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Hamiltonian treatment of time dispersive and dissipative media within the linear response theory

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Abstract

We develop a Hamiltonian theory for a time dispersive and dissipative (TDD) inhomogeneous medium, as described by a linear response equation respecting causality and power dissipation. The canonical Hamiltonian constructed here exactly reproduces the original dissipative evolution after integrating out auxiliary fields. In particular, for a dielectric medium we obtain a simple formula for the Hamiltonian and closed form expressions for the energy density and energy flux involving the auxiliary fields. The developed approach also allows to treat a long standing problem of scattering from a lossy non-spherical obstacle and, more generally, wave propagation in TDD media.

1. Introduction

There is an intrinsic ambiguity in identifying the field energy densities for radiation in a time dispersive and dissipative (TDD) medium as described by the linear response theory, e.g., in a dielectric medium described by the classical linear Maxwell equations with complex valued frequency dependent electric permittivity $\varepsilon(\omega)$ and magnetic permeability $\mu(\omega)$. Consequently, there are problems with the interpretation of the energy balance equation [12, Section 77; 1, Section 1.5a; 5, Section 6.8; 17]. There were a number of efforts [17,14,20] to construct a consistent macroscopic theory of dielectric media that accounts for dispersion and dissipation, based on more fundamental microscopic theories. At first sight, it seems that the introduction of a realistic material medium in an explicit form similar to [17,14,21] is the only way to model a TDD medium. In fact, that is not so and in this paper we describe a consistent macroscopic approach *within the linear response theory*. Full proofs of the statements outlined here will appear in a forthcoming paper [3].

A linear response TDD medium is an essentially open dissipative system, which in principle can be obtained by (i) eliminating some degrees of freedom from a more involved microscopic theory and (ii) making the approximation of linear response. Stopping short of introducing a microscopic theory we ask, *is there a conservative extended system which exactly reproduces the given linear TDD system after reduction?* In [2] we showed that indeed such an extension is (i) possible and (ii) essentially uniquely determined, under general conditions of causality, power dissipation,

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and minimality of the extension. Here we go further and construct a canonical Hamiltonian for such a conservative extension based only on the given TDD equations—without assumption on the underlying microstructure. In particular, we construct such a Hamiltonian for a dielectric medium as defined by complex $\varepsilon(\omega)$ and $\mu(\omega)$. The construction given here is not restricted to a dielectric medium, however, but holds for TDD systems with a certain mathematical structure—Eqs. (8)–(10)—including, in particular, elastic and acoustic media, and it can be extended to space dispersive dissipative systems. A somewhat related construction of the evolution equations for linear absorptive dielectrics was given in [27]. The range of validity of the proposed theory is the same as for the linear response, though nonlinear generalizations are clearly possible.

Other important benefits of the approach developed here are (i) The constructed Hamiltonian is an integral of a local energy density, which in the absence of TDD terms reduces to the local field energy. This permits us to derive an expression for the energy transport for TDD media. (ii) The present formulation allows to treat, in particular, a long standing problem of scattering from a lossy non-spherical scatter—analyzed by other methods with limited success [18]—by applying the well-developed scattering theory or conservative systems, see [22,26] and references therein. These applications will be discussed in detail in forthcoming work [3,4].

2. Construction of the Hamiltonian

We consider a system described by two canonical vector coordinates $p, q \in H$, with H a real Hilbert space. In the absence of TDD terms, the evolution is supposed to be induced by a Hamiltonian $A(p, q)$ of the form

$$A(p,q) = \tfrac{1}{2}\langle K_{\mathrm{p}}p, K_{\mathrm{p}}p\rangle + \tfrac{1}{2}\langle K_{\mathrm{q}}q, K_{\mathrm{q}}q\rangle, \tag{1}$$

with closed linear operators K_{p}, K_{q} from H into auxiliary spaces H_{p}, H_{q}, respectively. To manifest the conservation of energy, it is convenient to consider the evolution of

$$f_{\mathrm{p}} := K_{\mathrm{p}}p \in H_{\mathrm{p}}, \quad f_{\mathrm{q}} := K_{\mathrm{q}}q \in H_{\mathrm{q}}, \tag{2}$$

in place of p, q. In the absence of dissipation, these quantities evolve according to

$$\partial_t \begin{pmatrix} f_{\mathrm{p}} \\ f_{\mathrm{q}} \end{pmatrix} = \begin{pmatrix} 0 & -K \\ K^\dagger & 0 \end{pmatrix} \begin{pmatrix} f_{\mathrm{p}} \\ f_{\mathrm{q}} \end{pmatrix} \quad \text{zero dissipation}, \tag{3}$$

with $K := K_{\mathrm{p}}K_{\mathrm{q}}^\dagger$ a closed linear map from H_{q} to H_{p}. Note that

$$A(p,q) = \tfrac{1}{2}(\|f_{\mathrm{p}}\|^2 + \|f_{\mathrm{q}}\|^2) \tag{4}$$

is conserved due to the antisymmetry of the generator in (3).

The electromagnetic field in a non-dispersive inhomogeneous medium may be described in this framework, with $p=(4\pi)^{-1}\mathbf{A}$ (magnetic potential), $q=\mathbf{D}$ (electric displacement), $f_{\mathrm{p}}=(2\sqrt{\pi})^{-1}\mathbf{H}$ (magnetic field), and $f_{\mathrm{q}}=(2\sqrt{\pi})^{-1}\mathbf{E}$ (electric field). Identifying (2) with the material relations, we determine the action of the operators K_{w}:

$$K_{\mathrm{p}}\frac{\mathbf{A}}{4\pi}(\vec{r}) = (2\sqrt{\pi})\mu^{-1}(\vec{r})\cdot\left\{\nabla\times\frac{\mathbf{A}}{4\pi}(\vec{r})\right\}, \quad K_{\mathrm{q}}\mathbf{D}(\vec{r}) = \frac{1}{2\sqrt{\pi}}\varepsilon^{-1}(\vec{r})\cdot\mathbf{D}(\vec{r}), \tag{5}$$

where μ, ε are the static permeability and dielectric tensors, assumed real and symmetric. We take $(4\pi)^{-1}\mathbf{A}$ and $\mathbf{D}$ in the space $H = H_{\mathrm{curl}}$ of divergence free vector fields—which amounts to a choice of gauge and an assumption of no free charges. To complete the picture we define H_{p}, H_{q} to be weighted L^2 spaces with scalar products

$$\langle \mathbf{H}, \mathbf{H}\rangle_{H_{\mathrm{p}}} = \int \mathrm{d}^3\vec{r}\,\mathbf{H}(\vec{r})\cdot\mu(\vec{r})\cdot\mathbf{H}(\vec{r}), \quad \langle \mathbf{E}, \mathbf{E}\rangle_{H_{\mathrm{q}}} = \int \mathrm{d}^3\vec{r}\,\mathbf{E}(\vec{r})\cdot\varepsilon(\vec{r})\cdot\mathbf{E}(\vec{r}). \tag{6}$$

As a result

$$K_{\mathrm{p}}^\dagger = (2\sqrt{\pi})\nabla\times, \quad K_{\mathrm{q}}^\dagger = \frac{1}{2\sqrt{\pi}}P_{\mathrm{curl}}, \quad K = \mu^{-1}(\vec{r})\cdot\nabla\times, \quad K^\dagger = \varepsilon^{-1}(\vec{r})\cdot\nabla\times, \tag{7}$$

with P_{curl} the orthogonal projection of $(L^2)^3$ onto H_{curl}.

An alternative formulation of the general system (1) is suggested by the example of the EM field, namely to consider (2) as generalized material relations together with evolution equations

$$\partial_t \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 & -K_{\mathrm{q}}^\dagger \\ K_{\mathrm{p}}^\dagger & 0 \end{pmatrix} \begin{pmatrix} f_{\mathrm{p}} \\ f_{\mathrm{q}} \end{pmatrix}. \tag{8}$$

In turn, this suggests a natural modification incorporating dispersion and dissipation by replacing (2) with

$$f_{\mathrm{w}}(t) + \int_0^\infty \mathrm{d}\tau\, \chi_{\mathrm{w}}(\tau) f_{\mathrm{w}}(t-\tau) = K_{\mathrm{w}} w(t) \quad \text{for } w = p, q, \quad \mathrm{w} = \mathrm{p}, \mathrm{q}. \tag{9}$$

The TDD character of (9) comes from the *operator valued generalized susceptibilities* χ_{w}, $\mathrm{w} = \mathrm{p}, \mathrm{q}$, the integrals of which explicitly satisfy the *causality condition*: values of $K_{\mathrm{w}} w(t)$ depend only on $f_{\mathrm{w}}(t')$ for times $t' \leqslant t$.

Our main result is the following: *Assume the susceptibilities* χ_{w} *satisfy the following power dissipation condition* (*PDC*):

$$\mathrm{Im}\{\zeta \hat{\chi}_{\mathrm{w}}(\zeta)\} = \frac{1}{2\mathrm{i}} \{\zeta \hat{\chi}_{\mathrm{w}}(\zeta) - \zeta^* \hat{\chi}_{\mathrm{w}}(\zeta)^\dagger\} \geqslant 0, \quad \mathrm{w} = \mathrm{p}, \mathrm{q} \text{ for all } \zeta = \omega + \mathrm{i}\eta, \quad \eta \geqslant 0, \tag{10}$$

for all $\zeta = \omega + \mathrm{i}\eta$, $\eta \geqslant 0$, *where* $\hat{\chi}_{\mathrm{w}}$ *is the Fourier–Laplace transform of* χ_{w}:

$$\hat{\chi}_{\mathrm{w}}(\zeta) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\zeta t} \chi_{\mathrm{w}}(t), \quad \mathrm{w} = \mathrm{p}, \mathrm{q}. \tag{11}$$

Then it is possible to construct a Hamiltonian extension to (1), *which reduces to* (1) *in the limit of zero susceptibility*, *such that the subsystem* p, q *evolves according to* (8), (9).

The extended Hamiltonian $\mathscr{H}(P, Q)$ is a function of extended momentum P and coordinate Q variables, each taking values in a Hilbert space $\mathscr{H} \supset H$, and has the same structure as (1), i.e.,

$$\mathscr{H}(P, Q) = \tfrac{1}{2} \langle \mathscr{K}_{\mathrm{p}} P, \mathscr{K}_{\mathrm{p}} P \rangle + \tfrac{1}{2} \langle \mathscr{K}_{\mathrm{q}} Q, \mathscr{K}_{\mathrm{q}} Q \rangle, \tag{12}$$

with $\mathscr{K}_{\mathrm{p}}$, $\mathscr{K}_{\mathrm{q}}$ closed operators from $\mathscr{H}$ to $\mathscr{H}_{\mathrm{p}} \supset H_{\mathrm{p}}$, $\mathscr{H}_{\mathrm{q}} \supset H_{\mathrm{q}}$, which extend K_{p} and K_{q}, respectively (see (48) below).

Before presenting the general construction, let us illustrate it with the example of a linear TDD dielectric medium, described by the macroscopic Maxwell equations without external charges and currents

$$\partial_t \mathbf{D} = \nabla \times \mathbf{H}, \quad \partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \quad \nabla \cdot \mathbf{B} = 0, \quad \nabla \cdot \mathbf{D} = 0, \tag{13}$$

in units with $c, \varepsilon_0, \mu_0 = 1$. Here

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P}, \quad \mathbf{B} = \mathbf{H} + 4\pi \mathbf{M}, \tag{14}$$

with the polarization $\mathbf{P}$ and magnetization $\mathbf{M}$ given by linear response

$$\mathbf{P}(\vec{r}, t) = \int_0^\infty \mathrm{d}\tau\, \chi_{\mathrm{E}}(\vec{r}, \tau) \mathbf{E}(\vec{r}, t-\tau), \quad \mathbf{M}(\vec{r}, t) = \int_0^\infty \mathrm{d}\tau\, \chi_{\mathrm{H}}(\vec{r}, \tau) \mathbf{H}(\vec{r}, t-\tau). \tag{15}$$

The electric and magnetic susceptibilities should satisfy the PDC (10) for each $\vec{r}$, and for simplicity we take them to be real valued scalars. (The frequency domain susceptibilities $\widehat{\chi}_{\mathrm{F}}(\omega)$ may nonetheless be complex.)

Motivated by [2] and the Lamb model (see Fig. 1 below), we introduce canonical variables

$$P = ((4\pi)^{-1} \mathbf{A}(\vec{r}), \boldsymbol{\theta}_{\mathrm{E}}(\vec{r}, s), \boldsymbol{\varphi}_{\mathrm{H}}(\vec{r}, s)), \quad Q = (\mathbf{D}(\vec{r}), \boldsymbol{\varphi}_{\mathrm{E}}(\vec{r}, s), \boldsymbol{\theta}_{\mathrm{H}}(\vec{r}, s)), \tag{16}$$

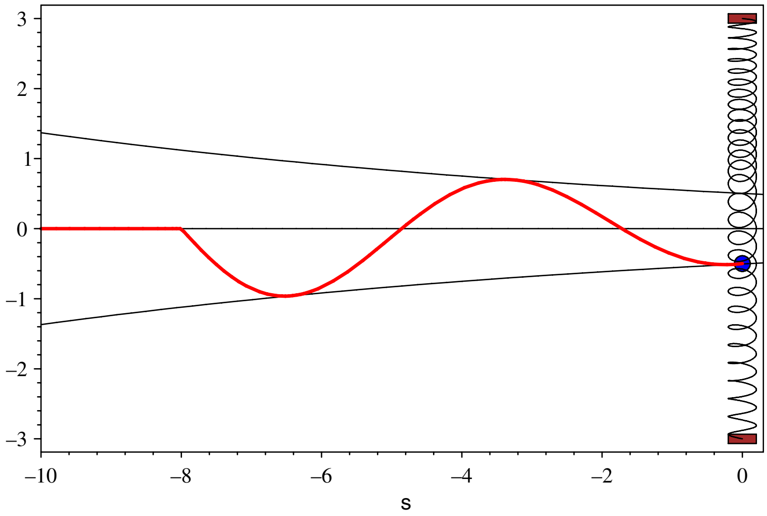

Fig. 1. The Lamb model, introduced in [10] to describe radiation damping, is a point mass attached to an infinite elastic string and a Hook's law spring. The point mass evolves as a classical linearly damped oscillator.

with $\mathbf{A}, \mathbf{D} \in H_{\text{curl}}$ and auxiliary vector fields $\boldsymbol{\varphi}_{\mathrm{F}}, \boldsymbol{\theta}_{\mathrm{F}}$, $\mathrm{F} = \mathrm{E}, \mathrm{H}$, which are functions of $\vec{r}$ and an auxiliary coordinate $-\infty < s < \infty$. For these variables we define a Hamiltonian

$$\mathscr{H}(P, Q) = \mathscr{T}(P) + \mathscr{U}(Q), \tag{17}$$

with,

$$\begin{aligned} \mathscr{T}(P) &= \frac{1}{2} \int \mathrm{d}^3\vec{r} \left| 2\sqrt{\pi}\, \nabla \times \frac{\mathbf{A}(\vec{r})}{4\pi} - \int_{-\infty}^{\infty} \mathrm{d}s\, \varsigma_{\mathrm{H}}(\vec{r}, s) \boldsymbol{\varphi}_{\mathrm{H}}(\vec{r}, s) \right|^2 \\ &+ \frac{1}{2} \int \mathrm{d}^3\vec{r} \int_{-\infty}^{\infty} \mathrm{d}s [|\boldsymbol{\theta}_{\mathrm{E}}(\vec{r}, s)|^2 + |\partial_s \boldsymbol{\varphi}_{\mathrm{H}}(\vec{r}, s)|^2], \end{aligned} \tag{18}$$

$$\begin{aligned} \mathscr{U}(Q) &= \frac{1}{2} \int \mathrm{d}^3\vec{r} \left| \frac{1}{2\sqrt{\pi}} \mathbf{D}(\vec{r}) - \int_{-\infty}^{\infty} \mathrm{d}s\, \varsigma_{\mathrm{E}}(\vec{r}, s) \boldsymbol{\varphi}_{\mathrm{E}}(\vec{r}, s) \right|^2 \\ &+ \frac{1}{2} \int \mathrm{d}^3\vec{r} \int_{-\infty}^{\infty} \mathrm{d}s [|\partial_s \boldsymbol{\varphi}_{\mathrm{E}}(\vec{r}, s)|^2 + |\boldsymbol{\theta}_{\mathrm{H}}(\vec{r}, s)|^2], \end{aligned} \tag{19}$$

where ς_{F}, $\mathrm{F} = \mathrm{E}, \mathrm{H}$, are scalar functions to be specified below.

The resulting Hamilton equations of motion for the extended Maxwell system are

$$\begin{aligned} &\partial_t \frac{\mathbf{A}(\mathbf{r}, t)}{4\pi} = -\frac{1}{4\pi} [\mathbf{D}(\mathbf{r}, t) - 2\sqrt{\pi} \langle \varsigma_{\mathrm{E}}, \boldsymbol{\varphi}_{\mathrm{E}} \rangle_s (\mathbf{r}, t)], \\ &\partial_t \boldsymbol{\varphi}_{\mathrm{H}}(\mathbf{r}, s) = -\boldsymbol{\theta}_{\mathrm{H}}(\mathbf{r}, s), \end{aligned} \tag{20}$$

$$\begin{aligned} &\partial_t \boldsymbol{\theta}_{\mathrm{E}}(\mathbf{r}, s) = \frac{1}{2\sqrt{\pi}} \varsigma_{\mathrm{E}}(\mathbf{r}, s) [\mathbf{D}(\mathbf{r}, t) - 2\sqrt{\pi} \langle \varsigma_{\mathrm{E}}, \boldsymbol{\varphi}_{\mathrm{E}} \rangle_s (\mathbf{r}, t)] + \partial_s^2 \boldsymbol{\varphi}_{\mathrm{E}}(\mathbf{r}, s), \\ &\partial_t \mathbf{D}(\mathbf{r}, t) = \nabla \times [\nabla \times \mathbf{A}(\mathbf{r}, t) - 2\sqrt{\pi} \langle \varsigma_{\mathrm{H}}, \boldsymbol{\varphi}_{\mathrm{H}} \rangle_s (\mathbf{r}, t)], \\ &\partial_t \boldsymbol{\theta}_{\mathrm{H}}(\mathbf{r}, s) = -\frac{1}{2\sqrt{\pi}} \varsigma_{\mathrm{H}}(\mathbf{r}, s) [\nabla \times \mathbf{A}(\mathbf{r}, t) - 2\sqrt{\pi} \langle \varsigma_{\mathrm{H}}, \boldsymbol{\varphi}_{\mathrm{H}} \rangle_s (\mathbf{r}, t)] - \partial_s^2 \boldsymbol{\varphi}_{\mathrm{H}}(\mathbf{r}, s), \\ &\partial_t \boldsymbol{\varphi}_{\mathrm{E}}(\mathbf{r}, s) = \boldsymbol{\theta}_{\mathrm{E}}(\mathbf{r}, s), \end{aligned} \tag{21}$$

where

$$\langle \bullet, \bullet \rangle_s = \int \bullet \bullet \, \mathrm{d}s. \tag{22}$$

We make the identifications:

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t), \tag{23}$$
$$\mathbf{H}(\mathbf{r}, t) = \mathbf{B}(\mathbf{r}, t) - 2\sqrt{\pi}\langle \varsigma_{\mathrm{H}}, \boldsymbol{\varphi}_{\mathrm{H}} \rangle_s(\mathbf{r}, t) = \mathbf{B}(\mathbf{r}, t) - 4\pi\mathbf{M}(\mathbf{r}, t), \tag{24}$$
$$\mathbf{E}(\mathbf{r}, t) = \mathbf{D}(\mathbf{r}, t) - 2\sqrt{\pi}\langle \varsigma_{\mathrm{E}}, \boldsymbol{\varphi}_{\mathrm{E}} \rangle_s(\mathbf{r}, t) = \mathbf{D}(\mathbf{r}, t) - 4\pi\mathbf{P}(\mathbf{r}, t),$$

with

$$\langle \varsigma_{\mathrm{H}}, \boldsymbol{\varphi}_{\mathrm{H}} \rangle_s(\mathbf{r}, t) = 2\sqrt{\pi}\mathbf{M}(\mathbf{r}, t), \quad \langle \varsigma_{\mathrm{E}}, \boldsymbol{\varphi}_{\mathrm{E}} \rangle_s(\mathbf{r}, t) = 2\sqrt{\pi}\mathbf{P}(\mathbf{r}, t), \tag{25}$$

resulting in the following equivalent system of extended Maxwell equations:

$$\partial_t \mathbf{H}(\mathbf{r}, t) = -\nabla \times \mathbf{E}(\mathbf{r}, t) + 2\sqrt{\pi}\langle \varsigma_{\mathrm{H}}, \boldsymbol{\theta}_{\mathrm{H}} \rangle_s(\mathbf{r}, t), \tag{26}$$
$$\partial_t \boldsymbol{\varphi}_{\mathrm{H}}(\mathbf{r}, s) = -\boldsymbol{\theta}_{\mathrm{H}}(\mathbf{r}, s), \quad \partial_t \boldsymbol{\theta}_{\mathrm{E}}(\mathbf{r}, s) = \frac{1}{2\sqrt{\pi}} \varsigma_{\mathrm{E}}(\mathbf{r}, s)\mathbf{E}(\mathbf{r}, t) + \partial_s^2 \boldsymbol{\varphi}_{\mathrm{E}}(\mathbf{r}, s),$$
$$\partial_t \mathbf{E}(\mathbf{r}, t) = \nabla \times \mathbf{H}(\mathbf{r}, t) - 2\sqrt{\pi}\langle \varsigma_{\mathrm{E}}, \boldsymbol{\theta}_{\mathrm{E}} \rangle_s(\mathbf{r}, t), \tag{27}$$
$$\partial_t \boldsymbol{\theta}_{\mathrm{H}}(\mathbf{r}, s) = -\frac{1}{2\sqrt{\pi}} \varsigma_{\mathrm{H}}(\mathbf{r}, s)\mathbf{H}(\mathbf{r}, t) - \partial_s^2 \boldsymbol{\varphi}_{\mathrm{H}}(\mathbf{r}, s), \quad \partial_t \boldsymbol{\varphi}_{\mathrm{E}}(\mathbf{r}, s) = \boldsymbol{\theta}_{\mathrm{E}}(\mathbf{r}, s).$$

Combining the first order Hamilton equations of motion for $\boldsymbol{\varphi}_{\mathrm{F}}$ and $\boldsymbol{\theta}_{\mathrm{F}}$ into a single second order equation for $\boldsymbol{\varphi}_{\mathrm{F}}$, $\mathrm{F} = \mathrm{E}, \mathrm{H}$, we obtain a driven wave equation

$$\{\partial_t^2 - \partial_s^2\}\boldsymbol{\varphi}_{\mathrm{F}}(\vec{r}, s, t) = \frac{1}{2\sqrt{\pi}} \varsigma_{\mathrm{F}}(\vec{r}, s)\mathbf{F}(\vec{r}, t), \quad \mathrm{F} = \mathrm{E}, \mathrm{H}. \tag{28}$$

Assuming $\boldsymbol{\varphi}_{\mathrm{F}}$ to be at rest ($\boldsymbol{\varphi}_{\mathrm{F}} = \partial_t \boldsymbol{\varphi}_{\mathrm{F}} = 0$) in the distant past, the solution to (28) is given by

$$\boldsymbol{\varphi}_{\mathrm{F}}(\vec{r}, s, t) = \frac{1}{4\sqrt{\pi}} \int_0^\infty \mathrm{d}\tau \int_{s-\tau}^{s+\tau} \mathrm{d}\sigma \, \varsigma_{\mathrm{F}}(\vec{r}, \sigma)\mathbf{F}(\vec{r}, t-\tau), \quad \mathrm{F} = \mathrm{E}, \mathrm{H}, \tag{29}$$

implying with (15) and (25) the following expression for the susceptibilities:

$$\chi_{\mathrm{F}}(\vec{r}, t) = \frac{1}{8\pi} \int_{-\infty}^\infty \mathrm{d}s \int_{s-t}^{s+t} \mathrm{d}\sigma \, \varsigma_{\mathrm{F}}(\vec{r}, s)\varsigma_{\mathrm{F}}(\vec{r}, \sigma), \quad \mathrm{F} = \mathrm{E}, \mathrm{H}. \tag{30}$$

The key fact is that, due to the PDC (10), it is possible to invert (30) and write ς_{F} as a function of χ_{F}. An explicit solution is

$$\varsigma_{\mathrm{F}}(\vec{r}, s) = \frac{2}{\sqrt[4]{2\pi}} \int_{-\infty}^\infty \mathrm{d}\omega \, \mathrm{e}^{-\mathrm{i}\omega s} \sqrt{\omega \, \mathrm{Im} \, \hat{\chi}_{\mathrm{F}}(\vec{r}, \omega + \mathrm{i}0)}, \quad \mathrm{F} = \mathrm{E}, \mathrm{H}. \tag{31}$$

Note that ς_{F} is real and invariant under $s \mapsto -s$.

The above discussion implies the following result on the extended system: *let the Hamiltonian* (17)–(19) *be given with* ς_{F} *defined by* (31) *for* χ_{F} *which obey* (10). *Then for any solution to the Hamilton equations of motion with* $\varphi_{\mathrm{F}}, \theta_{\mathrm{F}} \to 0$ *as* $t \to -\infty$, *the variables* $\mathbf{D}(\vec{r}, t)$ *and* $\mathbf{B}(\vec{r}, t) = \nabla \times \mathbf{A}(\vec{r}, t)$ *evolve according to the macroscopic Maxwell equations* (13)–(15).

Based on the constructed TDD Hamiltonian (17), we obtain an expression for the energy density of the EM field and the medium

$$\mathscr{E}(\vec{r},t)=\frac{1}{8\pi}\{|\mathbf{E}|^2+|\mathbf{H}|^2\}(\vec{r},t)+\frac{1}{2}\{\|\partial_s\boldsymbol{\varphi}_{\mathrm{H}}\|_s^2+\|\boldsymbol{\theta}_{\mathrm{H}}\|_s^2+\|\partial_s\boldsymbol{\varphi}_{\mathrm{E}}\|_s^2+\|\boldsymbol{\theta}_{\mathrm{E}}\|_s^2\}(\vec{r},t), \tag{32}$$

where

$$\|\bullet\|_s^2=\int|\bullet|^2\,\mathrm{d}s. \tag{33}$$

This results in the conservation law

$$\partial_t\mathscr{E}+\nabla\cdot\mathbf{S}=0, \tag{34}$$

with the familiar Poynting vector for the energy flux

$$\mathbf{S}(\vec{r},t)=\frac{1}{4\pi}\mathbf{E}(\vec{r},t)\times\mathbf{H}(\vec{r},t). \tag{35}$$

These identities follow from (17)–(19) and the general theory of Hamiltonian fields [11].

When the interaction ς is set to zero, the EM and auxiliary fields decouple and (32) reduces to

$$\mathscr{E}_0(\vec{r},t)=\mathscr{E}_{\mathrm{EM}}(\vec{r},t)+\mathscr{E}_{\mathrm{S}}(\vec{r},t), \tag{36}$$

with the energy density of the EM field

$$\mathscr{E}_{\mathrm{EM}}(\vec{r},t)=\frac{1}{8\pi}|\mathbf{D}|^2(\vec{r},t)+\frac{1}{8\pi}|\nabla\times\mathbf{A}|^2(\vec{r},t), \tag{37}$$

and the energy density of the auxiliary fields

$$\mathscr{E}_{\mathrm{S}}(\vec{r},t)=\tfrac{1}{2}\{\|\partial_s\boldsymbol{\varphi}_{\mathrm{H}}\|_s^2+\|\boldsymbol{\theta}_{\mathrm{H}}\|_s+\|\partial_s\boldsymbol{\varphi}_{\mathrm{E}}\|_s^2+\|\boldsymbol{\theta}_{\mathrm{E}}\|_s^2\}(\vec{r},t). \tag{38}$$

Subtracting (36) from (32) gives the energy shift due to the interaction of the EM field and the matter

$$\delta\mathscr{E}(\vec{r},t)=\frac{1}{8\pi}\{|\mathbf{E}(\mathbf{r},t)|^2-|\mathbf{D}(\mathbf{r},t)|^2+|\mathbf{H}(\mathbf{r},t)|^2-|\mathbf{B}(\mathbf{r},t)|^2\}. \tag{39}$$

In general, it is not possible to give an expression for the energy density $\mathscr{E}_{\mathrm{S}}(\vec{r},t)$ of the medium in terms of the instantaneous EM fields $\mathbf{E}(\vec{r},t)$ and $\mathbf{H}(\vec{r},t)$. However, using (29), (30) and the equations of motion we have calculated that

$$\partial_t\frac{1}{2}\{\|\partial_s\boldsymbol{\varphi}_{\mathrm{F}}\|_{\mathrm{s}}^2+\|\boldsymbol{\theta}_{\mathrm{F}}\|_{\mathrm{s}}^2\}(\vec{r},t)=\frac{1}{2\sqrt{\pi}}[\partial_t\langle\varsigma_{\mathrm{F}},\boldsymbol{\varphi}_{\mathrm{F}}\rangle(\vec{r},t)]\cdot\mathbf{F}(\vec{r},t) \tag{40}$$

$$=[\partial_t\mathbf{P}(\vec{r},t)]\cdot\mathbf{E}(\vec{r},t),\quad \mathrm{F}=\mathrm{E}, \tag{41}$$

with a similar expression for $\mathrm{F}=\mathrm{H}$.

The result (41) is the usual expression for the rate of change the density of EM energy stored in a dielectric. For a wave packet $\mathbf{E}(\vec{r},t)=\mathrm{Re}\,\{\mathrm{e}^{-\mathrm{i}\omega_0 t}\mathbf{E}_0(\vec{r},t)\}$ with $\mathbf{E}_0(\vec{r},t)$ a slowly varying function of t, we have

$$\partial_t\mathbf{P}(\vec{r},t)\approx\sqrt{2\pi}\,\mathrm{Re}\left\{-\mathrm{i}\omega_0\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)\mathrm{e}^{-\mathrm{i}\omega_0 t}\mathbf{E}_0(\vec{r},t)+\frac{\mathrm{d}\omega_0\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)}{\mathrm{d}\omega_0}\,\mathrm{e}^{-\mathrm{i}\omega_0 t}\partial_t\mathbf{E}_0(\vec{r},t)\right\}, \tag{42}$$

and thus

$$[\partial_t \mathbf{P}(\vec{r},t)]\cdot\mathbf{E}(\vec{r},t) \approx \frac{\sqrt{2\pi}}{2}\,\mathrm{Re}\left\{-\mathrm{i}\omega_0\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)|\mathbf{E}_0(\vec{r},t)|^2 + \frac{\mathrm{d}\omega_0\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)}{\mathrm{d}\omega_0}[\partial_t\mathbf{E}_0(\vec{r},t)]\cdot\mathbf{E}_0^*(\vec{r},t)\right\} + \text{terms with a factor of } \mathrm{e}^{-\mathrm{i}\omega_0 t} \text{ or } \mathrm{e}^{\mathrm{i}\omega_0 t}. \tag{43}$$

If we consider the *time averaged* power density, averaged over a time scale longer than $1/\omega_0$, the terms with oscillatory factors are very small and we have (with $\overline{\bullet}$ denoting time averaging):

$$\overline{[\partial_t \mathbf{P}(\vec{r},t)]\cdot\mathbf{E}(\vec{r},t)} \approx \sqrt{\frac{\pi}{2}}\left\{\frac{1}{2}\left[\frac{\mathrm{d}}{\mathrm{d}\omega_0}\,\omega_0\,\mathrm{Re}\,\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)\right]\partial_t|\mathbf{E}_0(\vec{r},t)|^2 + \omega_0\,\mathrm{Im}\,\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)|\mathbf{E}_0(\vec{r},t)|^2\right\}, \tag{44}$$

where we have assumed for simplicity that the slowly varying function $\mathbf{E}_0(\vec{r},t)$ is real. The first term on the r.h.s. of (44) is a total derivative, which when integrated gives the Brillouin formula for the time averaged energy density in a material medium (see [12, Section 80]):

$$\frac{\sqrt{2\pi}}{4}\left[\frac{\mathrm{d}}{\mathrm{d}\omega_0}\omega_0\,\mathrm{Re}\,\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)\right]|\mathbf{E}_0(\vec{r},t)|^2, \tag{45}$$

which neglects losses entirely, and hence is useful only if $\mathrm{Im}\,\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)$ is zero or so small as to be irrelevant. The second term of (44) is strictly positive and gives the contribution

$$\sqrt{\frac{\pi}{2}}\omega_0\,\mathrm{Im}\,\widehat{\chi}_{\mathrm{E}}(\vec{r},\omega_0)\int_{-\infty}^{t}|\mathbf{E}_0(\vec{r},\tau)|^2\,\mathrm{d}\tau \tag{46}$$

to the time averaged material energy density, which is non-decreasing in time and incorporates losses in an approximate way.

For a general system of the form (8)–(10), a TDD Hamiltonian can be constructed in the same way. We define canonical variables

$$P=(p,\theta_{\mathrm{q}},\varphi_{\mathrm{p}}),\qquad Q=(q,\varphi_{\mathrm{q}},\theta_{\mathrm{p}}), \tag{47}$$

with $\theta_{\mathrm{w}}(s)$, $\varphi_{\mathrm{w}}(s)$ functions of an auxiliary coordinate $-\infty<s<\infty$, taking values in the Hilbert spaces H_{w}, $\mathrm{w}=\mathrm{p},\mathrm{q}$. If $\chi_{\mathrm{w}}(t)=\chi_{\mathrm{w}}(t)^{\dagger}$ for all $t\geqslant 0$, the Hamiltonian is of the form (12), with

$$\begin{aligned}\mathscr{K}_{\mathrm{p}}P &= \left(K_{\mathrm{p}}p-\int_{-\infty}^{\infty}\mathrm{d}s\,\varsigma_{\mathrm{p}}(s)\varphi_{\mathrm{p}}(s),\theta_{\mathrm{q}},\partial_s\varphi_{\mathrm{p}}\right),\\ \mathscr{K}_{\mathrm{q}}Q &= \left(K_{\mathrm{q}}q-\int_{-\infty}^{\infty}\mathrm{d}s\,\varsigma_{\mathrm{q}}(s)\varphi_{\mathrm{q}}(s),\partial_s\varphi_{\mathrm{q}},\theta_{\mathrm{p}}\right),\end{aligned} \tag{48}$$

where

$$\hat{\varsigma}_{\mathrm{w}}(\omega)=(2\pi)^{-1/4}\sqrt{2\omega\,\mathrm{Im}\,\chi_{\mathrm{w}}(\omega+\mathrm{i}0)},\qquad \mathrm{w}=\mathrm{p},\mathrm{q}, \tag{49}$$

with $\sqrt{\bullet}$ the operator square root.

In particular, we can handle it this way: (i) Non-isotropic media, provided the tensors χ_{w} are real symmetric. (Gyrotropy could in principle be handled by a more involved construction with terms mixing momenta and coordinates.) (ii) Space dispersion, in which case terms depending on $\nabla\boldsymbol{\varphi}$ and $\nabla\boldsymbol{\theta}$ appear in the Hamiltonian. Details of the abstract construction and further examples will be given in forthcoming work [3].

3. Discussion and comparison with prior work

The need for a Hamiltonian description of a dissipative system has long been known, having been emphasized by Morse and Feshbach [19, Chapter 3.2] 40 years ago. They constructed, for a damped oscillator, an artificial Hamiltonian based on a "mirror-image" trick, incorporating a second oscillator with negative friction. The resulting Hamiltonian is quite unphysical: it is unbounded from below and under time reversal the oscillator is transformed into its "mirror-image." The artificial nature of this construction was described in [19, Chapter 3.2]: "By this arbitrary trick we are able to handle dissipative systems as though they were conservative. This is not very satisfactory if an alternate method of solution is known..."

The Hamiltonian we construct for TDD media can be viewed as a quite general "satisfactory solution" to the problem posed in [19, Chapter 3.2] since *we do not introduce negative friction* and, in particular, we do not make use of "mirror-images." Instead we couple a given TDD system to an effective model for the normal modes of the underlying medium. For the combined system we give a non-negative Hamiltonian with a transparent interpretation as the system energy. As regards the underlying microscopic theory, this is an effective Hamiltonian for those modes well approximated by linear response.

The evolution equations of the proposed theory come from a Hamiltonian and are thus time reversible. Nonetheless, an irreversible motion of the TDD system stems from the infinite heat capacity of the auxiliary system. This is demonstrated in its simplest form by the damped harmonic oscillator

$$m\partial_t^2 q(t) + \gamma\partial_t q(t) + kq(t) = 0, \tag{50}$$

which results from the TDD system

$$\partial_t \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} -f_{\mathrm{q}} \\ f_{\mathrm{p}} \end{pmatrix}, \quad \begin{pmatrix} f_{\mathrm{p}}(t) + \gamma \int_0^\infty f_{\mathrm{p}}(t-\tau)\,\mathrm{d}\tau \\ f_{\mathrm{q}}(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{m}} p(t) \\ \sqrt{k} q(t) \end{pmatrix}, \tag{51}$$

with $m, k, \gamma > 0$. The construction presented above reproduces in this simple case a model due to Lamb in 1900 [10]—see Fig. 1—in which the energy of an oscillator escapes to infinity along an attached flexible string. The theory proposed here illustrates that, from the standpoint of thermodynamics, dissipation in classical linear response is an idealization which assumes infinite heat capacity of (hidden) degrees of freedom.

In general, the auxiliary system, described by the fields $\{\varphi_{\mathrm{p}}, \varphi_{\mathrm{q}}, \theta_{\mathrm{p}}, \theta_{\mathrm{q}}\}$, is governed by a Hamiltonian $\mathrm{H_{hb}}(\varphi, \theta)$ of the following simple and universal form:

$$\mathrm{H_{hb}}(\varphi, \theta) = \frac{1}{2}\int_0^\infty [\|\theta(s)\|^2_{H_{\mathrm{p}}\oplus H_{\mathrm{q}}} + \|\partial_s \varphi(s)\|^2_{H_{\mathrm{p}}\oplus H_{\mathrm{q}}}]\,\mathrm{d}s. \tag{52}$$

The Hamiltonian $\mathrm{H_{hb}}(\varphi, \theta)$ in (52) is a *canonical heat bath* (justifying the index hb) as described in [6, Section 2; 25, Section 2].

The physical concept of an ideal or canonical heat bath originates in thermodynamics. Statistical mechanical models at the mathematical level of rigor were introduced, motivated, and described rather recently (to our best knowledge), see [7, Section 1; 6, Section 2; 25, Section 2] and references therein. The consensus among the references, on the basis of statistical mechanics, is that the generator of motion for a canonical heat bath must be $\mathrm{i}\times$ a self-adjoint operator with absolutely continuous spectrum with no gaps, i.e., the spectrum must be the entire real line $\mathbb{R}$, and the spectrum must be of a uniform multiplicity. These requirements lead to a system unitarily equivalent to the universal form Hamiltonian (52), [6, Section 2].

General statistical mechanics considerations indicate that for a system to behave according the thermodynamics it must be properly coupled to the heat bath. In particular, the coupling should involve all modes of the heat bath, [7, Section 1; 6, Section 2; 25, Section 2]. In our Hamiltonian setting the coupling is essentially $\langle K_{\mathrm{w}} w, T_{\mathrm{w}}\varphi_{\mathrm{w}}\rangle$, which is the *dipole approximation*, [25, Section 1,2], and the condition of coupling to all modes is the following constraint on the dissipation:

$$\overline{\bigcup_{\omega\in\mathbb{R}} \operatorname{Ran}\operatorname{Im}\widehat{\chi}_{\mathrm{w}}(\omega)} = H_{\mathrm{w}}, \quad \mathrm{w} = \mathrm{p}, \mathrm{q}. \tag{53}$$

There is some relation in spirit between our theory and a recently proposed hydrodynamic theory (HT) [16,9,8]. Both theories are self contained, macroscopic, and make no assumption on the underlying microstructure. However, the theory proposed here, unlike the HT, makes no use of parameters other than the susceptibilities of linear response theory. Furthermore, the present theory is truly conservative, with dissipative effects modeled by effectively irreversible energy transport to an auxiliary system, which may be conceived of as constructed from flexible strings. In contrast, the HT makes use of explicitly dissipative, nonconservative equations similar to those of Navier–Stokes.

A deeper relation can be found between the approach described here and the well known dilation theory which, in certain cases, provides a treatment for dissipation and resonance phenomena. We first give a brief account of the dilation theory, based on Pavlov's extensive review [23] as well as his more recent work [24]. For more detailed exposition on the subject we refer the reader to [23,24] and references therein.

The dilation theory was the first rather general approach to the construction of a spectral theory for dissipative operators. It is based on an abstract version of the Lax–Phillips scattering theory [13,15] which assumes that there are (i) a dynamical unitary evolution group $U_t = \mathrm{e}^{\mathrm{i}\Omega t}$ in a Hilbert space H where Ω is a self-adjoint operator in H; (ii) an "*incoming*" subspace $D_- \subset H$ invariant with respect to the semi-group U_t, $t < 0$, and an "*outgoing*" subspace $D_+ \subset H$ invariant with respect to the semi-group U_t, $t > 0$. The invariant subspaces (also called *scattering channels*) $D_\pm$ *are assumed to be orthogonal*. Then one introduces the "*observation*" subspace $K = H \ominus (D_- \oplus D_+)$ which is coinvariant in the sense that the restriction of U_t, $t > 0$, to K is a well defined semigroup on its own, namely for $t > 0$

$$Z_t = P_K U_t|_K = \mathrm{e}^{\mathrm{i}Bt} \quad \text{where } P_K \text{ is the orthogonal projection on } K. \tag{54}$$

In many interesting cases the generator B of the semigroup Z_t is dissipative, i.e., $\operatorname{Im} B \geqslant 0$ or, even, $\operatorname{Im} B > 0$. So the relation (54) provides an interesting scenario within the Lax–Phillips scattering theory for the rise of a dissipative operator. The dilation theory yields the spectral theory through the construction of generalized eigenmodes (the scattering theory) provided, of course, the conditions discussed above are satisfied.

Looking at the dilation theory from the point of view of open (dispersive and dissipative) systems, one can ask if the theory allows to find the unitary group $U_t = \mathrm{e}^{\mathrm{i}\Omega t}$ or, equivalently, the self-adjoint operator Ω being given the dissipative operator B? The answer is positive for rather large class of dissipative operators B. For example, if $B = \Omega_0 + \mathrm{i}a$, where Ω_0 is self-adjoint and $a \geqslant 0$ is bounded, a unique minimal dilation and its eigenmodes can effectively constructed [24, Theorem 3].

Hence when the dilation theory applies it provides a solid foundation for spectral studies. Unfortunately, the dilation theory does not apply to many important physical problems simply because its initial assumptions on the nature of the dissipation are too restrictive. For systems described by evolution equations (8)–(9) the dissipation always comes with the dispersion, and the dilation theory does not apply. Indeed, the most general form for a linear causal time-homogeneous *open system*, as analyzed in [2], is

$$m\partial_t v(t) = -\mathrm{i}Av(t) - \int_0^\infty a(\tau)v(t-\tau)\,\mathrm{d}\tau + f(t), \quad v(t) \in H_0, \tag{55}$$

where H_0 is a Hilbert space, $m > 0$ and Ω are self-adjoint operators in H_0, $f(t)$ is an external force and $a(t)$ is the *friction function*, subject to a PDC

$$\operatorname{Re} \int_0^\infty \int_0^\infty \overline{v(t)}a(\tau)v(t-\tau)\,\mathrm{d}t\,\mathrm{d}\tau \geqslant 0. \tag{56}$$

Only in the very special case of (55) when the friction is instantaneous (Markovian), i.e., $a(t) = a_0\delta(t)$, can one use the dilation theory as in [24, Theorem 3]. For many well studied dielectric media, such as Lorentz or Debye, not to mention media with generic frequency dependent electric susceptibilities, the relevant friction functions are not instantaneous. For such systems one must use a more general approach, such as developed in [2] and extended here and in [3].

It is interesting to point out, however, that coupling to a canonical heat bath (52) may be interpreted, as in the Lamb model, as "attaching an elastic string" at any point of loss. The attached strings are analogous to the scattering channels of the dilation theory, with the only difference being that our "strings" are coupled in more general ways than in the dilation theory. Thus, one can view our TDD Hamiltonian as a natural generalization of the constructions of the dilation theory.

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