the dielectric function is only valid above the real axis. Below the real axis η has the opposite sign. The zero is very illusive. If one approaches the zero from the upper half plane it makes a jump to the upper half plane when one crosses the real axis. This clearly shows that it is not safe to use equation (2), directly. If plotted the real part of the mode energies from equation (10) form two branches of modes, one acoustical (lower) and one optical (upper). The lower (upper) branch comes from putting $f_{\mathbf{k}}^1 = 0$ ($f_{\mathbf{k}}^2 = 0$). A first naive guess is that a good approximation of the interaction energy would be to just sum the real part of the zero-point energies for the modes. This might seem to be a good and simple shortcut to an approximate result. However, as we will see later, it turns out not to be such a good idea.

Let us now instead use equation (3) to find the energy contribution from each 2D wave vector. The total interaction energy per unit area is

$$E = \frac{1}{\Omega} \sum_{\mathbf{k}} E_{\mathbf{k}} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{1}{2\pi i} \oint dz \frac{\hbar}{2} z \frac{d}{dz} \ln f_{\mathbf{k}}(z), \quad (11)$$

where Ω is the total area of one half space. In an actual calculation we let this area go to infinity and the summation over \mathbf{k} turns into an integration. We first choose our contour to encircle the positive real axis. The contour then consists of two parts: an integration from zero to plus infinity performed just below the real axis; an integration from plus infinity to zero performed just above the axis. We may first perform an integration by parts in both contributions and end up with

$$E_{\mathbf{k}} = -\frac{1}{2\pi i} \frac{\hbar}{2} \oint dz \ln f_{\mathbf{k}}(z). \quad (12)$$

Then the integration below and above the axis are combined into one integral

$$E_{\mathbf{k}} = -\frac{1}{i} \frac{\hbar}{2} \int_0^{\infty} \frac{d\omega}{2\pi} \ln \frac{f_{\mathbf{k}}(\omega)^*}{f_{\mathbf{k}}(\omega)} = \sum_{l=1}^2 \frac{\hbar}{2} \int_0^{\infty} \frac{d\omega}{2\pi} 2 \tan^{-1} \{ \text{Im} [f_{\mathbf{k}}^l(\omega)] / \text{Re} [f_{\mathbf{k}}^l(\omega)] \}, \quad (13)$$

where the function \tan^{-1} is taken from the branch where $0 \leq \tan^{-1} \leq \pi$.

Let us now instead deform the integration contour into a semicircle in the right half plane with the center of the circle at the origin and the straight part parallel with and just to the right of the imaginary frequency axis,

$$E_{\mathbf{k}} = \frac{\hbar}{2} \int_0^{\infty} \frac{d\omega}{2\pi} 2 \ln \frac{f_{\mathbf{k}}'(\omega)}{4} = \frac{\hbar}{2} \int_0^{\infty} \frac{d\omega}{2\pi} 2 \ln \frac{f_{\mathbf{k}}(i\omega)}{4}. \quad (14)$$

The integration along the curved part of the contour vanishes when the radius goes to infinity. The 4 in the denominator takes care of this. The zeros and poles of the function $f_{\mathbf{k}}(\omega)$ in equation (9) do not change from the division by a factor of 4. Thus we end up with two integrals for the same thing: one along the real frequency axis; one along the imaginary axis. Now, we may simplify the integrands by letting $x = (\eta/2)/\omega_{\text{pl}}$ and expressing the frequency in terms of the plasma frequency. Equations (13) and (14) then reduce to

$$\begin{aligned} \frac{E_{\mathbf{k}}}{\hbar\omega_{\text{pl}}/2} &= \int_0^{\infty} \frac{d\omega}{2\pi} 2 \left\{ \tan^{-1} \left[\frac{2x(1 - e^{-kd})}{\omega(2\omega^2 + 8x^2 - 1 + e^{-kd})} \right] \right. \\ &\quad \left. + \tan^{-1} \left[\frac{2x(1 + e^{-kd})}{\omega(2\omega^2 + 8x^2 - 1 - e^{-kd})} \right] \right\} = \int_0^{\infty} d\omega F(\omega) \end{aligned} \quad (15)$$

and

$$\frac{E_{\mathbf{k}}}{\hbar\omega_{\text{pl}}/2} = \int_0^{\infty} \frac{d\omega}{2\pi} 2 \ln \frac{[2 + 1/\omega(\omega + 2x)]^2 - e^{-2kd}[1/\omega(\omega + 2x)]^2}{4} = \int_0^{\infty} d\omega G(\omega), \quad (16)$$

respectively. These two integrands $F(\omega)$ and $G(\omega)$ are shown in figure 1 for a wave vector with $kd = 0.5$, for the two parameter choices $x = 0.1$ and 0.01 .

In figure 2 we present the results from the different approaches. The solid curve is the exact result from equation (15) or (16) and the dashed curve shows the shortcut from just dropping the imaginary parts of the mode energies. The circles are the result from yet another approximation that we will discuss in section 4. The fact that equations (15) and (16) produce the same result proves that the poles and zeros are all on the real axis.

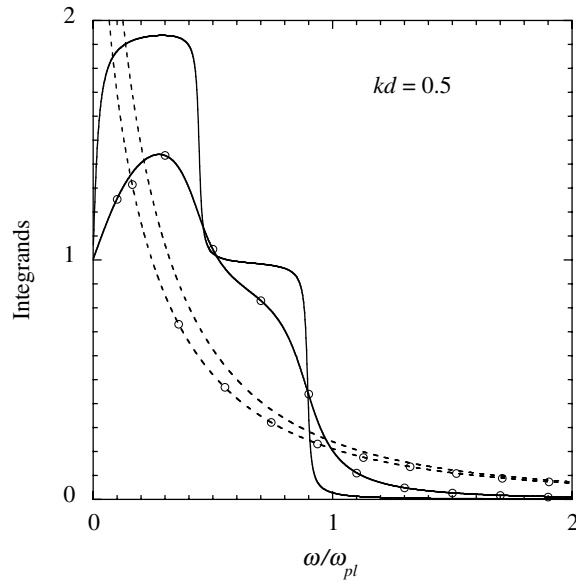


Figure 1. The solid and dashed curves are the integrands of equations (15) and (16), respectively. The curves with circles are for $x = 0.1$ and the others are for $x = 0.01$.

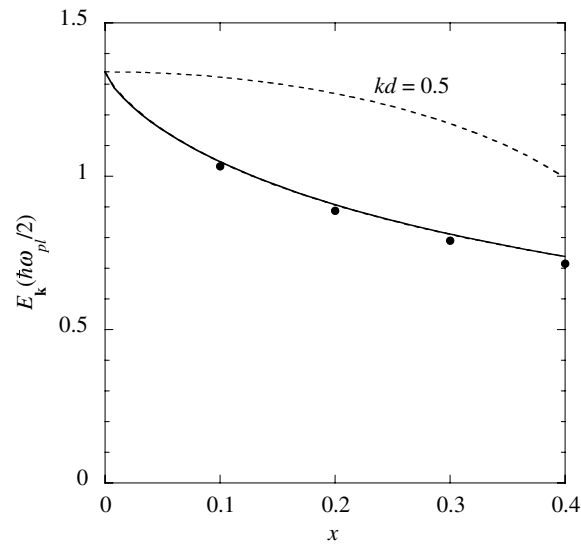


Figure 2. The contribution to the interaction energy from one wave vector with $kd = 0.5$. The solid curve is the exact result as calculated from either equation (15) or (16). The dashed curve is from neglecting the imaginary parts of the poles and zeros. The circles are the result from using equation (18) and the parameters given in the text.

4. A mode summation method that works

In the preceding section we found that the naive use of the mode-summation method failed. The question is whether the mode-summation method can be used at all in the case of

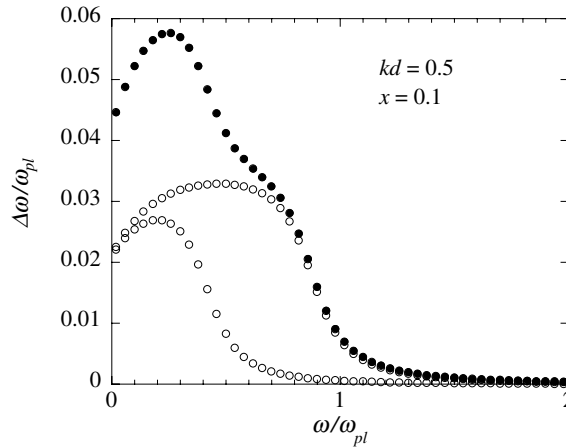


Figure 3. The energy shifts of the zeros away from the poles when the interaction is turned on. The open circles are the shifts of the modes corresponding to one of the two branch types. The filled circles is the combined effect. See the text for more details

dissipative materials. To investigate this we make a Lehman representation of the dielectric function,

$$\varepsilon(\omega) = 1 + \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{-2\text{Im}\varepsilon(\omega')}{\omega - \omega'} = 1 - \int_0^{\infty} \frac{d\omega'}{2\pi} \frac{8x}{[(\omega/\omega_{pl})^2 - (\omega')^2][(\omega')^2 + 4x^2]}. \quad (17)$$

The integral over frequency can be viewed as a limit of discrete frequency summations where the step size goes towards zero. In each summation the dielectric function has its poles and zeros on the axis. These points come closer and closer when we take the limit. The integrations over frequency and momentum should always be viewed as limits of discrete summations since the system is always finite in size and possible energy and momentum transfers are discrete.

Now if we approximate the integral of equation (17) with a discrete summation,

$$\varepsilon(\omega) \approx 1 - \frac{8x}{2\pi} \frac{\omega'_{\max}}{i_{\max}} \sum_{i=1}^{i_{\max}} [(\omega/\omega_{pl})^2 - (\omega'_i)^2]^{-1} [(\omega'_i)^2 + 4x^2]^{-1}, \quad (18)$$

where $\omega'_i = (i - 1/2)\omega'_{\max}/i_{\max}$, the dielectric function has a finite number of poles and zeros. Using this function in the expressions for the two factors $f_{\mathbf{k}}^1(\omega)$ and $f_{\mathbf{k}}^2(\omega)$ of equation (9) means that also these factors each have the same number of poles and zeros. Using equation (2) where the sum runs over these poles and zeros gives us an approximate result for $E_{\mathbf{k}}$, the contribution to the interaction energy from mode \mathbf{k} . The result becomes asymptotically the exact result when we let ω'_{\max} and i_{\max} go towards infinity. In figure 2 the first (last) two circles were calculated including 50 equidistant poles in the region below $2\omega_{pl}$ ($3\omega_{pl}$), i.e. $\omega'_{\max} = 2(3)$ and $i_{\max} = 50(50)$. Thus we have to find the frequency of 50 poles and 50 zeros. This is feasible and the result is in much better agreement with the exact result than what one obtains when just neglecting the imaginary part of the zeros and poles.

In this treatment all poles and zeros are real valued. We now have one acoustical and one optical branch in between each pair of neighbouring poles. When the interaction is turned off the zeros end up at the position of the lowest of the two poles. When the interaction is turned on they move up a distance and it is these shifts in frequency or energy that are their contributions to the interaction energy. In figure 3 we show as open circles these shifts for the

acoustical (the curve with left-most maximum) and optical branches. The combined shifts are shown as filled circles. We clearly see the resemblance of the filled circles to the integrand of equation (15), represented by the solid curve with circles in figure 1.

5. Summary and conclusions

The modes between two metal half-spaces are, in neglect of dissipation, distinct with real-valued energies. When dissipation is included it appears as if the modes move away from the real axis into the complex frequency plane. We have demonstrated that this is not so. The modes form a continuum on the real frequency axis and the direct use of the mode summation method is no longer feasible. The functions appearing in the condition for modes contain integrals over momentum or frequencies. Since the system is finite in size these integrals should be considered as discrete summations; the possible momentum and energy transfers in a finite system is discrete. In doing so all zeros and poles end up on the real axis. When one takes the limit when the volume goes to infinity the zeros and poles form a continuum of points on the real axis.

We have demonstrated two different contour integrations that can be used to find the result; the one we favour most ends up with an integration along the imaginary frequency axis; the other involves an integration along the real frequency axis.

We have further demonstrated that one may use an approximation in which this continuum of modes is replaced by a finite number of distinct modes and obtain reasonable good results using the mode-summation method. This gives a great improvement compared to the result from just neglecting the imaginary parts of the complex-valued energies of the apparent modes.

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