Scarf for Lifshitz

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Abstract  Polarization of dispersive and dissipative dielectric media with smoothed-out inhomogeneities is studied with the goal to clarify the question of renormalizability of electromagnetic stress–energy tensor. The stress tensor is computed with the Lifshitz approach to van der Waals forces in the non-retarded limit, which accounts for dominant effects at the distances from the interface shorter than the absorption wavelength. After the subtraction of the leading free space ultraviolet divergencies, there still remain two types of divergencies. First, contributions diverging in the sharp interface case become \textit{finite} once it is smoothed out. Second, new \textit{subleading} ultraviolet cut-off-dependent contributions appear due to the interface internal structure. The Hadamard expansion, based on the heat kernel method, is applied to systematically single out both finite and subleading contributions and to demonstrate incomplete renormalizability of the Lifshitz theory. The above approach also allows us to reveal the purely quantum mechanical nature of surface tension, which consists of finite cut-off-independent as well as cut-off-dependent contributions. The deduced theory of surface tension and its calculations for real dielectric media are favourably compared to the available experimental data. The problem of surface tension proves to be of a \textit{distinguished limit} type because the sharp interface formulation loses the critical information about the internal structure of an interface. The general theory offered here is illustrated with an exactly solvable model representing a smooth transition between two different dielectric media, which relies upon a solution of the Schrödinger equation with the Scarf potential.

1 Introduction

1.1 The circle of phenomena: quantum fluctuations of a vacuum and matter

While the basic elements of QFT—a vacuum, interaction between particles, and structure of simple atoms—are reasonably well understood, real matter and its interaction with quantum fluctuations of the vacuum are less so as the accurate modelling and prediction of its properties prove to be hard [1–3]. The structure and hence mechanical strength of condensed matter are determined by the forces acting between molecules $i$ and $j$—phenomenologically, this is often described by the canonical Lennard-Jones potential $\varphi_{\text{LJ}}^{ij} = 4\nu \left[ (r_m/r_{ij})^{12} - (r_m/r_{ij})^6 \right]$, which is an isotropic part of intermolecular interaction;

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here $\upsilon$ is the depth of the potential well and $2^{1/6}r_m \sim r_m$ is the intermolecular separation at which $\varphi_{LJ}$ has a minimum. The first term in $\varphi_{LJ}$ is a purely heuristic way of modelling a quantum repulsion of molecules due to the Pauli exclusion principle. The last term in $\varphi_{LJ}$—commonly known as the van der Waals (vdW) interaction $\varphi_{vdW} = -4\upsilon (r_m/r)^6$—can be rigorously justified by dipole–dipole (Keesom), dipole-induced dipole (Debye), and dispersion induced dipole-induced dipole (London) interactions.

It is the latter (dispersive) part of vdW forces—present in any matter and playing a role in a host of everyday phenomena such as adhesion, surface tension (ST), adsorption, wetting, crack propagation in solids, to name a few, and hence considered to be the most important [4]—which we will be dealing with here. As motivated by applications, about a century ago it was realized that the pressure $\Pi_D$ in thin liquid films is generally different from the pressure in the macroscopic bulk liquid due to the action of vdW potential forces. This disjoining Derjaguin’s pressure $\Pi_D = -A_H/(6\pi \ell^3)$ was originally calculated for pure substances and non-charged interfaces [5] via pairwise (additive) summation of intermolecular potential interactions $\varphi_{vdW}^\ell$; here $A_H$ is the Hamaker constant specific to a given combination of substances in contact. However, a rigorous account of the subject matter started with Casimir’s work [6,7], in whose original configuration two parallel perfectly conducting plates are separated by the vacuum, which gives rise to a finite pressure on the plates $\Pi_C = \hbar c/\pi^2((240\ell^4))$.

Driven by the discrepancy between experiments [8–10] and “additive” macroscopic theory [5,11,12], a rigorous derivation of the pressure, with $\Pi_D$ in the non-retarded and $\Pi_C$ in the retarded limits, was performed by Lifshitz [13] in the case of two parallel homogeneous dielectric media separated by the vacuum. His work recognized the genuine quantum nature and non-additivity of dispersion forces. Later, Dzyaloshinskii et al. (DLP) [14] generalized the Lifshitz theory by introducing another homogeneous medium instead of the vacuum as the intervening phase.

In the Lifshitz/DLP theory, the electromagnetic (EM) fluctuations are quantized in polarizable media. Because the range of influence of vdW forces is much larger than the interatomic distance, $r \gg r_m$ due to power-law decay $\varphi_{vdW} \sim r^{-6}$ in the non-retarded limit and $\varphi_{vdW} \sim r^{-7}$ in the retarded one, the calculation of the EM stress–energy tensor $T_{\mu\nu}$ in macroscopic bodies can be done exclusively based on their geometry and the classical EM linear response functions such as dielectric permittivity $\varepsilon$ and magnetic susceptibility $\mu$.

The predicted values of the Casimir–Derjaguin force were confirmed in the earlier experiments [8–10,15] and more recent precise measurements [16]. Nowadays the Casimir effect is considered to be important in many nano- and microelectromechanical systems [17]. Despite being of wide interest and the subject of a mature research area, there remain open questions regarding the divergence of the EM stress–energy tensor $T_{\mu\nu}$ inside the bodies and vacuum. Thus, a renaissance in studying Casimir–Derjaguin forces is driven by both theoretical and applied underpinnings.

1.2 The problem of divergencies: bulk and interfaces

While the Casimir–Derjaguin force arises from interactions between the fluctuating quantum fields and matter, traditionally the Casimir–Derjaguin problem is posed as the response of a fluctuating quantum field to externally imposed boundary conditions (BCs). Namely, in the standard treatment of the Casimir–Derjaguin effect one investigates the EM field only and considers, for example, the metal plates as perfect conductors represented by the corresponding BCs. While BCs are a very convenient mathematical idealization, physical materials cannot constrain arbitrarily high frequency components of a fluctuating quantum field or, equivalently, wavelengths much shorter than $r_m$. For example, for an imperfect conductor of
characteristic skin depth $\delta_s$, waves of sufficiently short wavelength $\lambda \lesssim \delta_s$ (high frequency) penetrate a significant distance before being attenuated and therefore do not 'see' the precise position of the boundary. In general, at a very high mode frequency $\omega$ all real media become transparent and indistinguishable from the vacuum $\varepsilon, \mu \rightarrow 1$.

The presence of an inhomogeneous structure, e.g. in the form of boundaries, without which Casimir and Derjaguin effects would not exist, leads to the distortion of the quantum state of the confined field containing no real force carriers and consisting entirely of zero-point fluctuations. Since the boundaries change the zero-point energy of the fluctuating fields, they give rise to forces between the rigid bodies or stresses on isolated surfaces.

Since the work of Casimir, it has been known that the sum over zero-point energies is highly divergent in the UV limit. Subtraction of the vacuum energy that is already present without the plates, i.e. not subject to the BCs, only removes the strongest UV divergence, which is quartic in the regularization parameter in three space dimensions [18]. This divergence does not affect the total force of interaction between bodies because its contribution to the energy does not depend on the separation distance between bodies. Similar subtractions can be found in the general theory of vdW forces by Lifshitz and DLP.

However, as became obvious from the local analysis, after this subtraction there are still remnant boundary-induced divergences in stresses and energy density as has been known for a long time [19–24]. One often considers this remaining effect as determined by the part of the zero-point energy [25], which is infrared (IR) and hence non-local being associated with the BCs. This is in contrast to the local nature of UV divergencies, the renormalization of which assumes that all local divergent terms can be combined with the bare coupling constants of the field theory to produce finite (renormalized) physically observable local characteristics of the system. In the case of a pure Maxwell field, i.e. not affected by the real media polarization, the stresses at the infinite plane boundary happen to be finite [26], only because of the special symmetry of the Maxwell field in this case, which allows for the diverging contributions from electric and magnetic fields to cancel each other locally. Dispersive media break this symmetry resulting in the stresses diverging at the sharp boundaries and may seem to imply diverging effects [27] such as ST.

There have been many attempts using various methods [28]—from point splitting [29], heat kernel expansion [30], proper time and wavenumber cut-off [31], zeta-function [32], dimensional [33] to other approaches [34,35]—to achieve local regularization near boundaries. As noted by Fulling [36], zeta-function and dimensional regularization methods hide the divergencies in an ad hoc way and yield global energies that may be inconsistent with the local $T^{\mu\nu}$. While the cut-off methods are naturally based on limiting the range of wavenumbers from above due to the microstructure of materials, the resulting cut-off-dependent values of stresses and energy density render the theory dissatisfying as well as leave some ambiguities in the interpretation of ST. It was also shown [36,37] that some versions of a finite UV cut-off near the Dirichlet boundary may lead to violation of a stress–energy tensor $T^{\mu\nu}$ conservation. There have been other formal solutions offered to cure the problem of boundary divergencies, e.g. to cancel them by introducing ad hoc surface-dependent counterterms [27,38,39].

Another approach put in practice is to replace sharp boundaries by steeply rising potential barriers [18,28,40–42], e.g. by modelling a wall with a potential such as the Dirac $\delta$-function [43–47] or a smooth power-law function [18,37,40]; in the case of a metal plate, the BCs are idealized by the $\delta$-function [25]. Graham et al. [44] constructed a model of an inhomogeneous medium by coupling the fluctuating field to a smooth background potential that implements the boundary condition in a certain limit. The same authors [45] considered the Casimir problem as the limit of a quantum fluctuating field $\phi(x)$ coupled to a smooth non-dynamical
background $\sigma(x)$ representing the material in the corresponding Lagrangian $\mathcal{L} \sim \sigma(x)\phi^2(x)$. However, in the Dirichlet limit when the external potential becomes sharply peaked, all modes of $\phi(x)$ vanish leading to divergent energy density at the sharp interface, i.e. in this limit the divergence cannot be removed by renormalization. Moreover, the Lagrangian for an effective theory of real media may not be written explicitly, which also renders the theory non-renormalizable from a practical point of view.

1.3 Paper outline

Regardless of the method for removing the boundary-induced divergencies remaining after the Lifshitz regularization, the lingering question is if they reflect physically significant cut-off dependence, e.g. related to tension of the interface (aka ST) [48], or are merely unphysical artefacts of the calculation method. The goal of the present study is to address the question of the space structure distortion (should it be a vacuum or matter) exhibited in the stress–energy tensor $T^\mu\nu$ diverging near the sharp boundary. The accompanying question is on the nature of ST, which may not be properly accounted for by the sharp interface models as it strongly depends on the details of the inter-molecular interactions near the interface [43–46]. To resolve all these quandaries, we revisit the idea of smoothing out the interface [21,23] as it corresponds to real physics: microscopically, the transition between phase densities and dielectric permittivities is never truly discontinuous. However, it is known that even for a smoothed-out interface there are UV divergencies of the stress tensor, which remain after renormalizations and have been previously deemed unphysical, thus requiring one to revisit the issue with proper renormalization and interpretation.

To make the theory specific we will focus here on the leading order effect—the non-retarded limit of vdW forces corresponding to Derjaguin’s disjoining pressure case [11, 12] when the materials involved are dielectrics, as formulated in Sect. 2 in the course of discussing the troubles with the Lifshitz theory. This Derjaguin’s limit enables a significant simplification of the algebra, hence making the analysis transparent and highlighting the nature of divergences.

To deal with the boundary-induced divergencies, we consider an interface between two media with a dielectric constant $\varepsilon(x)$ smoothed out over the characteristic width $w$ in one direction $z$ and apply the standard QFT methods of dealing with UV divergencies applicable in the bulk. As a result, the renormalization procedure is unambiguous, because the interface is just a smooth inhomogeneity. A particular choice of the interface inhomogeneity $\varepsilon(z)$ profile leading to the stationary Schrödinger equation with the Scarf potential $V(z)$ permits us to construct the pertinent propagator (Green’s function) in an analytic form (Sect. 3.3) and thus compute all stresses explicitly. Given the exact representation of the propagator, in line with the Wald axiomatic approach [49,50] it proves natural to use the heat kernel method with the Hadamard expansion [30,51] in the point-splitting regularization to extract finite contributions (Sect. 3.1). The heat kernel method is also applied in the proper time cut-off regularization to analyse the UV divergent contributions (Sect. 3.2). The resulting qualitative picture, though, is the same for all smoothed-out interfaces and hence our choice of the Scarf potential $V(z)$ is just a matter of convenience. The case of a sharp interface is recovered in the limit when its width $w$ vanishes: the stresses (59), which are finite in the case of a smoothed-out interface, grow in this limit and account for the divergencies (18b) that appear in the computations using the conventional sharp BCs approach (Sect. 2). However, in addition, there appear subleading divergent stresses (35c), which are absent in the solution of the sharp interface problem and account for the intrinsic interfacial structure. The laid out analysis also reveals the quantum mechanical nature of ST in a rigorous manner (Sect. 4).
with the concise expression (71,73) comparing favourably to the available experimental data (Sect. 4.2). Finally, the key findings of the paper are recapitulated in Sect. 5 and put in the context of previous studies.

2 The trouble with the Lifshitz theory

The underlying idea of the Lifshitz theory is similar to that of Casimir: instead of the vacuum gap of width \( \ell \) between two metal plates, the Maxwell field fluctuations are quantized in the vacuum gap between two polarizable dielectric media [13]. The corresponding energy of EM zero-point fluctuations is also formally divergent, which is not observable, but any variation of this energy results in an actual force between dielectrics. As in the case of Casimir’s study, subtraction of the vacuum energy \( \mathcal{E}^{\text{vac}}(\infty) \) when the dielectrics are absent cancels the contribution of all the modes outside the gap and results in a finite effect, \( \mathcal{E}^{\text{fin}}(\ell) = \mathcal{E}^{\text{vac}}(\ell) - \mathcal{E}^{\text{vac}}(\infty) \), which can be interpreted as the result of work against the Casimir–Derjaguin pressure between the plates when we change the distance \( \ell \) between them.

2.1 Non-retarded limit of the Lifshitz theory

The EM stress–energy tensor \( T^{\mu\nu} = F^{\mu\alpha} D^\nu_\alpha - \frac{1}{4} g^{\mu\nu} F_{\alpha\beta} D^{\alpha\beta} \) [52], where \( F^{\mu\nu} \) and \( D^{\mu\nu} \) are the Maxwell field and displacement tensors, correspondingly, and \( g^{\mu\nu} \) the Minkowski metric with signature \((-+++)\), in the equilibrium case when there are no fluxes takes the form

\[
T^{\mu\nu} = \begin{bmatrix} \varrho & 0 \\ 0 & -\sigma_{ij} \end{bmatrix}, \quad i, j = (x, y, z), \quad \mu, \nu = (t, x, y, z),
\]

where \( \varrho = T_{00} \) is the EM energy density and \( \sigma_{ij} \) the EM stress tensor with the standard convention on its signs. Throughout the text we will adopt the Planck units, in which \( \hbar = c = k_B = 1 \), and restore SI units whenever computations are performed. In dispersive media the Lifshitz theory is formally applicable to arbitrary wavelengths and frequencies. Both the electric and magnetic fields written in the frequency domain

\[
\tilde{D}_{0j}(\omega; x) = \varepsilon(\omega; x)\tilde{F}_{0j}(\omega; x), \quad \tilde{H}_{ij}(\omega; x) = \mu^{-1}(\omega; x)\tilde{F}_{ij}(\omega; x)
\]

contribute to the stresses. Dispersion forces are due to the molecules polarizability, which in turn is related to the frequency-dependent refractive index and thus dispersion. If the medium is dissipative, \( \varepsilon(\omega; x) \) and \( \mu(\omega; x) \) are necessarily complex with the imaginary parts being always positive, as they account for absorption of the EM waves propagating in the medium [14]. Absorption frequency \( \omega_a \) of the real media provides a natural length-scale \( \lambda_a = 2\pi/\omega_a \) where Casimir (retarded) effect transitions to Derjaguin (non-retarded) one, e.g. for water \( \lambda_a \approx 0.1 \mu\text{m} \). The non-retarded limit [53] corresponds to the case when the characteristic distance \( \ell \) (e.g. the size of the gap separating materials or the length scale on which the interaction is considered) is much smaller than the wavelength \( \lambda_a \) characteristic of these media absorption, \( \ell \ll \lambda_a \). One may interpret this inequality as resulting from the time \( \Delta t = \ell \) over which EM field propagates on the distance \( \ell \) being much smaller than the period of molecules vibrations. The Derjaguin limit corresponds to the leading order effect \( \sim \ell^{-3} \) on the distances \( \ell \ll \lambda_a \) compared to that of Casimir \( \sim \ell^{-4} \) valid for \( \ell \gtrsim \lambda_a \) [54], which

---

1 Because in the time domain the relation between the displacement vector \( D \) and the electric field vector \( E \) is nonlocal, \( D(t,x) = E(t,x) + \int_0^\infty f(\tau) E(t-\tau, x) \, d\tau \), while in the frequency-domain it becomes \( \tilde{D}(\omega; x) = \varepsilon(\omega)\tilde{E}(\omega; x) \), \( \varepsilon(\omega) = 1 + \int_0^\infty f(\tau) e^{i\omega\tau} \, d\tau \).
allows one to calculate the leading order contribution to ST based on the Derjaguin limit only (Sect. 4).

Thus, we are interested in the forces on the (short) distances, \( \ell \ll \lambda_{d\ell} \), where retarded effects are no longer important, so that the Maxwell equations \( \tilde{D}_{\mu \nu} = 0 \), which are local in the frequency domain, in the absence of free charges reduce to electrostatic approximation and hence the components of the vector potential simplify to \( A_0 = -\phi \) and \( A_I = 0 \) in the Coulomb gauge \( \nabla \cdot A_I \). This interaction is described by the non-retarded limit of the Lifshitz theory and the corresponding Green’s function for the mode with frequency \( \omega \) reduces to

\[
\hat{G}(\omega; x, x') \equiv \hat{G}_{00}(\omega; x, x') \quad \text{and satisfies the equation}
\]

\[
\hat{O} \hat{G} \equiv \nabla_i^\prime [\epsilon(\omega; x) \nabla_i \hat{G}(\zeta; x, x')] = \delta(x - x'),
\]

where \( \hat{O} = \delta^{ij} \partial_i \epsilon \partial_j \). Note that Eq. (3) reflects the fact that interaction of electric dipoles is important in the non-retarded limit only, which is why only spatial covariant derivatives appear, despite that the quantum fluctuations of Maxwell field are time-dependent. Such a consideration of the non-retarded limit of the Lifshitz theory from the very beginning, i.e. independent of the general case accounting for both retarded and non-retarded effects, is analogous to the previous study by Barash and Ginzburg [53] in the sharp interface formulation. The inverse Fourier transform of the solution to (3) corresponds to the Feynman Green’s function (propagator) \( G_F^{\beta}(t, x; t', x') \) which is an expectation value of time ordered product of field operators—in our case finite temperature quantum mean value 2:

\[
G_F^{\beta}(t, x; t', x') \equiv G_{00}^{\beta}(t, x; t', x') = \langle T A_0(t, x) A_0(t', x') \rangle.
\]

Here \( A_0 \) and upright equivalents of classical quantities elsewhere in the text will be understood as operators, the angle brackets \( \langle \ldots \rangle \) denote averaging w.r.t the ground state of the system and symbol \( T \) the chronological product. Fundamentally, the constructed Green’s function is a linear response to an external source introduced in the Maxwell equations, which was originally done by Lifshitz [13] and later by Schwinger et al. [56]. According to the linear response theory and fluctuation–dissipation theorem, the Green’s function—the correlation function (propagator)

\[
\tilde{G}(\omega; x, x') \equiv \tilde{G}_{00}(\omega; x, x') \quad \text{and satisfies the equation}
\]

\[
\hat{O} \tilde{G} \equiv \nabla_i^\prime \epsilon(\omega; x) \nabla_i \tilde{G}(\zeta; x, x') = \delta(x - x'),
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The Green’s function of a macroscopic system (as ours) at finite temperatures \( G^{\beta} \) differs from that at zero temperature \( G^{F} \) only in that the vacuum mean value of the product of fields is replaced by averaging over the Gibbs distribution of states at temperature \( T \), which in QFT for convenience is accounted for by the inverse temperature parameter \( \beta = 1/T \). In the coordinate space the thermal Green’s function \( G^{\beta}(t, x; t', x') \) can be obtained from the Feynman propagator \( G^{\beta}(t, x; t', x') \) (4) using the Wick rotation 3—substitution of \( t = -it_\epsilon \) in the Lorenzian Green’s function to produce a Euclidean one \( G^{\beta}(t_\epsilon, x, x') = -iG^{F}(it_\epsilon, x, x') \), which is periodic in the Euclidean compactified time \( t_\epsilon \) with the period \( \beta \). Here we took into account the homogeneity of the Green’s function in time \( t_\epsilon \) and inhomogeneity in space

2 For signs of various Green’s functions here and later in the text, we refer reader to Fursaev and Vassilevich [55] for our choice of the metric signature. For other choices of the metric, one may consult [51].

3 The sign convention [57,58] used here is dictated by the need to regularize the Feynman path integral via an analytic continuation from real \( t \) to complex \( t \) with negative imaginary part. However, the opposite sign convention is often used [54], which also transforms the Lorentzian into the Euclidean metric.
in view of the presence of boundaries. Due to the periodicity in \( t_E \), one can decompose \( G^\beta(t_E, x, x') \) in a Fourier time series:

\[
G^\beta(t_E, x, x') = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \hat{G}(\xi_n; x, x') e^{i\xi_n t_E},
\]

where \( \hat{G}(\xi_n; x, x') = \int_0^\beta G^\beta(t_E, x, x') e^{-i\xi_n t_E} dt_E \) are the Fourier components—the solutions of (3)—and \( \xi_n = 2\pi n/\beta \) the Matsubara frequencies; other variables (\( A_0 \), stress tensor \( \sigma \), etc.) are expanded similar to (5). Stress tensor of EM field and other physical quantities can be computed from the derivatives of the Green’s function (5) in the limit of coincident points \( t_E = 0, x = x' \). Note that although formally the resulting expressions are proportional to the temperature \( T \) as (5), they do not vanish when \( T \to 0 \), because in this limit the distance between Matsubara frequencies \( \xi_n \) shrinks and therefore the summation can be replaced with integration \( T \sum_n \ldots \to \int \frac{d\omega}{\pi} \ldots \) [54], which generally produces a non-vanishing and temperature-independent quantity proportional to the Planck constant \( h \) (in SI units).

Next, note that because of the Wick rotation, the frequency \( \omega \) in the dielectric permittivity becomes purely imaginary—with the help of the Kramers–Kronig formula we can express it as

\[
\varepsilon(i\xi; x) = 1 + \frac{2}{\pi} \int_0^\infty d\omega' \frac{\varepsilon'(\omega'; x)}{\omega'^2 + \xi^2}.
\]

Due to (6), the Fourier coefficients in (5) are symmetric, \( \hat{G}(\xi_n; x, x') = \hat{G}(\xi_n; x', x) \). In the context of the above transition from zero to a finite temperature Green’s function, it should be mentioned that the Lifshitz theory is valid when fluctuations are predominantly quantum [53,59], i.e. it must be \( T \ll \omega \), where \( \omega \) are the frequencies in the neighbourhood of absorption \( \omega_a \), since according to the fluctuation-dissipation theorem the main contribution to the interaction (and hence stresses) comes from this range of frequencies. For example, for water \( \omega_a \sim 2\pi \cdot 10^{15} \text{ rad s}^{-1} \) [4] and thus we get the upper bound temperature on the order of \( T \sim 10^3 \text{ K} \). Because the frequency \( \omega \) in the above inequality \( T \ll \omega \) is related to some characteristic time scale \( \tau = 2\pi/\omega \), the same inequality must be satisfied when applied to the time scale of the inhomogeneity, which in our case is related to the interface width \( \tau = w \).

In classical electrodynamics the total Helmholtz stress tensor in isotropic dielectric media is a sum of the isotropic mechanical (elastic) stress tensor of the medium \( \sigma_{ij}^{(m)} \) and the EM part \( \sigma_{ij}^{(el)} \) [60]:

\[
\sigma_{ij}^{(el)} = \sigma_{ij}^{(m)} + \sigma_{ij}^{(el)}, \quad \sigma_{ij}^{(el)} = p^{(el)} \delta_{ij}, \quad \sigma_{ij} = \varepsilon E_i E_j - \frac{1}{2} \delta_{ij} \left( \varepsilon - \rho \frac{\partial \varepsilon}{\partial \rho} \right) E_i E_j.
\]

where \( \rho \) is the medium mass density. The electrostriction effect, which is described by the \( \rho \partial \varepsilon/\partial \rho \) term in brackets, is of the same order as other terms, as can be seen from the Clausius–Mossotti formula [60] \( \rho \partial \varepsilon/\partial \rho = (\varepsilon - 1) (\varepsilon + 3)/3 \) leading to \( \varepsilon - \rho \partial \varepsilon/\partial \rho = - (\varepsilon^2 - 2\varepsilon - 2)/3 \). The stress tensor \( \sigma_{ij} \) in quantum electrodynamics can be obtained from the classical one (7) by substitution

\[
E_i(t, x) E_j(t', x') \rightarrow \langle E_i(t, x) E_j(t', x') \rangle,
\]

where \( \langle E_i E_j \rangle \) is a quantum average of the product of field operators; the resulting expression is valid for the fluctuating EM field, which is in a thermodynamic equilibrium with the medium. Since we are working in the frequency space as dictated by (3), we need to compute
The system consists of three parallel layers of dielectrics characterized by the corresponding $\varepsilon(i\zeta)$. The distance between two interfaces is $\ell$.

The quantum average $\langle E_i(\zeta, x)E_j(\zeta, x) \rangle$ for every mode $\zeta_n$. In terms of the thermal Green’s function its regularized version (achieved by point-splitting) takes the form

$$
\langle E_i(\zeta, x)E_j(\zeta, x') \rangle = \nabla_i \nabla_j \hat{G}(\zeta; x, x') ,
$$

where the Green’s function has a meaning of a quantum average

$$
\hat{G}(\zeta; x, x') = \langle A_0(\zeta; x)A_0(\zeta; x') \rangle .
$$

The quantum mean values are typically prone to UV divergencies. For our purposes it is convenient to use a point-splitting regularization as it helps us to regularize the quantities we are interested in and, at the same time, we can take advantage of the knowledge of the exact solution for the Green’s function. In this approach the quantum mean value of the stress–energy tensor (1) is expressed in terms of the derivatives of (5). Namely, for every Fourier component $\hat{\sigma}_{ij}(\zeta; x)$ of the stress, we write the regularized version of (7):

$$
\hat{\sigma}_{ij}(\zeta; x) = \left[ \hat{\sigma}_{ij}(\zeta; x, x') \right] \equiv \lim_{x' \to x} \frac{\partial}{\partial \rho} g_{ij} \hat{\sigma}_{ij}(\zeta; x, x') ,
$$

$$
\hat{\sigma}_{ij}(\zeta; x, x') = \sqrt{\varepsilon(i\zeta; x)} \varepsilon(i\zeta; x') \left( \nabla_i \nabla_j - \frac{1}{2} g_{ij} g_{kk} \nabla_k \nabla_k' \right) \hat{G}(\zeta; x, x')
$$

where $\varepsilon(i\zeta; x)$ is given by (6) and $g_{ij} = g_{ij}(x, x')$ the spatial parallel transport operator, which reduces to unity $g_{ij}(x, x') = \delta_{ij}$ since we work in the Cartesian coordinates $x, y, z$.

Because we use the point-splitting regularization in the $z$-direction orthogonal to the interface, the Euclidean time can be put to zero, $t_E = 0$, in (5) at the very beginning. Note that the choice of point-splitting in the $z$-direction is just a matter of convenience. Because the treatment of the static system at finite temperature is equivalent to the analysis in the Euclidean signature, other choices will lead to the same results for the renormalized finite physical observables.

2.2 Stresses between parallel plates

As an illustration we now briefly derive local stresses for a system consisting of the vacuum gap, $\varepsilon_3 = 1$, between two layers of homogeneous dielectrics, cf. Fig. 1, in which case there are no electrostriction effects in the gap. This example demonstrates the origin of divergent stresses near the sharp interface. Because in the $x$ and $y$-directions the problem is homogeneous, it is convenient to expand the Green’s function in the spatial Fourier modes

$$
\hat{G}(\zeta; x, x') = \int_{-\infty}^{\infty} \frac{d^2 q}{(2\pi)^2} e^{i q \cdot x} \hat{G}(\zeta, q; z, z') ,
$$
where $\mathbf{q} = (q_x, q_y)$. In every layer with constant $\varepsilon = \varepsilon_1, \varepsilon_2, \varepsilon_3$, the corresponding $\tilde{G}$ obeys

$$
\varepsilon(\partial^2_{zz} - q^2)\tilde{G}(\zeta, \mathbf{q}; z, z') = \delta(z - z'), \quad \mathbf{q} = |\mathbf{q}| = \sqrt{q_x^2 + q_y^2}.
$$

(13)

On the interfaces between the layers, the Green’s function has to satisfy the BCs which follow from the Maxwell equations, i.e. the continuity across the interface of the tangential component of the electric field strength $\mathbf{E}$ and of the normal component of the electric displacement field $\mathbf{D}$:

$$
\tilde{G}^{(1)}(z, z')|_{z=0} = \tilde{G}^{(1)}(z, z')|_{z=\ell}, \quad \tilde{G}^{(2)}(z, z')|_{z=\ell} = \tilde{G}^{(3)}(z, z')|_{z=\ell},
$$

(14a)

$$
\varepsilon_3 \partial_z \tilde{G}^{(3)}(z, z')|_{z=0} = \varepsilon_1 \partial_z \tilde{G}^{(1)}(z, z')|_{z=0}, \quad \varepsilon_2 \partial_z \tilde{G}^{(2)}(z, z')|_{z=\ell} = \varepsilon_3 \partial_z \tilde{G}^{(3)}(z, z')|_{z=\ell},
$$

(14b)

where for brevity we omitted dependence on $\zeta$ and $q$. The solution to (13, 14) in layer 3:

$$
\tilde{G}(z, z') = \tilde{G}^{(\text{div})}(z, z') + \tilde{G}^{(\text{ino})}(z, z'), \quad \text{where} \quad \tilde{G}^{(\text{div})}(z, z') = -\frac{1}{2q\varepsilon_3} \varepsilon - q|z - z'|,
$$

(15)

and the finite part $\tilde{G}^{(\text{ino})}(z, z')$, e.g. in layer 3 for $0 < z, z' < \ell$, follows from (15,16).

Then the renormalized components of the EM stress tensor $\sigma_{ij}^{(\text{fin})}(z)$ in medium 3 can be computed in the limit of coincident points according to (11):

$$
\sigma_{xx}^{(\text{fin})}(z) = \sigma_{yy}(z) = -\frac{1}{4\pi\beta} \sum_{n=-\infty}^{\infty} \varepsilon(i\zeta_n) \int_{0}^{\infty} dq \ q \ \left\{ \partial_z \partial_{z'} \tilde{G}^{(\text{fin})}(\zeta_n, q; z, z') \right\}|_{z=z'},
$$

(17a)

$$
\sigma_{zz}^{(\text{fin})}(z) = -\frac{1}{4\pi\beta} \sum_{n=-\infty}^{\infty} \varepsilon(i\zeta_n) \int_{0}^{\infty} dq \ q \ \left\{ \partial_z \partial_{z'} - q^2 \right\} \tilde{G}^{(\text{fin})}(\zeta_n, q; z, z')\right\}|_{z=z'},
$$

(17b)

Substituting here $\tilde{G}^{(\text{ino})}$ derived from (15, 16), we recover the non-retarded limit of the Lifshitz theory [13]:

$$
\sigma_{zz}^{(\text{ino})}(z) = \frac{1}{8\pi\beta} \sum_{n=-\infty}^{\infty} \int_{0}^{\infty} dq \ q^2 \frac{4(\varepsilon_1 - \varepsilon_3)(\varepsilon_2 - \varepsilon_3)}{(\varepsilon_1 + \varepsilon_3)(\varepsilon_2 + \varepsilon_3)e^{2q\ell} - (\varepsilon_1 - \varepsilon_3)(\varepsilon_2 - \varepsilon_3)},
$$

(18a)

$$
\sigma_{xx}^{(\text{ino})}(z) = \sigma_{yy}^{(\text{ino})}(z) = -\frac{1}{8\pi\beta} \sum_{n=-\infty}^{\infty} \int_{0}^{\infty} dq \ q \ \frac{4(\varepsilon_1 - \varepsilon_3)(\varepsilon_2 - \varepsilon_3)}{(\varepsilon_1 + \varepsilon_3)(\varepsilon_2 + \varepsilon_3)e^{2q\ell} - (\varepsilon_1 - \varepsilon_3)(\varepsilon_2 - \varepsilon_3)},
$$

(18b)

where $0 < z < \ell$. Obviously, the pressure in the $z$-direction $\sigma_{zz}^{(\text{ino})}(z)|_{0 < z < \ell}$ is finite, i.e. independent of the UV cut-off, and does not depend on $\zeta$; with the change of variable $2q\ell = p$ one can see that $\sigma_{zz}^{(\text{ino})} \sim \ell^{-3}$. The EM pressure in the gap (or a dielectric film [14]) corresponds to the excess mechanical pressure compared to the pressure outside the gap (film). When $\varepsilon_1 > \varepsilon_3$ and $\varepsilon_2 > \varepsilon_3$, it leads to attraction between plates. In the case when $\varepsilon_1 > \varepsilon_3$
and $\varepsilon_2 < \varepsilon_3$ it produces a repulsion force. When the gap (film) is thick, $\ell \to \infty$, this excess pressure vanishes. As for the tangent components of the pressure $\sigma_{\alpha\beta}^{(\text{fin})}(z) = \sigma_{\alpha\beta}^{(\text{fin})}(z)$, regardless how thick the gap is, they diverge as $z$ approaches interfaces at $z = 0$ and $z = \ell$ because the integral in (18b) over the momentum $q$ becomes divergent on the interfaces.

Note that while the non-retarded limit is defined by the inequality $\ell \ll \lambda$, it would be misleading to think of the frequencies $\zeta_n$ in the sums (18) as associated with real photons and that the latter are responsible for the origin of the stresses (18): for example, in vacuum there are no real photons, but only quantum zero-point fluctuations. While the free Maxwell equations do possess natural propagating modes (photons, on-shell solutions), we consider the off-shell solutions of the non-retarded approximation of the Maxwell equations with a source term (3). Electromagnetic oscillations are driven externally by quantum fluctuations of dipoles, and hence all frequencies are present despite that we consider the non-retarded limit (i.e. the $\delta$-function in Eq. (3), rewritten in the original time-space, is decomposed in the time Fourier series containing harmonics of all frequencies). Apparently, as opposed to propagating modes, which satisfy the dispersion relation $\omega = 2\pi/\ell$, the Matsubara frequencies $\zeta_n$ are off-shell quantities and do not obey this relation. Because we consider the case when zero-point quantum fluctuations dominate thermal ones (Sect. 2.1), excitation of natural modes is insignificant.

Intuitively, the divergence of the along-the-interface stresses (18b) can be appreciated on the example of the Casimir problem from the leakage of a point continuous spectrum of the along-the-interface wavenumber components $q$ of the total wavenumber $\mathbf{k} = (q, k_z)$ when the free space energy $\mathcal{E}_{\text{vac}}(\infty) = \frac{1}{(2\pi)^4} \int d^3k |\mathbf{k}| = \frac{1}{(2\pi)^2} \int d^2q \int dk_z \sqrt{q^2 + k_z^2}$ is subtracted from that of the finite width $\ell$ cavity $\mathcal{E}_{\text{vac}}(\ell) = \frac{1}{2} \sum_{n,q} \omega_{n,q}$. Here $\omega_{n,q} = \sqrt{q^2 + (n\pi/\ell)^2}$ and the summation is performed over all integers $n$, due to discreteness of the numeration of the point spectrum in the $z$-direction, and over all continuous wavenumbers $q$ in the $x$- and $y$-directions. The leakage occurs because of the square root in the dispersion relation $\omega \sim |\mathbf{k}|$, which, despite being linear, mixes the discrete $k_z$ and continuous wavenumbers $q$ in the difference $\mathcal{E}_{\text{vac}}(\ell) - \mathcal{E}_{\text{vac}}(\infty)$. This decomposition of the wavenumbers $\mathbf{k} = (q, k_z)$ and the dispersion relation $\omega \sim |\mathbf{k}|$ itself are analogous to the Klein–Gordon model

$$\phi_{tt} - \phi_{zz} + m^2 \phi = 0,$$

(19)

the free particle solution $\phi \sim e^{i(k_z z - \omega t)}$ of which yields the dispersion relation of our type, $\omega = \sqrt{k_z^2 + m^2}$, i.e. our wavenumbers $q$ play the role of a mass $m$ in the Klein–Gordon equation. If we think of equation (19) as governing oscillations of a string, then the second term is a restoring tension force from neighbouring points as in the standard wave equation, while the last term is a harmonic oscillator restoring force, which naturally grows with mass $m$, or equivalently with the wavenumber $q$ in our case. As explained above, this term can be unbounded due to sharp interface approximation when neglecting the microscopic structure of matter and leaks into the Casimir effect after the free space contribution $\mathcal{E}_{\text{vac}}(\infty)$ is subtracted. The same model (19) also explains the localization of the divergence near the interface: indeed, in the steady case we find $\phi(z; q) \sim e^{-mz}$ behaving as surface EM waves [53].
3 Trouble resolution: Scarf for Lifshitz

As we saw in Sect. 2.2, in the Lifshitz approach [13,14] the stress tensor contains a UV divergent part. This property is reflected in the fact that the stress tensor with separated points $\hat{\sigma}_{ij}(\zeta; x, x')$ diverges in the limit $x \rightarrow x'$. In accordance to a conventional QFT approach, it should be written as a sum of a UV divergent and regular parts

$$\hat{\sigma}_{ij}(\zeta; x, x') = \hat{\sigma}_{ij}^{(\text{div})}(\zeta; x, x') + \hat{\sigma}_{ij}^{(\text{fin})}(\zeta; x, x')$$  (20)

with similar decomposition applied to other quantities such as the energy density $\hat{\varrho}(\zeta; x, x')$ and the Green's function $\hat{G}(\zeta; x, x')$. The UV divergent contributions are present even in homogeneous media without boundaries. However, due to equilibrium of the media these formally diverging stresses must be balanced by mechanical ones. The observable regular stresses in a piecewise homogeneous system that is described by constant dielectric permittivities $\varepsilon(\zeta)$ are typically achieved through subtracting from the total Green's function a divergent part [13,14]

$$\hat{G}^{(\text{div})}(\zeta; x, x') = -\frac{1}{4\pi \varepsilon(i\zeta)|x-x'|}$$  (21)

associated with an infinite homogeneous medium having the constant dielectric permittivity $\varepsilon(i\zeta)$ equal to that of the corresponding phase. The resulting finite stresses $\hat{\sigma}_{ij}^{(\text{fin})}(\zeta; x, x')$ are then obtained by acting on $\hat{G}^{(\text{fin})}(\zeta; x, x') = \hat{G}(\zeta; x, x') - \hat{G}^{(\text{div})}(\zeta; x, x')$ by the same differential operator as in (11). Note that distinguishing the divergent part $\hat{G}^{(\text{div})}$ is based not on the divergence of $\hat{G}$ itself, but on the part of it that leads to diverging stresses $\hat{\sigma}_{ij}^{(\text{div})}$ in (20). Thus, after this regularization procedure, the obtained finite pressure tensor component (18a) orthogonal to the interface (18a) exactly reproduces the Lifshitz result. Evidently, this Lifshitz subtraction does not cure all divergencies in inhomogeneous media: the problem is that the local tangent pressure tensor components (18b) diverge on the interface.

3.1 Proper time regularization

In order to understand the role of UV divergent terms in the stress tensor, in the present section we start with Schwinger’s proper time regularization of the effective action [61], because it respects the symmetries of the system and keeps track of the divergent parts. Later on (Sect. 3.2) we will also use the point-splitting regularization, which, for purely technical reasons, happens to be more convenient for computations of the finite part of the stress tensor. There is no disagreement between different regularization schemes about finite contributions to the quantum stress tensor, which do not depend on regularization parameters. As for the divergent parts, they are dealt with differently in different regularization schemes. In renormalizable theories, the divergencies are removed by the introduction of corresponding counterterms in the bare Lagrangian of the system. Other methods simply omit divergent terms: for example, the zeta-function regularization automatically discards all divergencies, while the dimensional regularization keeps track of logarithmic divergencies and discards power law divergencies.

In our case of a real condensed matter system, we have to be vigilant and keep track of all divergent contributions. These UV divergent terms formally appear because the Lifshitz theory is effective, rather than microscopic, and hence deals only with low-energy phenomena of vdW forces by accounting for EM interactions of polarizable molecules only. Divergent terms depend on the microscopic structure of the media on the length scales $\lesssim r_m$ and can lead to physically observable effects. In particular, as we will show in Sect. 4, the main contribution...
3.1.1 Calculation of stresses

Schwinger’s proper time regularization [61] keeps information about all divergent terms and, as opposed to the point-splitting method, does not require averaging over all directions, which makes it the best choice for our analysis of divergent contributions. Using Schwinger’s approach the stress tensor of the system can be computed from the classical action and then quantization. While in our problem the metric is flat \( g_{ij} = \delta_{ij}, \ g_{tt} = -1, \) and \( \sqrt{g(x)} = 1, \) we provisionally keep it arbitrary which will be handy in further analysis of divergencies via the calculations based on variation with respect to \( g_{\mu\nu}, \) in particular, because the resulting Hilbert stress–energy tensor

\[
T^{\mu\nu} = \frac{2}{\sqrt{|g|}} \frac{\delta S}{\delta g_{\mu\nu}}, \quad T_{\mu\nu} = g_{\mu\alpha} g_{\nu \beta} T^{\alpha\beta}
\]  

(22)

is symmetric as opposed to the canonical stress–energy tensor requiring the Belinfante–Rosenfeld modification to make it symmetric. Note that in this variation 4D metric \( g_{\mu\nu}(t, x) \) depends on all coordinates, and only after the variation we can put \( g_{\mu\nu} = \text{diag}(-1, 1, 1, 1). \) As per (1), the spatial components of the stress–energy tensor define the stress tensor \( \sigma_{ij} = -T_{ij}, \) which is used in the theory of continuous media [52].

Given the standard logic of application of the Maxwell equations to general isotropic dielectric media with dispersion and dissipation (Sect. 2.1), i.e. consideration of each field mode \( A_0(\omega; x) \) with frequency \( \omega \) separately in the Fourier space, we first construct the EM free energy for each mode and then sum up over all the modes. In order to describe non-retarded effects it is sufficient to consider a vanishing magnetic field, what in the Coulomb gauge is equivalent to the choice \( A_i = 0. \) Since description of the system in equilibrium at finite temperature reduces to the Wick rotated \( t = -it_E \) formulation, the modes are the Fourier transforms over the periodic Euclidean time: \( A_0(\xi_n; x) = \int_0^\beta dt_E A_0(t_E, x) e^{-i\xi_n t_E}. \) Then, the classical electromagnetic action is a sum of contributions of all Matsubara modes

\[
S_E = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} S_n, \quad \text{with} \quad S_n = -\frac{1}{2} \int d^3 x \, \varepsilon(i\xi_n; x) \, \partial_k A_0(\xi_n; x) \, \partial^k A_0^*(\xi_n; x),
\]  

(23)

which is negative as it should be for dielectrics [62]; note that the free energy \( F \) is related to the action via \( S_E = \beta F, \) which is sometimes used for calculation of stresses [54]. Actually, this form is a more convenient physical description of dispersive media rather than a time-dependent one; the latter can be derived from (23) with the inverse Fourier transform of \( A_0(\xi_n; x), \) i.e. \( A_0(t_E, x) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} A_0(\xi_n; x) e^{i\xi_n t_E}. \)

For future analysis it is useful to rewrite the components (23) of the action as a functional of a three-dimensional (3D) metric \( g_{ij}(x) \)

\[
S_n = -\frac{1}{2} \int d^3 x \sqrt{g} \, \varepsilon(i\xi_n; x) \, g^{ij} \nabla_i A_0(\xi_n; x) \nabla_j A_0^*(\xi_n; x)
\]  

(24)

and the total action in the 3D-covariant form \( S^{(m)} = S^{(m)}_E + S^{(m)}, \) where \( S^{(m)} = \beta \int d^3 x \sqrt{g} \, L^{(m)}(\rho) \) is the ‘bare’ action of classical matter in the absence of external electric field, \( L^{(m)}(\rho) \) the ‘bare’ Lagrangian density as a function of the mass density \( \rho, \) \( g_{ij} \) an artificial 3D metric, and \( g = \det(g_{ij}) \). Variation of the metric \( \delta g_{ij} \) can be interpreted as a result of ST is explained by a specific divergent term which depends on both the cut-off parameter and the width \( w \) of the interface.
of deformation of a fixed mass volume element of the matter and, therefore, the dependence of $\varepsilon$ on the density $\rho$ can be replaced\(^4\) with that on the metric $g$.

After the Wick rotation, due to the change from the Minkowski to Euclidean action, it happens that the corresponding Euclidean stress–energy tensor on static backgrounds has the spatial components $T_{ii} = -\dot{T}_{ij} = \sigma_{ij}$. This trivial observation appears to be useful in application to the Lifshitz theory and Matsubara approach, which deal with systems in equilibrium and quantities defined as functions of imaginary frequencies. Then, for the equilibrium system in question we can derive the stress tensor $\sigma_{ij}$ by variation over time-independent 3D metric. To this end note that if the Lagrangian density $\mathcal{L}[g(t, x), A_0(t, x)]$ is a function of metric components $g_{0i}$ and $g_{ij}$, then its functional variations with respect to the spatial part of the metric satisfy the following equivalence relation

$$\int_0^\beta \mathrm{d}t \int d^3x \frac{\delta \mathcal{L}[t, x]}{\delta g_{ij}(t', x')} \Leftrightarrow \int d^3x \frac{\delta \mathcal{L}[x]}{\delta g_{ij}(x')};$$

(25)

here on the left hand-side the metric is a function of time and space, while on the right hand-side it is considered as a function of space only. The classical EM Hilbert stress tensor is obtained by variation of the action over the 3D metric

$$\sigma^{ij} = \frac{2}{\beta \sqrt{g}} \frac{\delta S}{\delta g_{ij}}, \quad \sigma_{ij} = g_{ik}g_{jl}\sigma^{kl}. \quad (26)$$

In the general case, the dielectric permittivity $\varepsilon(i\zeta; x)$ can also be a function of density $\rho$, i.e. it implicitly depends on the metric as well. Under deformations of an elementary volume $\sqrt{g} \, d^3x$, which keep the number of atoms in it fixed, the total mass in this volume is constant and hence $\delta[\sqrt{g} \rho] = 0 = \rho \delta \sqrt{g} + \sqrt{g} \delta \rho = -g^{ij} \sqrt{g} \delta g_{ij} + \sqrt{g} \delta \rho$. Using this relation we get

$$\frac{\delta \rho}{\delta g_{ij}} = -\frac{1}{2} \rho g^{ij}, \quad \text{so that} \quad \frac{\delta \varepsilon}{\delta g_{ij}} = \frac{\delta \varepsilon}{\delta \rho} \frac{\delta \rho}{\delta g_{ij}} = -\frac{1}{2} \frac{\delta \varepsilon}{\delta \rho} g^{ij}. \quad (27)$$

At the end, we obtain for the EM tensor, in consistency with the expressions elsewhere [62],

$$\sigma_{ij} = \frac{1}{\beta} \sum_n \sigma_{ij}(\eta_n), \quad \hat{\sigma}_{ij}(\eta) = \varepsilon \nabla_i A_0 \nabla_j A_0^* - \frac{1}{2} g_{ij} \left[ \varepsilon - \rho \frac{\partial \varepsilon}{\partial \rho} \right] \nabla_k A_0 \nabla^k A_0^*, \quad (28)$$

and the term proportional to the derivative of $\varepsilon$ w.r.t. the density accounts for the electrostriction effects.

Variation of the total action $S^{tot}$ over the metric produces

$$\sigma^{ij}_{\text{tot}} = \frac{2}{\beta \sqrt{g}} \frac{\delta S^{tot}}{\delta g_{ij}}, \quad \sigma^{(tot)}_{ij} = \sigma^{(m)}_{ij} + \sigma^{m}_{ij}, \quad (29)$$

where we perform variation with respect to the metric $g_{ij}$ with lower indices and $\sigma^{(m)}_{ij}(x) = -p^{(m)}(x)g_{ij}$ is the mechanical (elastic) stress tensor with $p^{(m)}(\rho) = L^{(m)} - \rho \partial_{\rho} L^{(m)}$ having the meaning of the ‘bare’ pressure of the medium. After the variation one can put $g_{ij} = \delta_{ij}$ and then recover (7). $S^{tot}$ can be formally treated as a Euclidean action [63], which in our case reduces to a sum over Matsubara frequencies of 3D actions. Then, QFT methods can be applied to its quantization. This action is the only effective functional we need to know as long as we are working in the framework of the Lifshitz theory in the non-retarded limit.

In order to compute stresses of quantum fluctuating electromagnetic field $\langle \sigma_{ij} \rangle$, one has to replace

$$\nabla_i A_0 \nabla_j A_0^* \to \langle \nabla_i A_0 \nabla_j A_0^* \rangle, \quad (30)$$

\(^4\) Consider deformation of a small volume with fixed number of molecules as an example.
where, as before, on the right-hand side $A_0$’s are to be understood as the field operators. The quantum mean value $\langle A_0(\xi; x)A_0^\dagger(\xi'; x') \rangle = \hat{G}(\xi; x, x')$ is the Euclidean Green’s function in 3D, and we have

$$\langle \nabla_i A_0(\xi; x) \nabla_j A_0^\dagger(\xi; x) \rangle = \nabla_i \nabla_j \hat{G}(\xi; x, x') \big|_{x'=x} \equiv \hat{G}_{ij}^{(\text{div})}(\xi; x).$$

The stress tensor takes the form (11) symmetrized in $x$ and $x'$. Since in the limit of coincident points it diverges, it should be regularized and local UV divergent terms extracted. For computation of the finite cut-off-independent part of the stress, one can safely use regularizations such as point-splitting, zeta-function, dimensional, Pauli–Villars, and other well-established in QFT techniques. Since for the exactly solvable Scarf potential we are able to compute the quantum mean value introduced in (11a), we determine the divergent contributions that are of interest to us, and since in the limit of coincident points it diverges, it should be regularized and local UV divergent terms extracted. For computing the finite cut-off-independent part of the stress, one can safely use regularizations such as point-splitting, zeta-function, dimensional, Pauli–Villars, and other well-established in QFT techniques. Since for the exactly solvable Scarf potential we are able to compute the quantum mean value introduced in (11a), we determine the divergent contributions that are of interest to us, and

$$\hat{G}_{ij}^{(\text{div})}(\xi; x) = -\frac{1}{(4\pi \epsilon)^{3/2}} \left[ \frac{\delta_{ij}}{3\lambda_0} \frac{1}{\epsilon} - \frac{\delta_{ij}}{48\lambda_0} \left( 28\partial \eta + 9\eta^2 \right) - \frac{1}{24\lambda_0} \left( 4\partial \eta \eta_i - 25\eta_i \eta_j \right) \right],$$

where $\lambda_0$ is the cut-off. Its substitution into the regularized stress tensor (11) leads to

$$\hat{G}_{ij}^{(\text{div})}(\xi; x) = \epsilon \left[ \hat{G}_{ij}^{(\text{div})} - \frac{1}{2} \delta_{ij} \left( 1 - \frac{\rho}{\epsilon} \frac{\partial \epsilon}{\partial \rho} \right) \hat{G}_k^{(\text{div})} \right].$$
It is convenient to collect terms of the same order in the cut-off parameter $\lambda_0$,

$$
\hat{\sigma}^{(\text{div})}_{ij}(\zeta; x) = \hat{\sigma}^{(\text{div})}_{ij}(\zeta; x) + \hat{\sigma}^{(\text{div})}_{ij}(\zeta; x), \quad \text{with}
$$

(35a)

$$
\hat{\sigma}^{(\text{div})}_{ij}(\zeta; x) = \frac{1}{(4\pi \varepsilon)^{3/2}} \frac{1}{\lambda_0^3} \delta_{ij} \left[ -\frac{1}{3} + \frac{1}{2} \left( 1 - \frac{\rho}{\varepsilon} \frac{\partial \varepsilon}{\partial \rho} \right) \right],
$$

(35b)

$$
\hat{\sigma}^{(\text{div})}_{ij}(\zeta; x) = \frac{1}{(4\pi \varepsilon)^{3/2}} \frac{1}{48\lambda_0} \delta_{ij} \left[ 28\rho \varepsilon + 9\eta^2 \right] \left( 1 - \frac{\rho}{\varepsilon} \frac{\partial \varepsilon}{\partial \rho} \right) (92\rho \varepsilon - 23\eta^2)
$$

+ \frac{\varepsilon}{(4\pi \varepsilon)^{3/2}} \frac{1}{24\lambda_0} \left[ 4\rho \varepsilon \eta - 25\eta \varepsilon \eta \right] + O(\lambda_0),
$$

(35c)

and also separate isotropic and anisotropic parts $\hat{\sigma}^{(\text{iso})}_{ij}(\zeta; x) = \delta_{ij} \hat{\sigma}^{(\text{iso})}_{ij}(\zeta; x) + \hat{\sigma}^{(\text{ani})}_{ij}(\zeta; x)$, omitting the terms vanishing in the limit $\lambda_0 \to 0$, where

$$
\hat{\sigma}^{(\text{iso})}_{ij}(\zeta; x) = \frac{1}{(4\pi \varepsilon)^{3/2}} \frac{1}{\lambda_0^3} \left[ -\frac{1}{3} + \frac{1}{2} \left( 1 - \frac{\rho}{\varepsilon} \frac{\partial \varepsilon}{\partial \rho} \right) \right]
$$

$$
\hat{\sigma}^{(\text{an})}_{ij}(\zeta; x) = \frac{1}{(4\pi \varepsilon)^{3/2}} \frac{1}{24\lambda_0} \left[ 4\rho \varepsilon \eta - 25\eta \varepsilon \eta \right].
$$

(36a)

(36b)

The total divergent stresses are calculated then according to

$$
\sigma^{(\text{div})}_{ij}(x) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \hat{\sigma}^{(\text{div})}_{ij}(\zeta_n; x),
$$

(37)

with similar expressions for $\sigma^{(\text{iso})}_{ij}(x)$ and $\sigma^{(\text{an})}_{ij}(x)$. Even though the split in isotropic and anisotropic parts in (36) is not unique, it does not lead to any physical ambiguity because both parts are always present in the sum together. We choose the simplest form for the anisotropic part which, when applied to the plane interface, reduces to the only non-vanishing component $\delta_{ij}$, $\hat{\sigma}^{(\text{an})}_{ij}(\zeta; x)$. It should be noted that the leading divergent terms (35b) including the electrostriction contribution are renormalized into the mechanical pressure as will be discussed in Sect. 3.1.2, while the subleading divergent terms (35c) dependent on $\eta$ are localized in the interfacial region and vanish when $\varepsilon = \text{const}$. The latter property of subleading stresses differentiates them from the finite ones $\hat{\sigma}^{(\text{an})}_{ij}$ which stay nontrivial outside the interface as the calculations in Sect. 3.3 will demonstrate. While the finite stresses are present in the sharp interface problem (18), the subleading stresses are clearly not, which will prove to be instrumental in explaining the origin of ST (Sect. 4).

### 3.1.2 Physical interpretation

Let us now discuss physical implications of the divergent part $\hat{\sigma}^{(\text{div})}_{ij}$ of the EM stress tensor $\sigma_{ij}$, which contributes to the total stress tensor (29). The Lifshitz theory treats media as continuous and hence is an effective theory that describes collective phenomena of microscopic interactions of polarizable molecules separated by the distance $r_m$. The leading divergency $\sim 1/r_m^3$ at this scale is isotropic and its contribution to a force acting on any volume element is given by the integral of a total derivative, which vanishes for any compact volume element. As mentioned earlier, the standard Lifshitz prescription is to subtract the stress of a homogeneous medium with the same constant $\varepsilon$ from the computed quantum result at every point. This prescription exactly corresponds to inclusion of the leading divergency to the
renormalization of the bare stress term \( \sigma_{ij}^{(m)} \). However, the subleading \( O(\lambda_0^{-1}) \) divergence in (35c) cannot be omitted as it leads to \( \sim 1/(r_m w^2) \) terms and does contribute to the ST (Sect. 4)—to distinguish from the leading UV divergence \( O(\lambda_0^{-3}) \) we call it a subleading UV divergence due to its local nature, but not an IR one despite the dependence on the characteristic scale of inhomogeneity. Appearance of subleading UV divergencies was noticed before in the Casimir problem of vacuum polarization between parallel plates without taking dispersion into account [66], which will be discussed in detail in Sect. 5.

As discussed in the Introduction, on the microscopic level the forces acting on interatomic/molecular distances are phenomenologically described by the Lennard-Jones potential \( \varphi_{\text{LJ}} \) combining the vdW interaction \( \varphi_{\text{vdW}}(r) \sim r^{-6} \) of polarized and polarizable molecules, the nature of which is the EM interactions including the ones of QM nature, and the \( r^{-12} \) term, which is a purely heuristic way of modelling short range \( O(r_m) \) quantum repulsion that stops two particles from being in the same location.\(^5\) Regardless of the nature of this short-range interaction, on the larger scales we are interested in, one may consider this interaction as that between billiard balls and hence isotropic. In other words, in the context of the macroscopic Lifshitz theory, i.e. when the microscopic details at the length-scales below \( r_m \) are not accounted for, repulsive molecular interactions are treated as that between points and thus lead to locally isotropic contributions to the effective stresses at the length-scales \( O(r_m) \). Therefore, in the effective theory [14] we can identify its role as the bare material stress tensor (7), where the isotropic pressure \( p \) can depend on the point \( x \). In equilibrium, this pressure is always adjusted in such a way that the local force density vanishes

\[
\nabla^j \sigma_{ij}^{(is)} = 0 \tag{38}
\]

everywhere in the bulk. Because we consider the system with a smooth inhomogeneous interface, which is static, the total local force density vanishes at every point inside the interface too. The terms in \( \hat{\sigma}_{ij}^{(iso)} \) are isotropic \( \sim \delta_{ij} \), including the electrostriction terms,\(^6\) should be combined with the bare \( \sigma_{ij}^{(m)} \) to produce the renormalized isotropic stress tensor

\[
\sigma_{ij}^{(ren)}(x) = -\delta_{ij} p^{(ren)}(x). \tag{39}
\]

This procedure exactly corresponds to renormalization in QFT, where \( p^{(m)} \) is formally defined by the microscopic “bare” Lagrangian of a classical theory of non-EM interactions. In condensed matter, however, not every system is renormalizable, because the structure of the classical theory is not always the same as the structure of quantum divergencies. This is exactly our case, because the term \( \sim \eta_i \eta_j \) in (35c) is not isotropic and together with finite terms proves to contribute to the ST (Sect. 4).

---

\(^5\) The power \(-12\) was chosen by Lennard-Jones for convenience: in reality, the actual potential may have a mixed polynomial-exponential form, cf. [67] and references therein. For example, in the case of helium atoms the repulsive interaction between them is caused by a depletion in electron density in the overlap region that descreens the nuclei from each other resulting in internuclear repulsion. In general, while the \( r^{-12} \) term is often attributed to the Pauli exclusion principle for fermions due to anti-symmetry of their wave functions resulting in an exchange interaction between identical particles (which also applies to bosons)—this interaction is different from Coulomb electrostatic repulsion and, in fact, stronger on shorter distances and ultimately responsible for the stability of matter [68,69]—it could also originate from the Heisenberg principle of uncertainty [70].

\(^6\) Physically, this absorption of electrostriction to the renormalized isotropic pressure follows from the chemical potential [14,62], which must be constant for media in equilibrium. One may think of the electrostriction stress as analogous to the gravity in the ocean compensated by the mechanical stresses in water: if it is balanced in the \( r \)-direction, then due to isotropy it must be balanced in the \( \theta \)-direction as well. Notably, the \( \theta \)-dependence of the electrostriction stress leads to non-uniform compression of the matter which is stronger near the interface. However, due to isotropy, electrostriction does not contribute to ST (Sect. 4).
In the light of the above discussion, we rearrange all the contributions to the stress tensor as

$$\sigma_{ij}^{(tot)} = \delta_{ij} \left[ -p^{(m)} + \sigma^{(iso)} + \sigma_{i}^{(fin)} + \sigma_{j}^{(fin)} \right]$$

where $\sigma_{ij}^{(fin)}$ is defined by (20) and will be calculated in Sect. 3.3. For our system $\epsilon(i\xi; x)$ is a function of $z$ only, in which case (32) reduces to $\eta_{i} = (0, 0, \eta)$ with $\eta = \epsilon^{-1} \partial \varepsilon / \partial \zeta$. We can write the $zz$-component of the stress tensor as

$$\sigma_{zz}^{(tot)} = \left[ -p^{(m)}(z) + \sigma^{(iso)}(z) \right] + \sigma_{z}^{(ani)} + \sigma_{z}^{(fin)}$$

while in the $x - y$ plane the stress is diagonal, so we need to know only the $xx$-component

$$\sigma_{xx}^{(tot)} = \left[ -p^{(m)}(z) + \sigma^{(iso)}(z) \right] + \sigma_{xx}^{(fin)}$$

The quantities in square brackets of (40, 41) correspond to isotropic contributions to the stress tensor. Because all quantities depend on the $z$-coordinate only, the equilibrium condition (38) reduces to

$$\partial_{z} \sigma_{zz}^{(tot)} = 0, \quad (42)$$

that is

$$\sigma_{zz}^{(tot)} = \lim_{z \to \pm \infty} \sigma_{zz}^{(tot)} \equiv -p_{0}^{(ren)} \quad (43)$$

where the constant $p_{0}^{(ren)}$ is the value of the renormalized (observable) pressure in both asymptotics $z \to \pm \infty$ and corresponds to $\lim_{z \to \pm \infty} \left[ -p^{(m)}(z) + \sigma^{(iso)}(z) \right]$. Note that in liquids and solids $p^{(m)} > 0$ since it originates from the repulsion between molecules, while the added EM terms are generally positive as they originate from attraction forces; altogether, we get $p_{0}^{(ren)} < 0$ since liquids and solids are a condensed matter (as opposed to gases), i.e. due to their cohesive nature $p_{0}^{(ren)}$ must be negative. Note that $p^{(m)}$ is a function of the $z$-coordinate only, but this dependence always compensates the $z$-dependence of $\sigma_{zz}^{(div)} + \sigma_{zz}^{(fin)}$. Thus, for the $xx$-component (41), we obtain

$$\sigma_{xx}^{(tot)} = -p_{0}^{(ren)} - \sigma_{zz}^{(ani)} + \sigma_{zz}^{(fin)} = \sigma_{xx}^{(ren)} \quad (44)$$

This tangent to the interface stress does depend on $z$, but in the asymptotic regions $z \to \pm \infty$ it approaches the same constant as $\sigma_{zz}^{(ren)}$

$$\sigma_{xx}^{(tot)} \to -p_{0}^{(ren)} \quad (45)$$

The nature of the divergent part $\sigma_{ij}^{(div)}(z, z')$ when $z' \to z$ requires an additional clarification. In QFT it is usually omitted or combined with the bare stress $\sigma_{ij}^{(m)}(z, z')$ of the classical theory of non-EM intermolecular interactions to produce a renormalized stress $\sigma_{ij}^{(ren)}(z, z') = \sigma_{ij}^{(m)}(z, z') + \sigma_{ij}^{(div)}(z, z')$, including subleading terms. The remaining part, which cannot be absorbed into the bare stresses, is then interpreted as the observable stress. This renormalization procedure works well for renormalizable theories, when all quantum UV divergencies can be absorbed in the redefinition of parameters of a “bare” classical theory.

Although condensed matter systems may not be renormalizable, it is logical to consider all microstructure-dependent terms as a renormalized mechanical stress tensor (39). As one can see from (35), divergent terms of quantum EM fluctuations consist of a leading universal part $\sigma_{ij}^{(div, u)}$ (discarded by Lifshitz [13] due to being independent of the distance $\ell$ between the bodies) and a subleading part $\sigma_{ij}^{(div, s)}$, which depends on the EM properties of the media. The second choice would be to combine with the bare mechanical stresses only the leading divergent terms to produce the renormalized mechanical stress tensor. In both approaches, far away from the interface the renormalized stress tensor takes the form (39). In the second approach the subleading divergent part, which depends on both the UV cut-off $\lambda_{0}$ and the gradient of $\epsilon$, leads to observable effects such as ST (Sect. 4). The presented here scheme of
regularization goes in parallel with the standard in QFT renormalization and can be formally lifted to the renormalization of a bare (material) Lagrangian $L^{(m)}$, which in our case cannot be written explicitly, by adding the counterterms $L^{(CT)}$, $L^{(m)} = L^{(ren)} + L^{(CT)}$, as was done in some model problems such as for scalar fields and $\delta$-potentials [45,46]. In spirit, the exploited renormalization is along the lines of the original Wilsonian approach [71], which is always defined with a physical cut-off, so that there is no fundamental difference between renormalizable and non-renormalizable theories. The non-renormalizable scales in our problem appear to be molecular $\lambda_0 \sim r_m$, which are not sources of any trouble if we are interested in the physics at scales above the cut-off as in the Lifshitz theory.

3.2 Point splitting regularization

We will use the point-splitting regularization in the $z$-direction, so that in the Green’s function (5) we put $t_\epsilon = 0$, $x = x'$, and $y = y'$. The resulting Green’s function $\bar{G}(\zeta, q; z, z')$ defined via (12) for every mode depends only on $q$ and satisfies the equation

$$\left[ \partial_z \epsilon(i\zeta; z) \partial_{z'} - q^2 \epsilon(i\zeta; z) \right] \bar{G}(\zeta, q; z, z') = \delta(z - z'), \quad q = \sqrt{q_x^2 + q_y^2}. \tag{46}$$

Let $\epsilon(i\zeta; z)$ change considerably only in the layer of width $w$ near $z = 0$. Then we can use this length-scale to introduce dimensionless quantities $\tilde{z} = w^{-1} z$, $k = w q$, $\bar{D}$, $\tilde{\sigma}_{ij}$ via

$$\bar{D}(\tilde{z}, \tilde{z}') = w^{-1}\tilde{G}(\zeta, wk; w\tilde{z}, w\tilde{z}'), \quad \tilde{\sigma}_{ij}^{(in)} = w^{-3} \tilde{\sigma}_{ij}^{(in)}, \quad \tilde{\sigma}_{ij}^{(dir)} = w^{-3} \tilde{\sigma}_{ij}^{(dir)}. \tag{47}$$

To remove the first-order derivative in (46), let us rescale $\bar{D}$ according to

$$\bar{\bar{D}}(\tilde{z}, \tilde{z}') = (\epsilon \epsilon')^{-1/2} \bar{D}(\tilde{z}, \tilde{z}'), \tag{48}$$

where $\bar{D}(\tilde{z}, \tilde{z}')$ obeys the simpler equation

$$\bar{\bar{O}} \bar{D}(\tilde{z}, \tilde{z}') = [\partial_{\tilde{z}}^2 - k^2 - V(\tilde{z})] \bar{D}(\tilde{z}, \tilde{z}') = \delta(\tilde{z} - \tilde{z}'), \tag{49}$$

with $k$ playing the role of an effective mass of the mode and the dimensionless potential $V(\tilde{z})$ given by the expression

$$V = \frac{1}{2} \partial_{\tilde{z}} \tilde{\eta} + \frac{1}{4} \tilde{\eta}^2, \quad \tilde{\eta} = \frac{\partial_{\tilde{z}} \tilde{\epsilon}}{\tilde{\epsilon}} = \frac{w}{\epsilon} \eta. \tag{50}$$

The Hadamard expansion of the Green’s function $\bar{D}(\tilde{z}, \tilde{z}')$ can be derived using the heat kernel representation

$$\bar{D}(\tilde{z}, \tilde{z}') = \int_0^\infty ds \ K(s|\tilde{z}, \tilde{z}'), \tag{51}$$

where the heat kernel $K(s|\tilde{z}, \tilde{z}')$ corresponding to the one-dimensional operator $\bar{\bar{O}}$ satisfies

$$[\partial_s - \bar{\bar{O}}] K(s|\tilde{z}, \tilde{z}') = -\delta(s)\delta(\tilde{z} - \tilde{z}'). \tag{52}$$

Its formal solution $K(s|\tilde{z}, \tilde{z}') = e^{\bar{\bar{O}} s} \delta(\tilde{z} - \tilde{z}')$ can be represented as a power series in the proper time parameter $s$:

$$K(s|\tilde{z}, \tilde{z}') = -\frac{1}{(4\pi s)^{1/2}} e^{-k^2 s - \frac{\epsilon - \epsilon'}{w} s^2} \left[ a_0(\tilde{z}, \tilde{z}') + a_1(\tilde{z}, \tilde{z}') s + a_2(\tilde{z}, \tilde{z}') s^2 + \ldots \right]. \tag{53}$$

Because from now on we will work mostly with the Fourier transforms of all quantities, we implicitly assume that they depend on the Matsubara frequencies $\omega_n$ and $q$, and, for simplicity, we omit these arguments in functions. Thus, in these notations we have $\epsilon(i\zeta; x) = \epsilon(x)$, $G(\zeta; x, x') = \hat{G}(x, x')$, etc. Since $\epsilon$ is already dimensionless, we use the same letter for the functions $\epsilon = \epsilon(\tilde{z}) = \epsilon(i\zeta; w\tilde{z})$. Springer
where \( a_n(\vec{z}, \vec{z}') \) are the Seeley-DeWitt coefficients. For the calculation of the divergent parts of the stress tensor, we need to know only the first two coefficients \( a_0(\vec{z}, \vec{z}') \) and \( a_1(\vec{z}, \vec{z}') \). For the operator defined by (3) the zero-order coefficient \( a_0(\vec{z}, \vec{z}') = 1 \), while the first-order coefficient \( a_1 \) we need to know only in the limit \( \vec{z} \to \vec{z}' \): \( a_1(\vec{z}, \vec{z}) = -V(\vec{z}) \). All higher order coefficients \( a_n(\vec{z}, \vec{z}') \) for \( n \geq 2 \) do not contribute to the divergent parts of the stress tensor \( \sigma_{ij}(\vec{x}, \vec{x}') \) in 3D because in the non-retarded regime the EM field reduces to the scalar potential \( A_0 \), which satisfies Eq. (3) with the 3D operator. Our procedure guarantees regularity of the contribution of each mode to the renormalized stresses and energy density. Of course, we have to find a sum over all modes with the Matsubara frequencies \( \zeta_n \), which may diverge in principle. However, for all realistic materials subject to Debye’s relaxation model \[72\]8

\[
\varepsilon(iz) = 1 + \frac{\varepsilon(0) - n^2}{1 + i\zeta/\omega_{\text{rot}}} + \frac{n^2 - 1}{1 + \zeta^2/\omega_{\text{rot}}^2},
\]

with \( \omega_{\text{rot}} \) being the rotational relaxation and \( \omega \), the main electronic absorption frequencies as well as \( n \) the refractive index, the summation (5) over Matsubara frequencies \( \zeta_n \) converges meaning that all the stresses become regular as soon as we take care of the 3D spatial divergencies, because the dielectric permittivity at high frequencies approaches that of the vacuum fast enough. Therefore, the UV behaviour of the system is governed by the properties of the 3D operator only. This is why the problems related to the coefficient \( a_2 \) \[75\], which describes logarithmic divergencies in 4D QFT, do not arise in the Lifshitz approach.

It is important to keep in mind that the UV divergencies of the stress tensor are stronger than those of the Green’s function. Therefore, in the Hadamard expansion of the Green’s function we have to include in \( G^{(\text{div})} \) all leading divergent terms and the first subleading term that after integration over the momenta \( k \) contribute to the divergent parts of the stress tensor in 3D \[76\]: even though the subleading term vanishes at the coincident points limit \( \vec{z} = \vec{z}' \), its derivatives do not. Retaining only divergent terms in the integral over \( s \) in (51) and substituting (50), we get the following structures

\[
D^{(\text{div})}(\vec{z}, \vec{z}') = -\frac{1}{2k} e^{-k|\vec{z}-\vec{z}'|} \left[ a_0(\vec{z}, \vec{z}') + a_1(\vec{z}, \vec{z}') \frac{1 + k|\vec{z} - \vec{z}'|}{2k^2} \right],
\]

\[
\partial_{\vec{z}} \partial_{\vec{z}'} D^{(\text{div})}(\vec{z}, \vec{z}') = -\frac{k}{2} e^{-k|\vec{z}-\vec{z}'|} \left[ -a_0(\vec{z}, \vec{z}') + a_1(\vec{z}, \vec{z}') \frac{1 - k|\vec{z} - \vec{z}'|}{2k^2} \right].
\]

Integration of these expressions over the momenta \( k \) is formally divergent, which reflects divergencies of the corresponding quantities in the coordinate space in the limit of coincident points of the part of the Green’s function \( \hat{G}(\vec{x}, \vec{x}') \) defined in (3), which leads to divergent stresses:

\[
\left[ \partial_{\vec{x}} \partial_{\vec{x}'} \hat{G}^{(\text{div})}(\vec{x}, \vec{x}') \right]_{\vec{x}=\vec{x}', \vec{y}=\vec{y}'} = \left[ \partial_{\vec{y}} \partial_{\vec{y}'} \hat{G}^{(\text{div})}(\vec{x}, \vec{x}') \right]_{\vec{x}=\vec{x}', \vec{y}=\vec{y}'} = \frac{1}{2w^2} \int_0^\infty \frac{dk}{2\pi} \frac{k^2 D^{(\text{div})}(\vec{z}, \vec{z}')} ,
\]

\[
\left[ \partial_{\vec{z}} \partial_{\vec{z}'} \hat{G}^{(\text{div})}(\vec{x}, \vec{x}') \right]_{\vec{x}=\vec{x}', \vec{y}=\vec{y}'} = \frac{1}{w^3} \int_0^\infty \frac{dk}{2\pi} k \partial_{\vec{z}} D^{(\text{div})}(\vec{z}, \vec{z}').
\]

These formulas provide us with a prescription how to extract divergencies of the stress–energy tensor (47) using the mode representation (5), which is consistent with the point-splitting approach in the coordinate space.

\[8\] This formula is usually deduced phenomenologically \[73\], but has a QM justification \[74\].
For computation of the divergent stresses, we need to know the divergent part of the unscaled Green’s function $D(x)$, which comes from (55a), its derivatives $\partial_\infty \partial_\infty D(x)$ and $k^2 D(x)$. Then, for the mode contributions to the diverging part of the stress tensor we have

$$
\hat{\tau}_{xx}(\zeta_n) = -\frac{1}{16\pi} \int_0^\infty dk e^{-k|\bar{z} - \bar{z}'|} \left[ k^2 + \frac{1}{2} \left( \frac{1}{2} \partial_\infty \eta - \frac{1}{4} \frac{\eta^2}{\varepsilon} \frac{\partial \varepsilon}{\partial \rho} \partial_\infty \eta \right) \right] \left( 1 + k |\bar{z} - \bar{z}'| \right),
$$

(57a)

$$
\hat{\tau}_{zz}(\zeta_n) = -\frac{1}{16\pi} \int_0^\infty dk e^{-k|\bar{z} - \bar{z}'|} \left[ -2k^2 + \left( \frac{1}{4} \frac{\eta^2}{\varepsilon} - \frac{1}{2} \frac{\rho}{\varepsilon} \frac{\partial \varepsilon}{\partial \rho} \partial_\infty \eta \right) \right] \left( 1 + k |\bar{z} - \bar{z}'| \right),
$$

(57b)

where the dependence of $\hat{\tau}_{ij}(\zeta)$ on the Matsubara frequencies $\zeta_n$ comes through $\varepsilon(i\zeta_n)$, while the finite stresses for every frequency mode $\zeta_n$ are computed from

$$
\hat{\tau}_{ij}(\zeta_n) = \hat{\tau}_{ij} - \hat{\tau}_{ij}(\zeta) - \int_0^\infty \frac{dk}{4\pi} \left[ \varepsilon \partial_i \partial_j D - \varepsilon \frac{\partial \varepsilon}{\partial \rho} \partial_i \partial_j \right] D,
$$

(58)

and the components of $\hat{\tau}_{ij}(\zeta)$ are given by (57). We also have to sum over all Matsubara frequencies in order to get the complete finite stress tensor for a particular dielectric:

$$
\sigma_{ij}^{(\text{fin})} = \frac{1}{\beta} \sum_{n=-\infty}^\infty \hat{\sigma}_{ij}^{(\text{fin})}(\zeta_n) = \frac{1}{\beta w^3} \sum_{n=-\infty}^\infty \hat{\tau}_{ij}^{(\text{fin})}(\zeta_n),
$$

(59)

while the diverging part is found from an analogous expression (37). Recall that the finite stress $\sigma_{ij}^{(\text{fin})}$ does not depend on the regularization scheme: both proper time cut-off and the point splitting Hadamard regularization lead to the same finite stresses. Also, note that the total stresses (58) contain the electrostriction contributions, which are isotropic and therefore do not contribute to the local force density.

In order to compute $\sigma_{ij}^{(\text{fin})}$, in the next section we consider a particular model of a smoothed-out interface for which the Green’s function can be constructed exactly. Among the exactly solvable models it is the one reducing to the Schrodinger equation with the Scarf potential [77], which satisfies all the properties necessary to account for a smoothed-out step-like transition between a dielectric medium and the vacuum or between two dielectric media.

3.3 Exact solution: the Scarf potential

As a particular model of a smoothed-out interface (cf. Fig. 2a) we consider

$$
\varepsilon(\bar{z}; \zeta) = e^{4c(\zeta)} \arctan(e^{-\zeta}),
$$

(60)

where $c > 0$ is a dimensionless constant. Since inside the dielectric and away from the interface $\bar{z} \rightarrow -\infty$ we have $\varepsilon(-\infty; \zeta) = \varepsilon_\infty(\zeta)$, the constant $c$ is given by the asymptotic value of the dielectric constant $c(\zeta) = \frac{1}{2\pi} \ln \varepsilon_\infty(\zeta)$, which depends on the Matsubara frequency $\zeta$. Then, the non-dimensional $\bar{\eta}$ introduced in (50) and the potential $V(\bar{z})$ become

$$
\bar{\eta}(\bar{z}) = -2c \frac{1}{\cosh \bar{z}}, \quad V(\bar{z}) = \frac{c^2}{\cosh^2 \bar{z}} + \frac{\sinh \bar{z}}{\cosh^2 \bar{z}},
$$

(61)

respectively; here we suppressed the dependence on $\zeta$ for brevity. This form of $V$ is known as the Scarf potential [77,78], cf. Fig. 2b.
We need to find the Green’s functions $D(z, z')$ (48) or, equivalently, $D(k; z, z')$ which satisfies Eq. (49) and should also vanish at $z \to \pm \infty$. To this end, we first have to determine the modes obeying the homogeneous part of equation (49)

$$\left[ \partial^2_z - k^2 - V(z) \right] u(z) = 0,$$

which has the form of the Schrödinger equation with the Scarf potential and can be solved in terms of hypergeometric functions. Two independent solutions to (62) are

$$u_1 = e^{\frac{\pi c}{Z}} Z^{-i\frac{c}{2}} F_1 \left(k, -k; \zeta; Z\right),$$

$$u_2 = e^{i\frac{\pi c}{2}} Z^{\frac{1}{2}+i\frac{c}{2}} (1 - Z^{i\frac{c}{2}}) F_1 \left(1 + k - \zeta, 1 - k - \zeta; 2 - \zeta; Z\right),$$

where $Z = \frac{1}{2}(1 - \sinh \overline{z})$ is a complex function of $\overline{z}$ and $\zeta = \frac{1}{2} - ic$ is a complex number.

The Green’s function satisfying (49) we are looking for has to be real. Naturally, there exist a pair of independent real solutions $v_1, v_2$, which are linear combinations of complex-valued $u_1$ and $u_2$:

$$v_1 := Au_1 - Bu_2,$$

$$v_2 := Cu_1 - Eu_2,$$

where the coefficients are complex

$$A = e^{\frac{\pi c}{Z}} \frac{1}{\Gamma(1 + k - \zeta) \Gamma(\zeta)},$$

$$B = e^{\frac{\pi c}{2} (1 + k - \zeta)} \frac{k}{\Gamma(k + \zeta) \Gamma(2 - \zeta)},$$

$$C = e^{-2i\pi \zeta} e^{-i\pi (1+k)} A,$$

$$E = e^{-i\pi (1+k)} B.$$  

The solution $v_1$ vanishes at $z \to +\infty$ and grows at $z \to -\infty$, while the solution $v_2$ grows at $z \to +\infty$ and vanishes at $z \to -\infty$.

The Wronskian of these two solutions can be computed analytically

$$W[v_1, v_2] = e^{\pi c} \left(1 + e^{-2\pi c}\right)^2 \frac{k}{2\pi \Gamma(k + \zeta) \Gamma(1 + k - \zeta)},$$

which is, evidently, also real despite the complex $\zeta$ entering the expression. Now we have everything at hand to construct the Green’s function $D(k; z, z')$ in (48):

$$D(k; z, z') = -\frac{v_1(z) v_2(z')}{W[v_1, v_2]},$$
Fig. 3 Stress distributions across the interfacial region for (a, b) water and (c, d) benzene. Model (54) for \( \varepsilon \) is used with the corresponding parameters [4] \( \varepsilon(0) = 80, n = 1.333, \omega_{rot} = 4\pi \cdot 10^{10} \text{ rad s}^{-1}, \omega_s = 6\pi \cdot 10^{15} \text{ rad s}^{-1} \) (water) and \( \varepsilon(0) = 2.28, n = 1.501, \omega_{rot} = 2.4\pi \cdot 10^{12} \text{ rad s}^{-1}, \omega_s = 6.4\pi \cdot 10^{15} \text{ rad s}^{-1} \) (benzene). (a, c) Finite contributions (59) without the prefactor \( \beta^{-1} w^{-3} \) along with the zero Matsubara frequency contribution only (thin lines); the finite electrostriction contribution \( \sigma_{ES}^{(fin)} \) is also shown separately (the electrostriction terms in (58) are singled out and renormalized with the corresponding counterparts in the divergent stresses according to (58)). (b, d) Subleading contributions \( \sigma_{xx}^{(div)} = \sigma_{(iso)}^{(iso)} \) and \( \sigma_{zz}^{(div)} = \sigma_{(iso)}^{(iso)} + \sigma_{(aniso)}^{(aniso)} \) calculated from (36a) and (36b) without the prefactor \( \beta^{-1} \lambda_0^{-1} w^{-2} \) and with both \( \eta \) and \( \bar{z} \) scaled with respect to the interface width \( w \).

where \( \bar{z}_{\text{max}} = \max(\bar{z}, \bar{z}') \) and \( \bar{z}_{\text{min}} = \min(\bar{z}, \bar{z}') \).

Substituting the constructed Green’s function (67, 48) in Eq. (58) and subtracting \( \hat{\tau}_{ij}^{(div)} \), as per (58), we find the finite stresses \( \hat{\tau}_{ij}^{(fin)} \) at each frequency \( \zeta_n \), which are then summed according to (59). The result of this procedure for two types of dielectrics—water and benzene chosen here as examples of polar and non-polar liquids, respectively—is shown in Fig. 3. Note that for computational purposes instead of (63) it is convenient to use hypergeometric functions of an inverse argument and separate representations for positive and negative \( \bar{z} \) because the corresponding hypergeometric functions have a branch cut \( 1/Z \in [1, \infty) \) on the real axis [79].

4 The quantum nature of surface tension

4.1 Calculation of surface tension

In order to define the ST, we consider a strip of infinite length in the \( z \)-direction and of unit length in the \( y \)-direction, with the normal \( n \) in the \( x \)-direction correspondingly. In the
asymptotic regions \( z \to \pm \infty \) the total stress tensor of a fluid is isotropic \((43,45)\), i.e. given by \( \sigma_{ij}^{(\text{tot})} = -\delta_{ij} p_0^{(\text{ren})} \). Note that because our system with a free interface is in a mechanical equilibrium, there is no net force in the \( z \)-direction acting on every volume element of the system \((42)\). Therefore \( \sigma_{zz}^{(\text{tot})} = -p_0^{(\text{ren})} = \text{const}^9 \) for all \( z \) as per \((43)\): below, above, and inside the smoothed-out interface. The leading order UV-divergent EM stresses \( \sigma_{ij} \) in the \( x, y \)-directions are compensated by the bare mechanical (elastic) stresses \( \sigma_{ij}^{(m)} \) producing an isotropic renormalized pressure \((39)\), which does not depend on the \( z \)-coordinate. The remaining subleading and finite parts of stresses in the \( x, y \)-directions do depend on \( z \). At the same time, all the quantities in the bulk do not depend on \( x \) and \( y \) due to translational invariance and the equilibrium condition \((38)\) in these directions is satisfied automatically for all \( z \). In the absence of the interface, i.e. when the entire space is filled with a homogeneous fluid, the force acting on the considered strip would be just \( \int_{-\infty}^{\infty} dz \ p_0^{(\text{ren})} > 0 \) since \( p_0^{(\text{ren})} < 0 \). Thus, the ST of the interface, in hydrodynamics and theoretical physics \([56]\) traditionally defined as a positive quantity because physically it corresponds to tensile stresses tending to compress the medium, is computed as the difference of the integral of \( \int_{-\infty}^{\infty} dz \ \sigma_{xx}^{(\text{tot})}(z) \) and the latter force:

\[
\gamma = \int_{-\infty}^{\infty} dz [\sigma_{xx}^{(\text{tot})}(z) + p_0^{(\text{ren})}] = \int_{-\infty}^{\infty} dz [\sigma_{xx}^{(\text{tot})}(z) - \sigma_{zz}^{(\text{tot})}].
\] (68)

The formula (68) is notable: despite that both EM (namely, the calculated here London) and non-EM (such as the ones responsible for the repulsive core in the Lennard-Jones potential, cf. Sect. 3.1.2) interactions contribute to the total energy of the interface, the equilibrium condition \((42)\) and its consequence \((44)\) enable us to express the total ST solely in terms of EM stresses. While above we provided a mechanistic derivation of (68), it is also in line with an energy-based derivation of (68) by Fisher \([1]\): the total energy per unit area of the interface is determined by the work of the ST forces, which is why the energy density per unit area of the interface exactly equals to \( \gamma \).

Due to the structure of (68), it is important to emphasize that any isotropic contributions, should they originate from electrostriction or other leading diverging terms in \((35b)\), cannot contribute to ST according to (68); these isotropic terms can affect only the (renormalized) mechanical pressure (Sect. 3.1.2). Because of the asymptotic behaviour \((45)\), only the region in the vicinity of the interface contributes to this integral. Remarkably, even if the interface is between a dielectric and the vacuum, polarization of the vacuum also contributes to ST—this is not an artefact of the theory as the measurable Casimir effect \([7]\) is also due to the vacuum polarization. Given that ST is dictated by the distribution of \( \sigma_{xx}^{(\text{tot})} - \sigma_{zz}^{(\text{tot})} \) across the interface, this behaviour is shown in Fig. 4 with separated finite \((a,d)\) and subleading \((b,e)\) contributions as well as the total stress difference \((c,f)\) compared to that obtained from the sharp interface problem \((18)\), which in the limit \( \ell \to \infty \) leads to

\[
\sigma_{xx}^{(\text{fin})} - \sigma_{zz}^{(\text{fin})} = -\frac{1}{32 \pi \beta w^3 \bar{z}^3} \sum_n \frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3}.
\] (69)

Note that (69) is an antisymmetric function of \( \bar{z} \) and hence it would be impossible to get a non-zero ST or contribution to it in the framework of the sharp interface formulation\(^{10}\) (Sect. 2)! This implies that the problem of calculating ST represents a distinguished limit:

\[9\] Recall that the pressure is the force per unit area of the wall should it be bounding the medium, while normal stress is the force per unit area acting on the medium itself.

\[10\] It must be also mentioned that the electrostriction contributions, which would have to be added to \((18)\) in the dielectric phase, cancel out in \((69)\) due to their isotropic nature cf. \((36a)\).
Fig. 4 The difference of stress distributions $\Delta \sigma = \sigma_{xx} - \sigma_{zz}$ across the interfacial region for (a–c) water and (d–f) benzene. (a, d) Finite contributions $\sigma_{xx}^{(in)} - \sigma_{zz}^{(in)}$ as per equations (59) without the prefactor $\beta^{-1} w^{-3}$ along with the zero Matsubara frequency contribution only (thin lines). (b, e) Subleading contributions $\sigma_{xx}^{(div)} - \sigma_{zz}^{(div)} = -\sigma_{zz}^{(ann)}$ calculated from (36a) and (36b) without the prefactor $\beta^{-1}\lambda_0^{-1} w^{-2}$ and with both $\eta$ and $z$ scaled with respect to the interface width $w$. (c, f) Finite contributions $\sigma_{xx}^{(fin)} - \sigma_{zz}^{(fin)}$ in the case of a sharp interface (dashed), as per equation (69) without the prefactor $\beta^{-1} w^{-3}$, are compared with the total $\Delta \sigma = \sigma_{xx} - \sigma_{zz}$ in the case of a smoothed-out interface, i.e. sum of finite (a, d) and subleading (b, e) contributions: $\Delta \sigma^{(fin)} + (w/\lambda_0) \Delta \sigma^{(div)}$. Here we took $\lambda_0 = r_m$ and the measured values $w = 4.49 \, \text{Å}$, $r_m = 3.1 \, \text{Å}$ for water and $w = 7.12 \, \text{Å}$, $r_m = 4.75 \, \text{Å}$ for benzene [80]

the result depends on whether one starts with a sharp interface formulation or first computes ST for a smoothed-out interface and then takes a limit to the sharp one. The presence of the distinguished limit is a reflection of the internal structure of the interface, which is lost in the sharp interface formulation: while the BCs (14) are recovered from (46) in the limit from smoothed out to sharp interface as follows from straightforward calculations with the theory of distributions, the stresses (11) involve derivatives of higher order of the Green’s function than in (14), which leads to the distinguished limit in the behaviour of stresses.

Also, one may consider a step-like interface of width $w$ with an intermediate dielectric constant $\varepsilon_2 < \varepsilon_3 < \varepsilon_1$. Analogous integration of $\sigma_{xx}^{(in)} - \sigma_{zz}^{(in)}$ over all $z$ leads to a non-zero $\gamma^{(in)} \sim w^{-2}$ diverging as $w \to 0$, rather than vanishing as in the single sharp interface case. This means that if some divergent terms are omitted in the calculation of stresses such as the subleading ones (35c), then the resulting ST would depend on the order of performing integration w.r.t. $z$ and taking a limit to the sharp interface. Only proper regularization, e.g. based on the heat kernel method used here, allows extraction of all terms remaining after subtraction of the leading divergencies: this enables one to extract both finite contributions that do not depend on the cut-off and subleading UV divergent ones that depend on it.

Let us next analyse the structure of $\sigma_{xx}^{(in)}(z)$ contributing to ST (68). As per Sect. 3.1, the EM contribution consists of the divergent and regular parts $\sigma_{ij} = \sigma_{ij}^{(div)} + \sigma_{ij}^{(fin)}$. The UV divergent part appears because of our treatment of media as continuous, which is why this
model is expected to work only down to the length-scales on the order of intermolecular distance \( r_m \). Thus, the UV divergent part is in fact a large, but finite quantity that depends on \( r_m \) or a cut-off parameter \( \lambda_0 \). The finite part \( \sigma_{\text{fin}}^{\text{UV}} \) describes the \( \lambda_0 \)-independent contribution of the vacuum polarization effects in inhomogeneous media. The equilibrium condition (38) tells us that all mechanical and EM forces counterbalance each other; in particular, in the \( z \)-direction we get (43). As per (68) and (44), the EM tangent pressure \( \sigma_{xx}^{\text{fin}} \) depends on \( z \) and contributes to the finite EM part of ST

\[
\gamma^{\text{(fin)}} = \int_{-\infty}^{\infty} dz \left[ \sigma_{xx}^{\text{(fin)}} - \sigma_{zz}^{\text{(fin)}} \right] = \int_{-\infty}^{\infty} dz \Delta \sigma^{\text{(fin)}},
\]

which is finite because \( \sigma_{xx}^{\text{(fin)}} \to 0 \) and \( \sigma_{zz}^{\text{(fin)}} \to 0 \) fast enough at \( z \to \pm \infty \). The finite part of surface tension \( \gamma^{\text{(fin)}} \) does not depend on the UV cut-off \( \lambda_0 \) and is proportional to \( w^{-2} \), where \( w > \lambda_0 \) is a characteristic width of the interface and \( \lambda_0 \) is the cut-off length-scale. This contribution is smaller than \( \gamma^{\text{(div)}} \), which is of the order of \( \sim 1/(\lambda_0 w) \). Also, while both \( \gamma^{\text{(div)}} \) and \( \gamma^{\text{(fin)}} \) in (71) seem to be proportional to temperature \( T = \beta^{-1} \), these quantities do not vanish in the limit \( T \to 0 \) as discussed in Sect. 2.1.

4.2 Comparison to experiments and further interpretation

To demonstrate the dependence of ST on the cut-off parameter \( \lambda_0 \) and identify the value of the latter required to fit to the experimentally measured ST, we used the calculations from

\[\gamma^{\text{(div)}} = -\int_{-\infty}^{\infty} dz \sigma_{zz}^{\text{(ani)}} \equiv \int_{-\infty}^{\infty} dz \Delta \sigma^{\text{(div)}} = \frac{23}{24(4\pi)^{3/2} \beta \lambda_0} \sum_n \int_{-\infty}^{\infty} dz \frac{\eta^2}{\varepsilon^{1/2}}. \]
Fig. 5 (a) On the interface width definition: \( w \) is the interface width scale, set in this figure to be 1; \( w^* \) is the experimentally measured width based on the length over which the density \( \rho(z) \) changes from 90 to 10% of the bulk value [81], which is assumed here to correlate with the profile of \( \epsilon(z) - 1 \). (b) Dependence of \( \gamma \) on the cut-off parameter \( \lambda_0^* \) for water at 287.5 K and benzene at 286 K according to formula (73); the data for the interface width \( w \) are taken from Fig. 4. The cut-off parameter required to obtain the corresponding correct ST (marked with a solid circle) at the reported temperature [80]: \( \lambda_0^* = 2.16 \) Å for 0.0737 N m\(^{-1}\) (water) and \( \lambda_0^* = 4.19 \) Å for 0.0298 N m\(^{-1}\) (benzene). For comparison, we also show the values of ST predicted by taking \( \lambda_0^* \) to be equal to the intermolecular distance (marked with empty circles) producing 0.0383 N m\(^{-1}\) for \( \lambda_0^* = 3.1 \) Å (water) and 0.0244 N m\(^{-1}\) for \( \lambda_0^* = 4.75 \) Å (benzene).

Fig. 4 along with equation (71) to produce in SI units

\[
\gamma = \frac{k_B T}{w^2} \left[ \int_{-\infty}^{\infty} d\tilde{z} \Delta \tilde{\sigma}^{(sa)} + \frac{w^*}{\lambda_0^*} \int_{-\infty}^{\infty} d\tilde{z} \Delta \tilde{\sigma}^{(sa)} \right],
\]  

(73)

where by introducing \( w^* \) and \( \lambda_0^* \) instead of the original quantities we took into account that the originally introduced scaling of \( z \) with respect to \( w \), which sets the length-scale in the problem, is different from the procedure used in experiments [81] to determine the (empirical) interfacial width \( w^* \); hence the non-dimensional expressions (with tildas) under the integral sign result from scaling with respect to \( w^* \). This fact is illustrated in Fig. 5a for the chosen interfacial profile (60); as a result, the cut-off parameter \( \lambda_0^* \) must also be rescaled to the same factor \( w^*/w \). Calculations for (60) show that as \( \epsilon \) drops from its value of 80 at zero frequency to 1 at high frequencies, the factor \( w^*/w \) varies in the range 3.29 – 3.69. Using \( w^*/w = 3.67 \) typical for the most values of \( \epsilon \) over the entire frequency domain, we plot (73) in Fig. 5b. It is notable that for the chosen substances the finite stresses contribution in (73) is actually negative.

The reported in Fig. 5b values of \( \gamma \) evaluated at \( \lambda_0^* = r_m \) are indicative of the validity of the theory, but the value of the cut-off parameter cannot be predicted within the framework of the Lifshitz theory as the physics behind \( \lambda_0 \) lies beyond its scope. While a more detailed comparison between theory and experiment would also require a more precise reconciliation with how the interface width \( w \) is measured in experiments [80,81], Fig. 5b demonstrates that all these differences can be absorbed into the cut-off parameter \( \lambda_0 \). The departure in the prediction is the largest in the case of water, i.e. about three times, which is because it is a polar liquid with strong hydrogen bonds.\(^{12}\)

\(^{12}\) First, this leads to the Keesom effect [82] contributing to vdW forces due to attraction of permanent dipoles with moments p—in the case of water the ratio of the Keesom to London energies of interaction
Despite that for water and benzene the determined values of the cut-off parameter $\lambda_0$ prove to be reasonably close to the intermolecular distance $r_m$ for a given substance, the true physics behind the cut-off parameter $\lambda_0$, responsible for the dependence on the alluded microscopic physics at the distances $\lesssim \lambda_0$ (Sect. 3.1), remains an open question. Since the Lifshitz theory is based upon the macroscopic dielectric permittivity $\varepsilon(\omega)$, which does not know about the origin of quantum EM fluctuations, one can equally assert that the cut-off parameter $\lambda_0$ may depend on the charge separation distance $\lambda_0$ of the fluctuating dipoles responsible for the EM stresses and hence ST. Since the latter can be estimated independently as the bond energy $\sim k_B$ divided by $r_m^2$, and the energy of fluctuating dipoles having moments $p = \lambda_d e$ due to polarization of molecules is $p^2/(4\pi \varepsilon_0 r_m^2)$, we find, for example, for water

$$
\lambda_d \sim \sqrt{4\pi \varepsilon_0 k_B T r_m^3/e^2} \approx 0.25 \text{ Å} \ll r_m = 3.1 \text{ Å}, \quad (74)
$$

where $e$ is the elementary (electron) charge. In particular, originally Dzyaloshinskii et al. [14] suggested that $\lambda_0$ might be considerably smaller than the interatomic spacing $r_m$. Regardless of the actual value, the dependence of ST on the cut-off parameter $\lambda_0$ may appear astonishing. Nevertheless, such kind of behaviour is typical for macroscopic models, which are not closed, e.g. the Navier–Stokes equations governing motion of a fluid or the Navier–Cauchy equations governing deformation of solids at macroscopic length–scales “remember” their microscopic origin through their respective dependence on viscosity or Lamé parameters, which can be accounted for by a microscopic theory only. This is a general property of macroscopic systems in which microscopic effects propagate to macroscopic scales. The cut-off parameter $\lambda_0$ plays such a role in the Lifshitz theory—as a “macroscopic” theory it remembers its origin at the microscopic scales $\lesssim \lambda_0$, at which fluctuations originate.

The cut-off dependence of ST was envisioned by Schwinger et al. [56] (see also [48]). These authors considered a sharp interface and found that the renormalized energies and hence contribution to ST, which appears to be nonzero if stresses are taken into account only on one side of the interface, as well as latent heat of liquid helium, are “cut-off dependent”. As we learned from the present study, stresses on both sides of the interface must be taken into account (73), and therefore the leading order contribution to ST due to non-retarded stresses, in the sharp interface formulation should vanish because of antisymmetry of the contributing stresses (69); also UV divergencies at a sharp interface are not well defined and in some cases may even cancel each ether locally [26] or in the integral sense [24]. Notably, while Schwinger et al. [56] reported the calculated magnitude of ST three times higher than the actual one $\gamma = 0.37 \text{ mN/m}$, our calculations produce $0.48 \text{ mN/m}$ based on the known interface thickness 6.5 Å [81] and interatomic distance 3.75 Å. More recently [70], in the context of quantum liquids, for which a bare Lagrangian exists, it was also noted that ST phenomena are the lowest-order corrections to the vacuum energy dependent on the intermolecular distance $r_m$—in our study the latter are the leading and the former are the subleading UV divergent terms in (35), which depend on the cut-off $\lambda_0$.

$\varphi_K/\varphi_L = 4p^4/(9h \beta T \alpha_0^2 \omega_0) \approx 6.32$, where $\alpha_0$ is the water molecular polarizability; most importantly, the hydrogen bond energy $3.82 \cdot 10^{-20} \text{ J}$ per bond is comparable to that of the latent heat of evaporation per molecule $6.78 \cdot 10^{-20} \text{ J}$ and much larger than $k_B T \approx 4.14 \cdot 10^{-21} \text{ J}$ thus indeed being capable of affecting the Footnote 12 continued value of ST. Second, the water molecule polarity may give rise to a local structure in the bulk and potentially at the interface thus, in particular, invalidating assumptions behind the isotropy of the dielectric permittivity upon which the Lifshitz theory is based—if one thinks of water molecules as permanent dipoles, they may orient themselves along the interface thus increasing ST as opposed to, say, surfactants, which, when added to water, stick their polar heads in water and thus orient themselves perpendicularly to the interface, thus decreasing ST due to repulsion between themselves.
Fig. 6 Scaling of interfacial tension $\gamma$ with interfacial thickness $w$ far from critical point (based on experimental data for Nitrobenzene-water [83] in the temperature range $T = 298$–$328$ K with $T_c = 513$ K and molecular dynamics simulations for water [84] in the temperature range $T = 268$–$373$ K with $T_c = 647$ K) and near critical point (based on experimental data for liquid Argon [85] in the temperature range $T = 85$–$120$ K with $T_c = 150.9$ K and sulphur–hexafluoride [86] in the temperature range $T = 305.952$–$318.573$ K with $T_c = 318.7$ K). All experiments used ellipsometry to study departures of reflection of polarized light from properties predicted by Fresnel’s equations. The power law scalings reported in the legend of the figure are obtained using least square fit to the data taking into account the errors reported in the above referenced papers.

We would like to point out that our theory of ST involving both subleading $\gamma^{(\text{div})} \sim \lambda_0 w^{-1}$ and finite $\gamma^{(\text{fin})} \sim w^{-2}$ contributions does not contradict the experimental [83,85,86] and molecular simulations [84] data available in the literature, cf. Fig. 6. Since the developed theory is applicable not only at zero temperature but also at finite temperatures (see the discussion in Sect. 2.1), formula (73) can be put in the context of known scalings below and near a critical point for corresponding substances. As one can gauge from Fig. 6 for nitrobenzene–water and water–vapour interfaces, far below the critical point the scaling $\gamma \sim w^{-m}$ is closer to $m = 1$ rather than $m = 2$. For temperatures approaching critical one, the exponent $m$ increases, e.g. for argon it becomes 1.66, and for temperatures very close to the critical point in the case of Sulfur-Hexafluoride it reaches 2, which is in accord to the critical phenomena scaling (capillary wave) theory [87] widely confirmed by experimental measurements [88,89]. In general, the interfacial thickness $w$ and tension $\gamma$ near a critical point scale as [88]

$$w \sim (T_c - T)^{-\nu} \quad \text{and} \quad \gamma \sim (T_c - T)^{\mu},$$

which from the classical theory of vdW [90] and Cahn-Hilliard [91] amount to the values $\nu = 1/2$ and $\mu = 3/2$. However, experimental measurements, cf. [88] and references therein, deviate appreciably yielding values closer to $\nu = 2/3$ and $\mu = 4/3$, e.g. for Sulphur-Hexafluoride, which is commonly used in electrical power industry for high-voltage circuit breakers and gas-insulated transmitters and therefore well-studied, one measures $\nu = 0.658 \pm 0.012$ and $\mu = 1.34 \pm 0.06$. Altogether, this yields $\gamma \sim w^{-2.04}$, which is close to the scaling of $\gamma^{(\text{fin})} \sim w^{-2}$ predicted in our work. Having said that, the difference between the subleading and finite contributions to ST far from a critical point is elusive: $w$ is normally just a few intermolecular distances $r_m$, so that both contributions are comparable, which is why ST can...
be reasonably estimated from the enthalpy of evaporation divided by $r_m^2$ producing the right order of magnitudes for a wide range of substances [92].

Next, to highlight the physics of ST, let us consider a crystal surface. While in the bulk the situation is isotropic, i.e. for the two orthogonal orientations of molecules in Fig. 7a, the vdW forces acting on the molecules are the same, in the case of the interface in Fig. 7b the vertically oriented pair no longer experiences the attraction from the upper space, while the horizontally oriented pair of molecules is now pulled apart by a force about half of that compared to the bulk configuration—altogether this leads to anisotropy in the pressure, i.e. it becomes a tensor as we also saw from the direct calculations (18,35). As a result, the matter is compressed near the interface, though anisotropically [93], and therefore the near-the-interface region acts like a skin. In liquids, of course, the behaviour of the intermolecular distance and hence the density profile is more complicated compared to that in crystals as a liquid phase must transition to its vapour state in a less abrupt fashion. The fact that the normal and tangent components of renormalized pressure are different near the interface indicates that a liquid in its vicinity starts behaving more like a solid. This anisotropy is an inherent property of inhomogeneous media, e.g. atmosphere, ocean, and rocks stratified under gravity field, though would require exotic conditions under which the length-scale of inhomogeneity is comparable to the range of Derjaguin or Casimir effects.

Despite being convincing, the classical considerations of the effect of vdW forces in the above paragraph are based on pairwise molecular interaction $\phi_{\text{vdW}}^{ij} = -4\nu (r_m/r_{ij})^6$, i.e. require molecules $i$ and $j$ to be present, and therefore fail to account for the vacuum polarization. Moreover, as we observed in the previous section Sect. 4.1, the Lifshitz theory with a sharp interface gives null ST due to antisymmetry of the stress (69). It is only the physically justified smoothed-out interface formulation is capable to properly account for the vacuum polarization and hence the ST phenomena. Therefore, all theories based on an effective Lennard-Jones-type intermolecular potential should it be combined with statistical approach (molecular distribution functions) [1,3,94–97] or direct molecular simulations [98–102] cannot truly capture the quantum-mechanical nature of the underlying local stresses and hence ST. Therefore, it is not surprising that ST calculated with these approaches often results in values substantially different from experimentally measured as (i) the involved
vdW forces cannot be accounted for by addition of the individual intermolecular potentials due to screening effects—the fact realized by Lifshitz [13]—and (ii) the quantum mechanical effects prove to play a significant role in settling the value of ST.

Lastly, the gained understanding of the stress distributions in Fig. 3 being concentrated in the neighbourhood of the interface brings up yet another physical interpretation of ST phenomena: if one considers molecules as dielectric dipoles in the fluctuating EM field, then, after averaging the intensity over fluctuations, they (molecules) are dragged in the direction of the gradient of the EM fluctuations intensity, i.e. to the interfacial region. As also envisioned above from the (pairwise) vdW intermolecular potential considerations, this effect naturally results in a higher molecular density near the interface, i.e. it acts as optical tweezers governed by an analogous underlying physical mechanism.

5 Discussion

First, let us recap the basic elements of the presented here story in simple terms. The key effect addressed in our study—divergence of the EM stresses acting along the interface—can be gleaned even from the pairwise summation [95] of intermolecular vdW potentials

$$\phi_{ij} = -\frac{4}{\upsilon (r_m/r_{ij})^6},$$

which for the stress $\sigma_{xx}(x_P)$ along the interface at a point $x_P = (x_P, y_P, z_P)$ located at the distance $\ell$ from the interface, cf. Fig. 7b, leads to

$$\sigma_{xx}(x_P) = -12 \upsilon r_m^6 \int_{-\infty}^{0} dz \int_{-\infty}^{+\infty} dx dy \frac{(x_P - x)^2}{|x_P - x|^8} = -\frac{\pi \upsilon r_m^6}{3 \ell^3},$$

and obviously diverges as one approaches the interface $\ell \to 0$, qualitatively being analogous to the result from the Lifshitz theory (69). Based on a similar calculation one can compute the disjoining pressure $\Pi_D(\ell)$, as it was originally done by Derjaguin [5], but the Hamaker constant $A_H$ would be incorrect because non-additive effects are neglected in this approach. While the Lifshitz theory accounts for non-additivity, the divergence remains, which comes from the nonphysical nature of the sharp interface associated with the jump in $\varepsilon$ and the high wavenumber (momenta) $q$ in the along-the-interface direction of the virtual photons contribution to the stress spectral representation leading to the divergent integrand $\sim q^2$ in (18).

In reality, however, there must be a cut-off [14] at some $q_{\text{max}}$, which is considerably smaller than the reciprocal of the interatomic spacing $r_m^{-1}$. The equivalence of the wavenumber $q$- divergence to that due to sharp interface limit is easy to see from Eq. (46) for the Fourier components of the Green’s function when interface is smeared on the length-scale $w$:

$$\left\{ \partial_z \left[ \varepsilon(z/w) \partial_z \right] - q^2 \right\} \tilde{G} = \delta(z - z');$$

clearly, the problem is scale-free under the transformations $z \to w\tilde{z}$ and $q^2 \to w^2q^2$, thus indicating that the limit of a sharp interface $w \to 0$ is equivalent to that of $q \to \infty$.

As mentioned in the Introduction, in the context of QFT studies the presence of divergencies near boundaries has been known for a long time along with the lack of a universal approach to deal with these divergencies, regardless of whether the transition between media $\varepsilon(z)$ is sharp as in the Lifshitz theory [23] or piecewise continuous with discontinuous derivatives at the interface between media [21,29,34,35], and whether the inhomogeneous media are dispersive [29] or non-dispersive [21,31,34,103]. In particular, it was realized that one cannot approximate a smoothed-out interface with a step-like discretization [23] and “though there have been many illuminating endeavors, more effort is still needed to find proper renormalization methods for the inhomogeneous cases” [35]. We believe that quantum microscopic
properties of the media dictate the application of proper regularization schemes which should respect symmetries, e.g. local isotropy of fluids, and not bring any new artificial features to the system. If \( \varepsilon(z) \) is step-like or piecewise continuous, so that its derivatives are discontinuous at the interface between media, the local isotropy is broken and stresses are ill-defined at the interface as follows from the developed here expressions (36,57). This is why in the literature there has been a lot of controversy about divergent stresses on the interface. Smooth interfaces or “soft walls” [37] do not suffer with this problem and should be used to define an appropriate limit to the idealized sharp interface models.

Therefore, to resolve the technical difficulties encountered previously in the literature, in this paper we studied the vacuum polarization in inhomogeneous media with an embedded smoothed-out interface. Because the problem of UV divergent terms appears already for a single sharp interface, we consider a model of a single smoothed-out interface. We used the heat kernel representation, proper time cut-off regularization, and the Hadamard expansion of the Green’s function to systematically determine its corresponding parts leading to divergent stresses. The heat kernel technique was also used by Bordag et al. [31] to study UV-divergencies in the EM effective action in the case of inhomogeneous dielectric media without dispersion. Here we considered dispersive media in the non-retarded (Deryaguin) limit, in which the operator containing only spatial derivatives appears, though the quantum fluctuations of the polarizable atoms’ dipole moments are time-dependent. At the scales smaller than \( \lambda_0 \), the non-retarded limit gives the chief contribution, while that of retarded transverse electromagnetic modes is negligibly small. Given the equivalence of the Green’s function at finite temperatures \( G^\beta \) and that at zero temperature \( G^F \) after Wick’s rotation, we expanded all time-dependent quantities in the Fourier series over the Matsubara modes. Then the quantization scheme reduces to the spectral theory of the 3D operator (3). We found that while there is no Casimir force acting normally to the interface, the vacuum polarization still plays an important role in the origin of ST. The value of total pressure in the liquid, cannot be determined solely by the effective theory—the microscopic physics must be invoked for that [70]. Polarization contributions to the stress tensor of an inhomogeneous system depend on the cut-off \( \lambda_0 \leq r_m \) as well as the characteristic scale \( w \) of inhomogeneity, i.e. the width of the interface, and can be classified as follows. (i) The leading UV contribution to the pressure is of the order \( \lambda_0^{-3} \), does not depend on the geometry of the system, is homogeneous and structurally the same as for the vacuum. For this reason it does not lead to any observable effects. The standard Lifshitz procedure is to truncate these terms. (ii) The subleading UV divergent term, which is on the order of \( \lambda_0^{-1} w^{-2} \), is related to ST of the interface and can be measured in experiments. (iii) The finite contribution \( w^{-3} \) is due to vDW interactions, does not depend on the UV cut-off scale \( \lambda_0 \), but also contributes to ST. In the case when \( w \sim \lambda_0 \), the subleading and finite contributions can be comparable. (iv) Retardation effects are insignificant at small scales \( w \ll \lambda_0 \) and become important only at the scales \( \gtrsim \lambda_0 \). This classification is in accordance with the one proposed by Volovik [70] for a description of quantum effects in quantum liquids. It is important to emphasize that while our renormalization technique is in essence the same as that used by Casimir and Lifshitz—namely, subtraction of the divergent free space contribution (with the value of dielectric permittivity \( \varepsilon(x) \) corresponding to a given point \( x \)—the presence of a smoothed-out interface leads not only to finite stresses (59), but also subleading divergent stresses (35c) dependent on the cut-off parameter and absent in the sharp interface case; both finite and subleading stresses in turn contribute to ST (71,73) favourably compared here with the available experimental data (Sect. 4.2).

Notably, observation of subleading contributions was also made by Ravndal [66] in the context of calculations of the Casimir energy between parallel plates without taking dispersion
into account. Namely, if the Casimir energy of a scalar field between the plates separated by a distance $\ell$ with Dirichlet boundary conditions is considered, the regularized energy density consists of three terms: (i) the leading UV divergent term $3\Lambda^4/(2\pi^2)$, where $\Lambda$ is the cut-off wavenumber beyond which the theory is inapplicable; (ii) the subleading UV divergent term $\Lambda^3/(4\pi\ell)$; (iii) and the pure Casimir term $-\pi^2/(1440\ell^4)$. For the Neumann boundary conditions, also when a scalar field is considered, the leading UV divergent and Casimir terms are the same, while the subleading term appears with the opposite sign. In the case of the EM field between perfectly conducting parallel plates, the transverse electric multipoles correspond to the Dirichlet modes while the transverse magnetic multipoles correspond to the Neumann modes [26,104,105]. It happens that for perfectly conducting plane plates the EM stress–energy tensor divergencies cancel and only finite Casimir effect survives [26]. However, this cancellation is not universal, but applicable only to Casimir effect with retardation as an artefact of idealized BCs in nondispersive media. In a system of realistic dielectrics with dispersion the role of magnetic field is negligible at small length-scales $\lesssim \lambda_a$, in which case (as opposed to the limit $\gtrsim \lambda_a$) there is no compensation of divergent terms coming from quantum fluctuations of interacting electric dipoles which depend on an inhomogeneity of the system. As we showed, this effect has observable physical consequences and together with the finite vdW terms leads to ST (Sect. 4).

In summary, we demonstrated that in the sharp interface formulation it is impossible to obtain ST due to asymmetry of the stresses (69). Hence, in order to reveal the origin of ST, one must consider a smoothed-out interface, the internal structure of which (cf. Fig. 4) explains the ST phenomena. Without proper renormalization, i.e. if one disregards all diverging contributions, ST could be even negative. Hence, subleading cut-off-dependent divergent terms must be kept to produce the correct ST, which is also consistent with the a priori fact that the Lifshitz theory cannot be fully renormalizable as it is an effective [106] and not a closed one (cf. discussion in Sect. 4.1). The Lifshitz theory can be seen as an outer solution of a general problem involving microscopic scales as well. Based on Kaplun’s extension theorem [107], it must have a region of validity overlapping at the scales $O(r_m)$ with the inner solution corresponding to a microscopic theory operating at the length scales $\leq r_m$. This implies that the Lifshitz theory can be applied down to the intermolecular scales $O(r_m)$. While the cut-off parameter $\lambda_0$ can be determined theoretically by matching these inner and outer solutions, should a microscopic theory exist, it can also be determined empirically as done here (Sect. 4.1). The theoretical basis for such a matching comes from the employed here proper time regularization scheme (Sect. 3.1), which also makes the Coulomb potential regularized at small distances provided the cut-off parameter $\lambda_0$ is finite. Hence, when applied to dipole–dipole interaction, this regularization makes the effective potential between dipoles to be attractive at large distances and repulsive at the distances on the order of $\lambda_0$, the behaviour qualitatively similar to the Lenard-Jones potential. This observation also explains why the properly regularized Lifshitz theory with a finite cut-off parameter $\lambda_0$ can match a microscopic theory and remain quite accurate at the intermolecular distances. As demonstrated in the present work (Sect. 4), applicability of the Lifshitz theory at the length-scales $O(r_m)$ also explains its ability to capture the ST phenomena accurately. While the idea of cut-off dependence of stresses “remains provocative yet unresolved” [108], it consistently reappeared in the literature [29,56] and in the present work as well.

Extension of the theory laid out here and applicable in the Derjaguin (non-retarded) limit to the general case including next-order of magnitude retarded (Casimir) effects would be a

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13 This is typical for non-closed theories, e.g. the Navier–Stokes equations require the empirically measured viscosity coefficient.
straightforward, though technically involved, generalization of the present work. A priori, it is clear that the contribution of Casimir effects to ST should be an order of \((\lambda_0/\lambda_a)^2\) correction to the ST values predicted here in the Derjaguin approximation. Calculations of stresses and ST can also be improved by using more accurate spectral data for dielectric constants \([109]\) instead of the simplified formula \((54)\) and accounting for finite temperature corrections. The proposed approach for computation of ST can be used for finding its values in solids as well, which are not only difficult to measure in practice, but also differ from surface energies and may vary with a direction along the solid surface \([110]\).

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### A Heat kernel calculations

Let us define the new field
\[
\phi = g^{-1/4} \Phi = \varepsilon^{3/4} \Phi
\]  
(78)
and the corresponding Green’s function
\[
\mathbb{G}(\zeta; x, x') = \langle \phi(x)\phi(x') \rangle = g^{-1/4}(x) g^{-1/4}(x') \hat{G}(\zeta; x, x'),
\]  
(79)
where \(\phi(x)\) is the operator corresponding to the field \(\phi(x)\). Then, the inner product for this new field takes the covariant form
\[
\oint \mathbb{G}(\zeta; x, x') = \frac{\delta(x - x')}{\sqrt{g}}, \text{ where } \oint = g^{-1/4}(x) \hat{G}^{1/4}(x).
\]  
(80)
Taking into account that
\[
\partial_j \varepsilon^{-3/4} = \varepsilon^{-3/4} \left( \partial_j - \frac{3}{4} \eta_j \right)
\]  
(81)
\[
\partial_i \partial_j \varepsilon^{-3/4} = \varepsilon^{-3/4} \left( \partial_i \partial_j - \frac{3}{4} \eta_i \partial_j - \frac{3}{4} \eta_j \partial_i - \frac{3}{4} (\partial_i \eta_j) + \frac{9}{16} \eta_i \eta_j \right),
\]  
(82)
the new operator \(\oint\) becomes
\[
\oint = \varepsilon \delta^{ij} \left( \partial_i \partial_j - \frac{1}{2} \eta_i \partial_j \right) - \frac{3}{4} \varepsilon \delta^{ij} \left( \partial_i \eta_j + \frac{1}{4} \eta_i \eta_j \right).
\]  
(83)
Note that
\[
\nabla_k \eta^k = \varepsilon \delta^{ij} \left( \partial_i \eta_j - \frac{1}{2} \eta_i \eta_j \right) = g^{ij} \left( \partial_i \eta_j - \frac{1}{2} \eta_i \eta_j \right)
\]  
(84)
and the covariant Laplacian in metric \(g_{ij}\) reads
\[
\triangle = g^{ij} \nabla_i \nabla_j = \frac{1}{\sqrt{g}} \partial_i \left( g^{ij} \sqrt{g} \partial_j \right) = g^{ij} \left( \partial_i \partial_j - \frac{1}{2} \eta_i \partial_j \right).
\]  
(85)
Therefore, we obtain the covariant form for the operator in (80)
\[
\oint = \triangle - \nabla, \text{ where } \nabla = \frac{3}{4} \left( \nabla^k \eta_k + \frac{3}{4} \eta^k \eta_k \right) = \frac{3}{4} \varepsilon \delta^{ij} \left( \partial_i \eta_j + \frac{1}{4} \eta_i \eta_j \right).
\]  
(86)
which is Hermitian with the covariant measure $\sqrt{g}$. The potential $\mathcal{V}$ can also be obtained following the computations in [31,64], which require the knowledge of the Christoffel symbols

$$
\Gamma_{jk}^i = -\frac{1}{2} [\delta_{ij} \eta_k + \delta_{ik} \eta_j - \delta_{jk} \eta_i], \quad g^{jk} \Gamma_{jk}^i = \frac{1}{2} \varepsilon \eta_i,
$$

and the connection

$$
\omega_i = \frac{1}{2} [\eta_i + g_{ik} \varepsilon^{mn} \Gamma^k_{mn}] = \frac{3}{4} \eta_i.
$$

Heat kernel corresponding to operator $\hat{Q}$ is $\hat{K}(s|x, x') = g^{1/4}(x)g^{1/4}(x')\mathbb{K}(s|x, x')$, where

$$
\mathbb{K}(s|x, x') = -e^{s\mathcal{Q}} = -\frac{\Delta^{1/2}(x, x')}{(4\pi s)^{3/2}} e^{-\frac{\sigma(x, x')}{2s}} (a_0(x, x') + s a_1(x, x') + \ldots);
$$

here $s$ is the proper time, $\sigma(x, x')$ a world function defined as one half of the square of geodesic distance between points in the metric $g_{ij}$ and $\Delta^{1/2}(x, x') \equiv g^{-1/2}(x)\mathcal{Q}(x, x')g^{-1/2}(x')$, where $\mathcal{Q}(x, x') = -\det (-\sigma_{\mu\nu})$ is the van Vleck–Morette determinant. For the computation of the heat kernel of this operator, we need to know $\Delta^{1/2}(x, x'), a_0(x, x')$, and $a_1(x, x')$ and their derivatives. In particular they include the curvature terms:

$$
R_{ij} = \frac{1}{2} \delta_{ij} \eta_i + \frac{1}{4} \eta_i \eta_j + \frac{1}{4} \delta_{ij} \delta^{km} (2 \partial_k \eta_m - \eta_k \eta_m), \quad R = 2 \varepsilon \delta^{km} (\partial_k \eta_m - \frac{1}{4} \eta_k \eta_m);
$$

here we used the relations

$$
\eta_{i;j} = \partial_j \eta_i + \eta_i \eta_j - \frac{1}{2} \delta_{ij} \delta^{km} \eta_k \eta_m, \tag{90a}
$$

$$
\eta^{k}_{;k} = \varepsilon \delta^{ij} (\partial_j \eta_i - \frac{1}{2} \eta_i \eta_j), \quad \partial_i (g^{1/4}) = -\frac{3}{4} \varepsilon^{-3/4} \eta_i. \tag{90b}
$$

The regularized Green’s function (79), in the original notation, assumes the form

$$
\hat{G}_{\lambda_0}(\zeta; x, x') = \int_{\lambda_0}^{\infty} ds \hat{K}(s|x, x') = g^{1/4}(x)g^{1/4}(x') \int_{\lambda_0}^{\infty} ds \mathbb{K}(s|x, x'),
$$

where $\lambda_0$ is the cut-off parameter, and can be expanded as

$$
\hat{G}_{\lambda_0}(\zeta; x, x') = -\int_{\lambda_0}^{\infty} ds \frac{\Delta^{1/2}(x, x')}{(4\pi s)^{3/2}} e^{-\frac{\sigma(x, x')}{2s}} (a_0(x, x') + s a_1(x, x') + \ldots) \tag{92}
$$

Derivation of the regularized stress tensor then reduces to the following steps:

i) Compute $\Delta^{1/2}(x, x'), a_0(x, x')$, and $a_1(x, x')$;

ii) Compute the second partial derivative of the Green’s function $\partial_x \partial_x' \hat{G}_{\lambda_0}(\zeta; x, x')$;

iii) Take the limit $x = x'$;

iv) Integrate over the proper time $s$ and then expand the result in the cut-off $\lambda_0$;

v) Compute $\hat{\sigma}_{ij}(\zeta; x)$ by substituting the result to (11).

For the quantities in the limit of coincident points, we introduce notation $[\ldots] = (\ldots)_{x=x'}$. The expressions that we need to compute divergent parts (33) of the Green’s function $\hat{G}_{\lambda_0}(\zeta; x, x')$ are [111]

$$
[\sigma] = 0, \quad [\sigma_{ij}] = 0, \quad [\sigma_{ij'}] = 0, \quad [\sigma_{ij}] = g_{ij}, \quad [\sigma_{ij'}] = -g_{ij}, \tag{93a}
$$

$$
[a_0] = 1, \quad [a_{0;ij}] = 0, \quad [a_{0;ij'}] = 0, \quad [a_1] = \frac{1}{6} R - \nabla, \quad [a_{1;ij}] = \frac{1}{2} \left( \frac{1}{6} R_{ij} - \nabla_{ij} \right). \tag{93b}
$$
\[ \Delta_{1/2} = 1, \quad [(\Delta_{1/2})_{ij}] = 0, \quad [(\Delta_{1/2})_{ij}] = -\frac{1}{6} R_{ij}, \quad (93c) \]

\[ \partial_i \partial_j \left( \frac{1}{4} g^{1/4}(x) g^{1/4}(x') \Delta_{1/2} \right) = e^{-3/2} \left( \frac{9}{16} \eta_i \eta_j - \frac{1}{6} R_{ij} \right). \quad (93d) \]

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