# Non-Hermitian Hamiltonian Approach for Electromagnetic Wave Propagation and Dissipation in Dielectric Media

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***Abstract*—Using the formal analogy between a certain class of Maxwell equations and the Schrdinger equation, we derive the effective Hamiltonian operator that governs the propagation of electromagnetic (EM) wave modes inside nonconducting linear media, which include a large range of nanophotonic and plasmonic waveguides. It turns out that this Hamiltonian is essentially non-Hermitian, and thus requires a special treatment. We formulate the density operator approach for dynamical systems with non-Hermitian Hamiltonians, and derive a master equation that describes the statistical ensembles of EM wave modes. The method provides a theoretical instrument which can be used when designing the next generation of quantum EM devices for sensitive and non-invasive measurements.**

***Index Terms*—electromagnetic wave propagation, non-Hermitian Hamiltonians, density operator, open systems.**

## I. Introduction

Notwithstanding the long history of studies, the propagation of electromagnetic (EM) wave inside nonconducting media remains an important and rapidly developing topic. Apart from an obvious theoretical value, it finds numerous applications in the designs of the nanoscale photonic and plasmonic devices, structures and metamaterials, such as lasers, spasers, modulators, waveguides, optical switches, laser-absorbers, coupled resonators and quantum wells.

During the past decade there has been growing interest in studying those systems by means of the formal analogy between Maxwell equations in nonconducting media and Schrödinger-type equations, dubbed here as the Maxwell-Schrödinger (MS) map. In this analogy, Maxwell equations are rewritten in the form of the matrix Schrödinger equation, except that the role of time is played by the coordinate along the direction of wave propagation (usually, $z$-coordinate), the Hamiltonian operator is non-Hermitian (NH), and the Planck constant is replaced by an effective one [1]. Therefore, a class of the physical systems that allow such mapping is broadly referred as non-Hermitian materials and waveguides. Moreover, inside this class one can select the subclass of physical systems and phenomena for which the corresponding Hamiltonian operator is pseudo-Hermitian and has parity-time (PT) symmetry [2]. This pseudo-Hermiticity manifests itself in various phenomena, such as non-reciprocal light propagation and Bloch oscillations, invisibility and loss-induced transparency, power oscillations, optical switching, coherent perfect absorptions, laser-absorbers, plasmonic waveguides, unidirectional tunneling, loss-free negative refraction, and so on. These processes can be studied using a general theory of pseudo-Hermitian and PT-symmetric Hamiltonians [3], [4].

However, the class of non-Hermitian materials and waveguides is much larger than its pseudo-Hermitian subclass. Indeed, as a result of the interaction of EM waves with their environment (which can be very diverse and uncontrollable), the description of their propagation requires the usage of the NH Hamiltonians of different kinds, not necessarily pseudo-Hermitian. In other words, this propagation must be described within the framework of a general theory of open quantum systems [5]. According to that theory, for such situations one needs to engage the full description of the (quantum) statistical ensemble of EM wave modes. In turn, it requires the usage of the density matrix, instead of a state vector, as a main object of theory. Therefore, MS map must be used to develop the corresponding generalization, which is going to be the main goal of this talk . Although the density-operator approach for quantum systems driven by NH Hamiltonians has been long since known (see, for instance, the monograph [6]), it has been further developed in the works [7]–[11]. In this report we adapt the formalism [7]–[11] for the purposes of describing the EM wave propagation inside nonconducting materials and waveguides in presence of dissipative effects induced by environment, as well as for extracting physical information and predicting new phenomena.

## II. Maxwell-Schrödinger analogy

Let us consider EM wave propagating inside a nonconducting isotropic linear medium. For this situation, there are no free charges and currents, therefore, Maxwell equations acquire a simple form:

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial}{\partial t}(\mu \mathbf{H}) = 0, \tag{1}$$

$$\nabla \times \mathbf{H} - \frac{1}{c}\frac{\partial}{\partial t}(\varepsilon \mathbf{E}) = 0, \tag{2}$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \nabla \cdot (\mu \mathbf{H}) = 0, \tag{3}$$

where $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$ and $\mathbf{H} = \mathbf{H}(\mathbf{r}, t)$ are electric and magnetic fields, respectively, while the cross and dot denote the vector and scalar products, respectively. Here $c = 1/\sqrt{\varepsilon_0\mu_0}$, $\varepsilon_0$ and $\mu_0$ being, respectively, the vacuum permittivity and permeability, whereas $\varepsilon$ and $\mu$ are the relative permittivity and permeability (complex-valued functions of coordinates, in general); as per usual, one can also express them via the medium's electric and magnetic susceptibilities: $\varepsilon = 1 + \chi_e$ and $\mu = 1 + \chi_m$.

Further, if we align $z$-axis with the direction of wave's propagation then, assuming the harmonic time dependence of the electric and magnetic fields, $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(x, y, z) \exp(-i\omega t)$, $\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(x, y, z) \exp(-i\omega t)$ , one can decompose them into the transverse and longitudinal (along $z$-axis) components: $\mathbf{E} = \mathbf{E}_\perp + \mathbf{e}_z E_z$, $\mathbf{H} = \mathbf{H}_\perp + \mathbf{e}_z H_z$, $\nabla = \nabla_\perp + \mathbf{e}_z \frac{\partial}{\partial z}$, where $\mathbf{e}_n$ is the basis vector along the $n$th axis. One can show that the vectors $\mathbf{E}_\perp$ and $\mathbf{H}_\perp$ are essentially two-dimensional: $\mathbf{E}_\perp \cdot \mathbf{e}_z = \mathbf{H}_\perp \cdot \mathbf{e}_z = 0$. Correspondingly, Maxwell equations take the form (from now on we adopt the units where $c = 1$):

$$i\mathbf{e}_z \times \frac{\partial}{\partial z}\mathbf{E}_\perp = \hat{L}_m \mathbf{H}_\perp, \tag{4}$$

$$i\mathbf{e}_z \times \frac{\partial}{\partial z}\mathbf{H}_\perp = -\hat{L}_e \mathbf{E}_\perp, \tag{5}$$

$$E_z = (i\varepsilon\omega)^{-1}\mathbf{e}_z \cdot (\nabla_\perp \times \mathbf{H}_\perp), \tag{6}$$

$$H_z = -(i\mu\omega)^{-1}\mathbf{e}_z \cdot (\nabla_\perp \times \mathbf{E}_\perp), \tag{7}$$

where we denote the following differential operators:

$$\hat{L}_e = \varepsilon\omega - \omega^{-1}\nabla_\perp \times \mu^{-1}\nabla_\perp \times, \tag{8}$$

$$\hat{L}_m = \mu\omega - \omega^{-1}\nabla_\perp \times \varepsilon^{-1}\nabla_\perp \times . \tag{9}$$

Using the 2D property $\mathbf{e}_z \times \mathbf{e}_z \times = -1$, the equations (4) and (5) can be written in the matrix form

$$i\frac{\partial}{\partial z}\begin{pmatrix}\mathbf{E}_\perp \\ \mathbf{H}_\perp\end{pmatrix} = \hat{\mathcal{H}}'\begin{pmatrix}\mathbf{E}_\perp \\ \mathbf{H}_\perp\end{pmatrix}, \tag{10}$$

where we denote the operator

$$\hat{\mathcal{H}}' = \hat{\sigma}_2\hat{\mathcal{D}} = \begin{pmatrix} 0 & -\mathbf{e}_z \times \hat{L}_m \\ \mathbf{e}_z \times \hat{L}_e & 0 \end{pmatrix}, \tag{11}$$

and

$$\hat{\mathcal{D}} \equiv \hat{\sigma}_2\hat{\mathcal{H}}' = \begin{pmatrix} \hat{L}_e & 0 \\ 0 & \hat{L}_m \end{pmatrix} \tag{12}$$

is the auxiliary operator.

One can check that the operator (11) is non-Hermitian, even when both $\varepsilon$ and $\mu$ are real-valued. The degree of non-Hermiticity of the theory's Hamiltonian becomes even larger if we write (10) in the form that is fully analogous to the Schrödinger equation, for we must rewrite it in terms of normalized values. Using the Dirac's bra-ket notations for the inner product, defined as the integral over the waveguide's effective cross-section (*i.e.*, the region outside of which all the EM wave's fields vanish), and introducing the norm

$$\mathcal{N}^2 \equiv \langle \mathbf{E}_\perp | \mathbf{E}_\perp \rangle + \langle \mathbf{H}_\perp | \mathbf{H}_\perp \rangle \equiv \int dxdy \left( |\mathbf{E}_\perp|^2 + |\mathbf{H}_\perp|^2 \right), \tag{13}$$

we can define the following ket vector

$$|\Psi\rangle \equiv \frac{1}{\mathcal{N}}\begin{pmatrix}\mathbf{E}_\perp \\ \mathbf{H}_\perp\end{pmatrix}, \tag{14}$$

which is automatically normalized to one, $\langle\Psi|\Psi\rangle = 1$, and thus it can be regarded as a proper state vector in some appropriate Hilbert space. In terms of this state vector the equation (10) acquires the Schrödinger form

$$i\hbar_w \frac{\partial}{\partial z}|\Psi\rangle = \hat{\mathcal{H}}|\Psi\rangle, \tag{15}$$

where we denote the operator

$$\hat{\mathcal{H}} \equiv \hbar_w \left(\hat{\mathcal{H}}' + \hat{\mathcal{H}}_\mathcal{N}\right) = \hbar_w \left(\hat{\sigma}_2\hat{\mathcal{D}} - i\Gamma_\mathcal{N}\hat{\mathcal{I}}\right), \tag{16}$$

where $\hat{\mathcal{I}}$ and $\hat{I}$ are, respectively, the identity operator and the $2 \times 2$ identity matrix, and the coefficient

$$\Gamma_\mathcal{N} = \frac{\partial}{\partial z}\ln|\mathcal{N}| \tag{17}$$

is in general a real-valued function of $z$ (as well as a functional of the fields). Here by $z$ we assume the value $z/c$, and the "Planck" constant $\hbar_w$ is an effective scale constant of the dimensionality energy×time, which is introduced for a purpose of preserving the correct dimensionality of the relevant terms in the emergent Schrödinger equation (the ambiguity of $\hbar_w$ is yet another manifestation of the absence of the fundamental length scale in Maxwell equations). Further, it should be noticed the appearance of the additional term in the Hamiltonian (16), $\hat{\mathcal{H}}_\mathcal{N} \equiv -i\Gamma_\mathcal{N}\hat{\mathcal{I}}$, which is essentially anti-Hermitian and proportional to the identity operator.

Thus, equations (14)-(16) represent the formal map between Maxwell equations for nonconducting linear media and the differential equation of the Schrödinger type, which opens up the possibility of using quantum mechanical notions (with certain reservations, of course) for the purposes of a theory of EM wave propagation inside different dielectric materials, including waveguides.

## III. Statistical mechanics of wave modes

What we have done in the previous section is merely a way of rewriting Maxwell equations for waves in nonconducting media in the Schrödinger form (15). In this section we will proceed with an important generalization: we go beyond those equations and introduce the quantum-type density matrix approach adapted for describing the propagation of EM waves inside nonconducting media. This will allow us to describe not only separate wave modes ("pure states", in quantum-mechanical terminology) or their superpositions ("entangled pure states") but also their statistical ensembles ("mixed states"). The latter are crucial for introducing the dissipative effects since the purity of the states is not necessarily preserved in presence of dissipative environments [12].

The main difference of the proposed approach from the standard non-Hermitian quantum-statistical one [7]–[11] is that the role of the time variable is played here by the third coordinate, $z/c$. In other words, instead of time evolution of quantum states the method will describe the distribution of EM wave energy along the propagation axis. This, however, does not pose much difference from the technical viewpoint, and most of concepts can be borrowed and applied for the purposes of the EM theory.

Finally, due to the fact that in this theory both the speed of light and effective Planck constant are scale constants, from now on we work in units where $\hbar_w = \hbar = c = 1$.

### A. Master equation

To begin with, if a Hamiltonian is a non-Hermitian operator, then it can be decomposed into its Hermitian and anti-Hermitian parts, respectively:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_+ + \hat{\mathcal{H}}_- = \hat{\mathcal{H}}_+ - i\hat{\Gamma}, \tag{18}$$

where we use the notations

$$\hat{\mathcal{H}}_\pm \equiv \frac{1}{2}\left(\hat{\mathcal{H}} \pm \hat{\mathcal{H}}^\dagger\right) = \pm\hat{\mathcal{H}}_\pm^\dagger, \tag{19}$$

and the Hermitian operator

$$\hat{\Gamma} \equiv i\hat{\mathcal{H}}_- = \hat{\Gamma}^\dagger \tag{20}$$

is usually dubbed the *decay operator*. For instance, for the Hamiltonian (16) one easily computes that

$$\hat{\mathcal{H}}_+ = \hat{\mathcal{H}}'_+ = \frac{1}{2}\left(\hat{\sigma}_2\hat{\mathcal{D}} + \hat{\mathcal{D}}^\dagger\hat{\sigma}_2\right), \tag{21}$$

$$\hat{\Gamma} = \hat{\Gamma}' + \Gamma_{\mathcal{N}}\hat{\mathcal{I}} = \frac{i}{2}\left(\hat{\sigma}_2\hat{\mathcal{D}} - \hat{\mathcal{D}}^\dagger\hat{\sigma}_2\right) + \Gamma_{\mathcal{N}}\hat{\mathcal{I}}, \tag{22}$$

where we imply the notations from the previous section. This decomposition means that within the total system, described by $\hat{\mathcal{H}}$, one can single out the Hermitian subsystem, described by $\hat{\mathcal{H}}_+$, whereas the operator $\hat{\Gamma}$ can be regarded as describing the energy exchange of this subsystem with its environment.

The quantum-statistical approach means here that the probability-conserving "evolution" (distribution along the propagation direction) of such a system is described by the (reduced) density operator, which contains information not only about superpositions of the EM wave modes but also about the statistical uncertainty of their distribution inside a medium. Such uncertainty can be caused, for instance, by the interaction of the wave with its environment, which usually happens inside realistic dielectric media. An example would be the thermal randomness that arises in the statistical mixture of large numbers of EM wave modes, each with a certain classical probability, switching from one to another due to thermal fluctuations. In such cases, unpolarized light ("mixed state") appears, which is in fact not the superposition of several polarized modes ("pure states"), but their statistical ensemble. Thus, the density matrix contains all the information necessary to calculate any measurable property of polarized or unpolarized radiation propagating inside realistic media with or without dissipation. Besides, one of its advantages is that for each mixed state there can be many statistical ensembles of pure states but only one density matrix.

An equation for the density matrix can be directly derived from any equation that has the Schrödinger form, see, for instance, Ref. [6]. Using Eq. (15), one can show that our NH system is fully described by the so-called non-normalized density operator $\hat{\Omega}$, which is defined as a solution of the operator equation of the Liouvillian type,

$$\frac{d}{dz}\hat{\Omega} = i\left(\hat{\Omega}\hat{\mathcal{H}}^\dagger - \hat{\mathcal{H}}\hat{\Omega}\right) = -i\left[\hat{\mathcal{H}}_+, \hat{\Omega}\right] - \left\{\hat{\Gamma}, \hat{\Omega}\right\}, \tag{23}$$

where square and curly brackets denote the commutator and anti-commutator, respectively. One can see that, as $z$ varies, the trace of $\hat{\Omega}$ is not conserved,

$$\frac{d}{dz}\mathrm{tr}\,\hat{\Omega} = -2\langle\hat{\Gamma}\rangle_\Omega, \tag{24}$$

where we denoted

$$\langle\hat{\Gamma}\rangle_\Omega = \mathrm{tr}(\hat{\Gamma}\,\hat{\Omega}), \tag{25}$$

therefore, $\hat{\Omega}$ cannot be regarded as a proper density operator in statistical sense. In order to define one, in Ref. [7] we introduced the operator

$$\hat{\rho} = \hat{\Omega}/\mathrm{tr}\,\hat{\Omega}, \tag{26}$$

which is automatically normalized (the physical meaning of this procedure will be discussed later), therefore, it can be used for computing expectation values, correlation functions and other observables.

In principle, in Eq. (23) one can change from $\hat{\Omega}$ to $\hat{\rho}$, and obtain the equation for the normalized density operator itself

$$\frac{d}{dz}\hat{\rho} = -i\left[\hat{\mathcal{H}}_+, \hat{\rho}\right] - \left\{\hat{\Gamma}, \hat{\rho}\right\} + 2\langle\Gamma\rangle\hat{\rho}, \tag{27}$$

where the notation

$$\langle A\rangle = \mathrm{tr}(\hat{\rho}\,\hat{A}) \tag{28}$$

will be used for denoting the expectation value of any given operator $\hat{A}$ with respect to the normalized density operator. It should be noted, however, that Eq. (27) contains slightly less information about the system (18) than (23) because the procedure (26) erases the information about the overall factor of $\hat{\Omega}$ including its trace. This missing piece of information can be useful, e.g., when studying the initial conditions or entropic properties of the system.

From the mathematical point of view, Eq. (27) is both nonlocal and nonlinear with respect to the density operator $\hat{\rho}$. Though, this does not pose a significant problem from the technical point of view, since one can always use Eq. (26) as an ansatz for getting a linear equation. Thus, Eqs. (23)-(27), together with the definition for computing the expectation values (28), represent the map that allows us to describe the distribution of system (18) along $z$ direction in terms of the matrix differential equation, which mathematical structure resembles the one of the conventional master equations of the Lindblad kind. According to this map, the Hermitian operator $\hat{\mathcal{H}}_+ = (\hat{\mathcal{H}} + \hat{\mathcal{H}}^\dagger)/2$ takes over a role of the system's Hamiltonian (cf. the commutator term in equations (23) or (27) above) whereas the decay operator $\hat{\Gamma} = i(\hat{\mathcal{H}} - \hat{\mathcal{H}}^\dagger)/2$ induces additional terms in the evolution equation that are supposed to account for NH effects. In other words, a theory with the non-Hermitian Hamiltonian $\hat{\mathcal{H}}$ is dual to a theory with the Hermitian Hamiltonian $(\hat{\mathcal{H}} + \hat{\mathcal{H}}^\dagger)/2$ but with the modified equation, which thus becomes the master equation of a special kind. This equivalence not only reveals new features of the dynamics driven by non-Hermitian Hamiltonians but also facilitates the application of such Hamiltonians for open quantum systems [8].

### B. Entropy

Apart from purity $\mathrm{tr}\hat{\rho}^2$ and linear entropy $S_L = 1 - \mathrm{tr}\hat{\rho}^2$, there exists another characteristic value describing the amount of disorder and statistical uncertainty in a system – the quantum entropy of the Gibbs type. In Ref. [10] it was shown that for a system driven by NH Hamiltonian one can introduce two types of quantum entropy: the conventional Gibbs-von-Neumann one

$$S_{\mathrm{vN}} \equiv -k_B \langle \ln \hat{\rho} \rangle = -k_B \mathrm{tr} \left( \hat{\rho} \ln \hat{\rho} \right), \tag{29}$$

and the NH-adapted Gibbs-von-Neumann one

$$S_{\mathrm{NH}} \equiv -k_B \langle \ln \hat{\Omega} \rangle = -k_B \mathrm{tr}(\hat{\rho} \ln \hat{\Omega}) = -k_B \frac{\mathrm{tr}(\hat{\Omega} \ln \hat{\Omega})}{\mathrm{tr}\, \hat{\Omega}}, \tag{30}$$

where $k_B$ is the Boltzmann constant. The two notions of entropy are related by the formula

$$S_{\mathrm{NH}} = S_{\mathrm{vN}} - k_{\mathrm{B}} \ln (\mathrm{tr}\, \hat{\Omega}), \tag{31}$$

therefore, the difference between $S_{\mathrm{NH}}$ and $S_{\mathrm{vN}}$ is a measure of deviation of $\mathrm{tr}\, \hat{\Omega}$ from unity. One can see that the entropy $S_{\mathrm{NH}}$ combines both the normalized and "primordial" (non-normalized) density operators, and thus can signal the expected thermodynamic behavior of an open system. The entropy $S_{\mathrm{NH}}$ also seems to be more suitable for describing the gain/loss processes that are related to the probability's non-conservation.

## IV. Conclusion

Using the formal analogy between the Schrödinger equation and a certain class of Maxwell equations, we have generalized the theory of EM wave's propagation in nonconducting linear media – in order to be able to describe not only separate wave modes (or their linear superpositions) but also the statistical ensembles of modes, referred as mixed states in quantum mechanics. It turns out that the Hamiltonians, which govern the dynamics of such ensembles, are in general not just pseudo-Hermitian or parity-time-symmetric but essentially non-Hermitian and thus require a special systematic treatment. Using the density operator approach for general non-Hermitian Hamiltonians developed in our earlier works, we have demonstrated that the non-Hermitian terms play an important role in the physics of wave propagation.

The proposed approach applies to a large class of nonconducting media and nanoscale photonic and plasmonic materials and waveguiding devices, where it provides a powerful tool to construct and study different models, as well as to derive the observables of different kinds: correlation functions, entropy, energy density and transmitted power, *etc*. This results in a consistent and thorough understanding of whether and how one can control the dissipative effects in different nonconducting media, which lead to decoherence and energy and information loss during propagation of EM waves. The control over these effects is especially important for the development of the next generation of quantum electromagnetic devices, including those which use the quantum interference of multimode EM beams in order to improve the sensitivity and non-invasivity of measurements, quantum amplifiers and radars being just some examples here [13]. For instance, the uncontrolled spontaneous transition of pure modes into statistical ensembles during beam's propagation would inevitably result in an increase of statistical uncertainty and hence lead to higher degrees of dissipation and noise. Further studies of such quantum-statistical effects is a fruitful direction of future research.

Last but not least, one can use this approach both ways: it also provides a methodology of how one can use EM waves in nonconducting media for experimental testing of the heuristic concepts and ideas of the non-Hermitian formalism in general, such as non-normalized and normalized density operators, master equations with anti-commutators, nonlinear and nonlocal terms, different notions of entropy, to mention just a few examples.


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