

Quantum Electromagnetics: A New Look, Part II*

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1 Introduction

In Part II, quantum electromagnetics (quantization of electromagnetic fields) will be extended to the anisotropic inhomogeneous medium case. This, as far as we know, has not been done before. Furthermore, connection with the mode decomposition approach will be made including the anisotropic inhomogeneous medium case. Two kinds of modes will be identified: the traveling wave case and the standing wave case. Each of them presents a different picture of the modes, and their physical pictures will be explained.

Next, the case of impressed sources will be introduced in both classical and quantum Hamiltonian mechanics. This is similar to the concept of impressed current sources in classical electromagnetics. Moreover, for a linear time invariant system, it can be shown that the solution can be more compactly written by the introduction of the Green's function as in the classical electromagnetics case [9, 10]. The illustrations of the use of Green's functions in both the vector and scalar potential cases will be given. The methods outlined in this part portend well for the development of new quantum technologies.

2 Anisotropic, Inhomogeneous Medium Case

Quantum electromagnetics for the anisotropic inhomogeneous medium case has not been presented in the literature before, even though it has been presented for the isotropic inhomogeneous medium case [2, 3]. Here, we present the lossless, reciprocal, anisotropic inhomogeneous medium case using the generalized Lorenz gauge. The generalized Lorenz gauge is not new and many past works have been referred to in [5]. Some works that have recently come to our attention are [6, 7]. Furthermore, the treatment of the lossy case is complicated and beyond the scope of this work [9–11]. It requires the coupling of a quantum system to a noise bath to maintain the Hermiticity of the system. Moreover, the introduction of loss, from the Kramers-Kronig relation [12], implies the dispersive nature of the medium. Before starting, however, some new notations will be introduced to lessen the algebra involved.

2.1 New Hamilton Equations

At this juncture, it is convenient to define the Hamiltonian density such that

$$H_A = \int d\mathbf{r} \mathcal{H}_A(\Pi(\mathbf{r}, t), \mathbf{A}(\mathbf{r}, t)) \quad (2.1)$$

Moreover, the functional derivatives with respect to the Hamiltonian always introduce the delta functions. Therefore, the sifting property of the delta function will remove the integral over the Hamiltonian density. With this in

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mind, the Hamiltonian density and the equations of motion can be re-derived and rewritten more succinctly as

$$\frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t} = \frac{\partial \tilde{\mathcal{H}}_A}{\partial \mathbf{\Pi}(\mathbf{r}, t)}, \quad \frac{\partial \mathbf{\Pi}(\mathbf{r}, t)}{\partial t} = -\frac{\partial \tilde{\mathcal{H}}_A}{\partial \mathbf{A}(\mathbf{r}, t)} \quad (2.2)$$

In this notation, the tilde above implies that the integration by parts has been performed so that the transpose of the operator can be easily found.

The generalized Lorenz gauge [5] in this case is

$$\nabla \cdot [\bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)] = -\chi(\mathbf{r}) \partial_t \Phi(\mathbf{r}, t) \quad (2.3)$$

yielding the decoupled potential equations as

$$\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}, t) - \chi(\mathbf{r}) \partial_t^2 \Phi(\mathbf{r}, t) = 0 \quad (2.4)$$

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}(\mathbf{r}, t) + \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \partial_t^2 \mathbf{A}(\mathbf{r}, t) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)) = 0 \quad (2.5)$$

where $\chi(\mathbf{r}) = \alpha |\bar{\boldsymbol{\varepsilon}} \cdot \bar{\boldsymbol{\mu}} \cdot \bar{\boldsymbol{\varepsilon}}|$, and α is an arbitrary constant. Here, $\bar{\boldsymbol{\varepsilon}}(\mathbf{r})$ and $\bar{\boldsymbol{\mu}}(\mathbf{r})$ are real symmetric tensors because of the reciprocal and lossless conditions.

The Hamiltonian density for the vector potential for anisotropic inhomogeneous medium case is

$$\begin{aligned} \mathcal{H}_A = \frac{1}{2} [\partial_t \mathbf{A}(\mathbf{r}, t)] \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot [\partial_t \mathbf{A}(\mathbf{r}, t)] + \frac{1}{2} [\nabla \times \mathbf{A}(\mathbf{r}, t)] \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{A}(\mathbf{r}, t)] \\ + \frac{1}{2} [\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)]^2 \chi^{-1}(\mathbf{r}) \end{aligned} \quad (2.6)$$

The scalar potential Hamiltonian density for the same case is

$$\mathcal{H}_\Phi = \frac{1}{2} [\nabla \Phi(\mathbf{r}, t)] \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot [\nabla \Phi(\mathbf{r}, t)] + \frac{1}{2} \chi(\mathbf{r}) [\partial_t \Phi(\mathbf{r}, t)]^2 \quad (2.7)$$

The total Hamiltonian density is then

$$\mathcal{H} = \mathcal{H}_A - \mathcal{H}_\Phi \quad (2.8)$$

The difference is needed as it can be shown that the above, after using integration by parts and Lorenz gauge, is equivalent to

$$\tilde{\mathcal{H}} = \frac{1}{2} [\mathbf{E}(\mathbf{r}, t) \cdot \mathbf{D}(\mathbf{r}, t) + \mathbf{H}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t)] \quad (2.9)$$

where the tilde implies that integration by parts has been used to arrive at the above form for the Hamiltonian density. The conjugate momenta for the vector and scalar potentials are defined as

$$\mathbf{\Pi}(\mathbf{r}, t) = \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \partial_t \mathbf{A}(\mathbf{r}, t), \quad \Pi_s(\mathbf{r}, t) = \chi(\mathbf{r}) \partial_t \Phi(\mathbf{r}, t) \quad (2.10)$$

Then, the total Hamiltonian density is

$$\begin{aligned} \mathcal{H} = \mathcal{H}_A - \mathcal{H}_\Phi = \frac{1}{2} \mathbf{\Pi}(\mathbf{r}, t) \cdot \bar{\boldsymbol{\varepsilon}}^{-1}(\mathbf{r}) \cdot \mathbf{\Pi}(\mathbf{r}, t) + \frac{1}{2} [\nabla \times \mathbf{A}(\mathbf{r}, t)] \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{A}(\mathbf{r}, t)] + \frac{1}{2\chi(\mathbf{r})} [\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)]^2 \\ - \frac{1}{2} [\nabla \Phi(\mathbf{r}, t)] \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot [\nabla \Phi(\mathbf{r}, t)] - \frac{1}{2\chi(\mathbf{r})} \Pi_s^2(\mathbf{r}, t) \end{aligned} \quad (2.11)$$

From the Hamilton equations, then

$$\frac{\partial \tilde{\mathcal{H}}_A}{\partial \mathbf{\Pi}} = \bar{\boldsymbol{\varepsilon}}^{-1}(\mathbf{r}) \cdot \mathbf{\Pi}(\mathbf{r}, t) = \partial_t \mathbf{A}(\mathbf{r}, t) \quad (2.12)$$

$$\frac{\partial \tilde{\mathcal{H}}_A}{\partial \mathbf{A}(\mathbf{r}, t)} = -\partial_t \mathbf{\Pi}(\mathbf{r}, t) = \nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}(\mathbf{r}, t) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla [\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)] \quad (2.13)$$

where integration by parts and the fact that $\bar{\boldsymbol{\varepsilon}}(\mathbf{r})$ and $\bar{\boldsymbol{\mu}}(\mathbf{r})$ are real symmetric tensors have been used to arrive at the above form. Combining the above yields the equation of motion for the vector potential:

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}(\mathbf{r}, t) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)) + \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \partial_t^2 \mathbf{A}(\mathbf{r}, t) = 0 \quad (2.14)$$

Similarly for the scalar potential part, only the scalar potential and its conjugate momentum are perturbed yielding,

$$\frac{\partial \tilde{\mathcal{H}}_\Phi}{\partial \Pi_s(\mathbf{r}, t)} = \chi^{-1}(\mathbf{r}) \Pi_s(\mathbf{r}, t) = \partial_t \Phi(\mathbf{r}, t) \quad (2.15)$$

$$\frac{\partial \tilde{\mathcal{H}}_\Phi}{\partial \Phi(\mathbf{r}, t)} = -\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}, t) = -\partial_t \Pi_s(\mathbf{r}, t) \quad (2.16)$$

where lossless reciprocal medium has been assumed here. Combining the above yields the equation of motion for the scalar potential:

$$\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}, t) - \chi(\mathbf{r}) \partial_t^2 \Phi(\mathbf{r}, t) = 0 \quad (2.17)$$

2.2 The Quantum Case

With the mathematical tools and algebra being developed, the generalization to the quantum case is rather straightforward. To arrive at the quantum description of the system, the conjugate variables are first elevated to become quantum operators like the free-space case. Then the commutators between the conjugate quantum operators as obtained in Part I, (8.8) and (8.15), are reproduced here

$$\left[\hat{\Pi}_s(\mathbf{r}, t), \hat{\Phi}(\mathbf{r}', t) \right] = i\hbar \delta(\mathbf{r} - \mathbf{r}') \hat{I} \quad (2.18)$$

and

$$\left[\hat{\mathbf{\Pi}}(\mathbf{r}, t), \hat{\mathbf{A}}(\mathbf{r}', t) \right] = i\hbar \delta(\mathbf{r} - \mathbf{r}') \hat{\mathbf{I}} \quad (2.19)$$

They induce derivative properties in the Heisenberg equations of motion as shown in Part I.

With the introduction of quantum Hamilton equations of motion previously, similar equations for the coupled harmonic oscillator case for anisotropic inhomogeneous medium case can be derived. One needs only to replace the field variables in equations in (2.4) to (2.7) with operators. Then the total Hamiltonian density and Hamiltonian will become operators as well.

The state of the quantum system is now determined by a state vector whose time evolution is governed by the Schrödinger equation, but with the appropriate Hamiltonian for anisotropic inhomogeneous medium. The quantum equations of motion for the vector and scalar potential can be shown to be

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \hat{\mathbf{A}}(\mathbf{r}, t) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \hat{\mathbf{A}}(\mathbf{r}, t)) + \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \partial_t^2 \hat{\mathbf{A}}(\mathbf{r}, t) = 0 \quad (2.20)$$

$$\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla \hat{\Phi}(\mathbf{r}, t) - \chi(\mathbf{r}) \partial_t^2 \hat{\Phi}(\mathbf{r}, t) = 0 \quad (2.21)$$

Again, the above quantum operators act on a fixed quantum state which defines the state of the system at $t = 0$, as these are Heisenberg operators.

3 Mode Decomposition Picture

The mode decomposition approach gives a different physical picture of the oscillatory fields of the coupled harmonic oscillators as a collection of lone harmonic oscillators. Hence, it is very useful for seeing the connection between

classical harmonic oscillators and quantum harmonic oscillators. The mode decomposition approach has been described in most literature for the free space case. It is also the standard way of connecting classical electromagnetics with quantum electromagnetics, as have been presented in many textbooks referenced in Part I of this work.

Previously, it has been shown that the quantum equations of motion can be obtained directly from the quantum Hamiltonian without going through mode decomposition. It can be shown that the two approaches yield the same result, and hence, are equivalent. The mode decomposition approach has not been presented for the case of dispersionless, anisotropic, inhomogeneous media. Therefore, it will be presented here. For simplicity, the scalar potential case will be presented first.

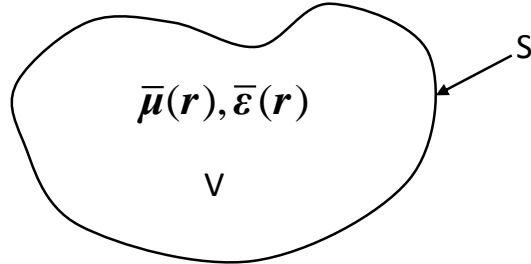


Figure 1: The mode decomposition picture is valid for cavity of arbitrary shape filled with lossless anisotropic inhomogeneous medium.

3.1 Scalar Potential Case

The equation of motion for the scalar potential case for anisotropic inhomogeneous media has been derived in (2.17). Using the separation of variables, one lets

$$\Phi(\mathbf{r}, t) = s_k(t)\Phi_k(\mathbf{r}) \quad (3.1)$$

Consequently, using it in (2.17) gives

$$\partial_t^2 s_k(t) = -\Omega_k^2 s_k(t) \quad (3.2)$$

$$\nabla \cdot \bar{\epsilon} \cdot \nabla \Phi_k(\mathbf{r}) + \Omega_k^2 \chi(\mathbf{r}) \Phi_k(\mathbf{r}) = 0 \quad (3.3)$$

In the above, $\Phi_k(\mathbf{r})$ represents an eigenmode of equation (3.3) with eigenvalue Ω_k^2 . Due to the Hermiticity of the operators involved, one can easily prove the orthogonality of these eigenmodes and the realness of the eigenvalue Ω_k^2 [13]. The Hermiticity is retained with Neumann, Dirichlet, or mixed boundary conditions when solving (3.3). For domain of some special shapes, periodic boundary condition can be imposed [14]. Therefore, one defines an orthonormal relation using Dirac notation as described in Appendix A as

$$\langle \Phi_{k'} | \chi | \Phi_k \rangle = \int d\mathbf{r} \Phi_{k'}^*(\mathbf{r}) \chi(\mathbf{r}) \Phi_k(\mathbf{r}) = \delta_{k'k} \quad (3.4)$$

On this note, one can expand in general a time varying field as

$$\Phi(\mathbf{r}, t) = \sum_k s_k(t) \Phi_k(\mathbf{r}) = \sum_k s_k^*(t) \Phi_k^*(\mathbf{r}) \quad (3.5)$$

The second equality follows from the realness of $\Phi(\mathbf{r}, t)$ on the left-hand side. Using the above eigenmode expansion of $\Phi(\mathbf{r}, t)$, it follows that the integral of the first term of the scalar potential Hamiltonian density in (2.7) is

$$\int d\mathbf{r} \nabla \Phi(\mathbf{r}, t) \cdot \bar{\epsilon}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}, t) = \sum_{k, k'} s_k(t) s_{k'}^*(t) \int d\mathbf{r} \nabla \Phi_k(\mathbf{r}) \cdot \bar{\epsilon}(\mathbf{r}) \cdot \nabla \Phi_{k'}^*(\mathbf{r}) \quad (3.6)$$

$$= \sum_k |s_k(t)|^2 \Omega_k^2 \quad (3.7)$$

The last equality can be shown using integration by parts, (3.3), boundary condition, and the orthogonality relationship (3.4). They together imply that

$$\int d\mathbf{r} [\nabla\Phi_k(\mathbf{r})] \cdot \bar{\boldsymbol{\varepsilon}} \cdot [\nabla\Phi_{k'}^*(\mathbf{r})] = - \int d\mathbf{r} [\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla\Phi_k(\mathbf{r})] \Phi_{k'}^*(\mathbf{r}) = \Omega_k^2 \int d\mathbf{r} \Phi_k(\mathbf{r}) \chi(\mathbf{r}) \Phi_{k'}^*(\mathbf{r}) \quad (3.8)$$

$$= \Omega_k^2 \delta_{kk'} \quad (3.9)$$

By the same token, one can show that the integral of second term of the scalar potential Hamiltonian density in (2.7) is

$$\int d\mathbf{r} \chi(\mathbf{r}) (\partial_t \Phi(\mathbf{r}, t))^2 = \sum_k |\partial_t s_k(t)|^2 \quad (3.10)$$

As a result, the Hamiltonian for the scalar potential then becomes

$$H_\Phi = \frac{1}{2} \sum_k [|P_{k,\Phi}(t)|^2 + |Q_{k,\Phi}(t)|^2] \quad (3.11)$$

where

$$P_{k,\Phi}(t) = \partial_t s_k(t), \quad Q_{k,\Phi}(t) = s_k(t) \Omega_k \quad (3.12)$$

3.2 Vector Potential Case

For the vector potential case, again by the separation of variables, letting

$$\mathbf{A}(\mathbf{r}, t) = \alpha_k(t) \mathbf{A}_k(\mathbf{r}) \quad (3.13)$$

yields

$$\partial_t^2 \alpha_k(t) = -\Omega_k^2 \alpha_k \quad (3.14)$$

As a result, the equation of motion (2.5) becomes

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}_k(\mathbf{r}) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r})) - \Omega_k^2 \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r}) = 0 \quad (3.15)$$

The Hermiticity of the above operators ensures the realness of the eigenvalue Ω_k^2 , and orthonormality relation can be defined as [13]

$$\langle \mathbf{A}_{k'} | \bar{\boldsymbol{\varepsilon}} | \mathbf{A}_k \rangle = \int d\mathbf{r} \mathbf{A}_{k'}^*(\mathbf{r}) \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r}) = \delta_{k'k} \quad (3.16)$$

As in the scalar potential case, different boundary conditions can be used to arrive at the above. Moreover, one can expand a general field as

$$\mathbf{A}(\mathbf{r}, t) = \sum_k \alpha_k(t) \mathbf{A}_k(\mathbf{r}) = \sum_k \alpha_k^*(t) \mathbf{A}_k^*(\mathbf{r}) \quad (3.17)$$

Using the above in the second and third terms in the integral of the Hamiltonian density given by (2.6), leads to

$$\begin{aligned} & \int d\mathbf{r} [\nabla \times \mathbf{A}(\mathbf{r}, t) \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}(\mathbf{r}, t) + (\nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t))^2 \chi^{-1}(\mathbf{r})] \\ &= \sum_{k,k'} \alpha_k(t) \alpha_{k'}^*(t) \int d\mathbf{r} [\nabla \times \mathbf{A}_k(\mathbf{r}) \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}_{k'}^*(\mathbf{r}) + \nabla \cdot \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{A}_k(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{A}_{k'}^*(\mathbf{r}) \chi^{-1}(\mathbf{r})] \\ &= \sum_k |\alpha_k(t)|^2 \Omega_k^2 \end{aligned} \quad (3.18)$$

In the above, integration by parts, (3.15), boundary condition, and the orthogonal relation (3.16) have been used to give,

$$\begin{aligned}
& \int d\mathbf{r} [\nabla \times \mathbf{A}_k(\mathbf{r}) \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}_{k'}^*(\mathbf{r}) + \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r}) \chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_{k'}^*(\mathbf{r})] \\
&= \int d\mathbf{r} \mathbf{A}_k(\mathbf{r}) \cdot [\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}_k(\mathbf{r}) - \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r}))] \\
&= \Omega_k^2 \int d\mathbf{r} \mathbf{A}_k(\mathbf{r}) \cdot \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{A}_{k'}^*(\mathbf{r}) = \Omega_k^2 \delta_{kk'}
\end{aligned} \tag{3.19}$$

And using (3.16) and (3.17) in the integral of the first term of the Hamiltonian density given by (2.6), then

$$\int d\mathbf{r} \partial_t \mathbf{A}(\mathbf{r}, t) \cdot \bar{\boldsymbol{\varepsilon}}(\mathbf{r}) \cdot \partial_t \mathbf{A}(\mathbf{r}, t) = \sum_k |\partial_t \alpha_k(t)|^2 \tag{3.20}$$

Therefore, from (3.18) and (3.20), the Hamiltonian for the vector potential is

$$H_A = \frac{1}{2} \sum_k [|P_{k,\mathbf{A}}(t)|^2 + |Q_{k,\mathbf{A}}(t)|^2] \tag{3.21}$$

where

$$P_{k,\mathbf{A}}(t) = \partial_t \alpha_k(t), \quad Q_{k,\mathbf{A}}(t) = \alpha_k(t) \Omega_k \tag{3.22}$$

3.3 Total Hamiltonian for Mode Decomposition

The scalar and vector potentials are related by the generalized Lorenz gauge. As a result, the scalar potential eigenmodes are related to the vector potential eigenmodes. Therefore, $s_k(t)$, $\partial_t s_k(t)$ are related to $a_k(t)$, $\partial_t a_k(t)$. The total Hamiltonian of the system for anisotropic inhomogeneous medium is the integral of (2.8), and is defined to be

$$H = H_A - H_\Phi \tag{3.23}$$

By comparing (3.5) and (3.17), and that by taking the divergence of (3.15), making it very similar to (3.3), it can be shown that

$$\nabla \cdot \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{A}_k(\mathbf{r}) = c_k \chi(\mathbf{r}) \Phi_k(\mathbf{r}) \tag{3.24}$$

Here, c_k is needed because $\mathbf{A}_k(\mathbf{r})$ and $\Phi_k(\mathbf{r})$ are orthonormal functions, and they cannot be directly related by the generalized Lorenz gauge. It is to be noted that the divergence operator maps a 3-vector into a scalar, the above can give rise to 3 degrees of degeneracy for the scalar potential $\Phi_k(\mathbf{r})$. By further taking the magnitude square of the above equation, (3.24), multiplying it by $\chi(\mathbf{r})$, integrating over space, and using the orthonormality relation of $\Phi_k(\mathbf{r})$, and making use of (3.19), one obtains

$$\int d\mathbf{r} [\nabla \times \mathbf{A}_k(\mathbf{r})] \cdot \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{A}_k^*(\mathbf{r})] = \Omega_k^2 - |c_k|^2 \tag{3.25}$$

For a lossless medium, $\bar{\boldsymbol{\mu}}(\mathbf{r})$ is a Hermitian positive definite tensor. The positive definiteness of the left-hand side ensures that $\Omega_k^2 > |c_k|^2$. By connecting the vector and scalar potential via the Lorenz gauge, one can hence show that

$$\partial_t s_k(t) = -c_k \alpha_k(t), \quad \partial_t \alpha_k(t) = \frac{\Omega_k^2}{c_k} s_k(t) \tag{3.26}$$

Using these, one can further show that

$$H = H_A - H_\Phi = \frac{1}{2} \sum_k [|\partial_t \alpha_k(t)|^2 + |\alpha_k(t)|^2 \Omega_k^2 - |\partial_t s_k(t)|^2 - |s_k(t)|^2 \Omega_k^2] \quad (3.27)$$

Again, as aforementioned, due to the degeneracies introduced by the map (3.24), the scalar potential modes could be counted multiple times in the above index k . Using (3.26) in the above, one arrives at

$$H = \frac{1}{2} \sum_k \left(1 - \frac{|c_k|^2}{\Omega_k^2}\right) [|\partial_t \alpha_k(t)|^2 + |\alpha_k(t)|^2 \Omega_k^2] \quad (3.28)$$

The above is a positive definite quantity from (3.25). Accordingly, the total Hamiltonian can be similarly expressed as

$$H = \frac{1}{2} \sum_k [|P_k(t)|^2 + |Q_k(t)|^2] \quad (3.29)$$

where

$$P_k(t) = \left(1 - \frac{|c_k|^2}{\Omega_k^2}\right)^{1/2} \partial_t \alpha_k(t), \quad Q_k(t) = \left(1 - \frac{|c_k|^2}{\Omega_k^2}\right)^{1/2} \alpha_k(t) \Omega_k \quad (3.30)$$

The Hamiltonian expounded in (3.29) represents the sum of Hamiltonians of many lone harmonic oscillators. This makes it easy to connect them to the lone quantum harmonic oscillators.

It is to be noted that $|P_k|^2$ is arrived at by subtracting the potential energy of the scalar potential Φ from the kinetic energy of the vector potential, and vice versa for $|Q_k|^2$. It shall be shown next that $|P_k|^2$ and $|Q_k|^2$ correspond to the energy stored in the electric field and magnetic field, respectively.

The above motivates the definition of orthonormalized electric field modes such that

$$\mathbf{E}_k(\mathbf{r}) = \left(1 - \frac{|c_k|^2}{\Omega_k^2}\right)^{-1/2} \left(\mathbf{A}_k(\mathbf{r}) + \frac{c_k}{\Omega_k^2} \nabla \Phi_k(\mathbf{r}) \right) \quad (3.31)$$

with the property that

$$\langle \mathbf{E}_k | \bar{\boldsymbol{\epsilon}} | \mathbf{E}_{k'} \rangle = \delta_{kk'} \quad (3.32)$$

Then the expansion of the electric field is

$$\mathbf{E}(\mathbf{r}) = \sum_k P_k(t) \mathbf{E}_k(\mathbf{r}) \quad (3.33)$$

Similarly, one can define orthonormalized magnetic field modes such that

$$\mathbf{H}_k(\mathbf{r}) = (\Omega_k^2 - |c_k|^2)^{-1/2} \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \nabla \times \mathbf{A}_k(\mathbf{r}) \quad (3.34)$$

with the property that

$$\langle \mathbf{H}_k | \bar{\boldsymbol{\mu}} | \mathbf{H}_{k'} \rangle = \delta_{kk'} \quad (3.35)$$

Then the expansion of the magnetic field is

$$\mathbf{H}(\mathbf{r}) = \sum_k Q_k(t) \mathbf{H}_k(\mathbf{r}) \quad (3.36)$$

So it is clear that $|P_k(t)|^2$ and $|Q_k(t)|^2$ correspond to energy stored in the electric field modes and magnetic field modes, respectively. One can also easily substitute the above mode decompositions for \mathbf{E} and \mathbf{H} into (2.9) to arrive at (3.29).

3.4 Longitudinal Modes

Because the total Hamiltonian H equals to $H_A - H_\Phi$, the energy in the vector potential Hamiltonian has excess energy compared to the energy in the \mathbf{E} and \mathbf{B} Hamiltonian. The reason can be attributed to the existence of the longitudinal modes. These modes can even have zero electromagnetic field, but non-zero scalar and vector potentials. For the zero magnetic field, the corresponding vector potential is curl free, or that $\mathbf{B} = \nabla \times \mathbf{A}$ is zero. The case of zero electric field is less obvious but can be constructed easily for the traveling wave modes in free space. The electric field is given by

$$\mathbf{E} = -\nabla\Phi - \partial_t\mathbf{A} \quad (3.37)$$

For a traveling plane wave mode with oscillation frequency of Ω_k , the corresponding mode is

$$\mathbf{E} = -i\mathbf{k}\Phi + i\Omega_k\mathbf{A} \quad (3.38)$$

If one chooses $\mathbf{k}\Phi = \Omega_k\mathbf{A}$ or that \mathbf{A} points in the \mathbf{k} direction, this mode has zero corresponding electric field. The oscillations of these modes are also called the longitudinal photons.

For the general anisotropic inhomogeneous medium case, the scalar potential oscillates according to the following equation:

$$\nabla \cdot \bar{\epsilon} \cdot \nabla \Phi_k(\mathbf{r}) + \Omega_k^2 \chi(\mathbf{r}) \Phi_k(\mathbf{r}) = 0 \quad (3.39)$$

A corresponding vector potential can be constructed such that

$$\mathbf{A}_k = \frac{i}{\Omega_k} \nabla \Phi_k \quad (3.40)$$

Such a longitudinal mode has no corresponding electromagnetic field! The energy of such modes has to be removed from the Hamiltonian of the vector potential in order to equate it to the energy of the electromagnetic field.

3.5 Traveling Wave Modes versus Standing Wave Modes

In the previous section, the total Hamiltonian has been expressed in terms of individual Hamiltonian of each mode. The total energy of each mode is denoted as the sum of $|P(t)|^2$ and $|Q(t)|^2$, be it the scalar potential case, the vector potential case, or the \mathbf{E} and \mathbf{H} fields case. The time behavior of these two energies will differ depending on the nature of the mode: whether if it is a traveling wave mode, or a standing wave mode.

From the eigenequations for the modes, it is seen that their eigenvalues are real. This implies that if Φ_k is a solution, so is Φ_k^* sharing the same eigenvalue. Since Φ_k^* corresponds to a time reversed solution, two cases are possible here: (i) It is a standing wave, and Φ_k is real valued or constant phase so that its complex conjugation is the same mode. (ii) It is a traveling wave so that its time reversed solution is traveling in the opposite direction.

3.5.1 Traveling Wave Modes

The mode decomposition picture for free space is often expressed in terms of traveling wave modes. For instance, take the example of the scalar potential case, with periodic boundary condition, an orthonormal traveling wave mode in a volume V can be written as

$$\Phi_{\boldsymbol{\kappa}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{\kappa} \cdot \mathbf{r}} \quad (3.41)$$

By the use of the periodic boundary condition in a cuboid volume $V = a \times b \times d$, $\boldsymbol{\kappa}$ can be discretized and made countably infinite in number. Then [14]

$$\boldsymbol{\kappa} = \hat{x}\kappa_x + \hat{y}\kappa_y + \hat{z}\kappa_z, \quad \kappa_x = 2l\pi/a, \quad \kappa_y = 2m\pi/b, \quad \kappa_z = 2p\pi/d, \quad (3.42)$$

$$\kappa^2 = \boldsymbol{\kappa} \cdot \boldsymbol{\kappa} = (2l\pi/a)^2 + (2m\pi/b)^2 + (2p\pi/d)^2 = \Omega_{\boldsymbol{\kappa}}^2/c^2 \quad (3.43)$$

where (l, m, p) are integer triplets, and c is the velocity of light in free space. The general solution to (3.2) is

$$s_{\mathbf{\kappa}}(t) = s_{\mathbf{\kappa},+}e^{-i\Omega_{\kappa}t} + s_{\mathbf{\kappa},-}e^{i\Omega_{\kappa}t} \quad (3.44)$$

Thus,

$$\Phi(\mathbf{r}, t) = \sum_{\mathbf{\kappa}} s_{\mathbf{\kappa}}(t)\Phi_{\mathbf{\kappa}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{\kappa}} (s_{\mathbf{\kappa},+}e^{-i\Omega_{\kappa}t}e^{i\mathbf{\kappa}\cdot\mathbf{r}} + s_{\mathbf{\kappa},-}e^{i\Omega_{\kappa}t}e^{i\mathbf{\kappa}\cdot\mathbf{r}}) \quad (3.45)$$

Since $\Omega_{-\kappa} = \Omega_{\kappa}$ from (3.43), the first and second sums physically represent plane wave modes propagating in all directions, and hence, only one of the two sums suffices to express the modal expansion of a general traveling wave solution. Therefore, when only one sum is needed to capture this physics, and it can be expressed as

$$\Phi(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{\kappa}} s_{\mathbf{\kappa}}(0)e^{-i\Omega_{\kappa}t}e^{i\mathbf{\kappa}\cdot\mathbf{r}} \quad (3.46)$$

Alternatively, the above can be rewritten as

$$\Phi(\mathbf{r}, t) = \frac{1}{2\sqrt{V}} \sum_{\mathbf{\kappa}} [s_{\mathbf{\kappa}}(0)e^{-i\Omega_{\kappa}t}e^{i\mathbf{\kappa}\cdot\mathbf{r}} + s_{\mathbf{\kappa}}^*(0)e^{i\Omega_{\kappa}t}e^{-i\mathbf{\kappa}\cdot\mathbf{r}}] \quad (3.47)$$

The second term comes from that the left-hand side of (3.46) is real-valued, hence taking its complex conjugation yields the same value. The last form is preferred so as to keep each mode real-valued. So for a traveling wave mode, the amplitude $s_{\mathbf{\kappa}}(t) = s_{\mathbf{\kappa}}(0)e^{-i\Omega_{\kappa}t}$ is already a rotating wave. Moreover, using the above to find $|P_{k,\Phi}|^2$ and $|Q_{k,\Phi}|^2$, they are always constants of time and equal to each other. The same phenomenon is observed when one converts the vector potential modes to traveling wave modes. The same goes for the electric and magnetic field modes. Another example of a traveling wave mode is a Bloch-Floquet mode [14]. If the periodic boundary condition is applied to the anisotropic inhomogeneous medium case, then Bloch-Floquet modes will ensue.

3.5.2 Standing Wave Modes

For a standing wave mode, Φ_k is equi-phase, and without loss of generality, Φ_k can be assumed real. In this case, to guarantee the realness of Φ in (3.1), then $s_k(t)$ must be real. Therefore, the general solution for $s_k(t)$ is

$$s_k(t) = b_k \cos(\Omega_k t + \theta_k), \quad \partial_t s_k(t) = -\Omega_k b_k \sin(\Omega_k t + \theta_k) \quad (3.48)$$

where b_k and θ_k are real. It is clear that $|\partial_t s_k(t)|^2 + \Omega_k^2 |s_k(t)|^2$ is a constant of time. Then, using the definitions of $|P_{k,\Phi}|^2$ and $|Q_{k,\Phi}|^2$, it is clear that the corresponding Hamiltonian for the scalar potential, H_{Φ} defined in (3.11), is also a constant of time. In this case, the Hamiltonian for each individual mode is analogous to a lone harmonic oscillator where $|P_{k,\Phi}|^2$ and $|Q_{k,\Phi}|^2$ correspond to the ‘‘potential’’ and ‘‘kinetic’’ energies stored. Their time variations correspond to the swapping of these two energies, as in a pendulum or a simple harmonic oscillator.

The same argument can be applied to $\alpha_k(t)$ and $\partial_t \alpha_k(t)$, showing that $|\partial_t \alpha_k(t)|^2 + \Omega_k^2 |\alpha_k(t)|^2$ is time independent, and convincing one that the Hamiltonian for the vector potential, H_A in (3.21), is a constant of time. By the same token, this can be applied to the total Hamiltonian in (3.29).

3.6 Constancy of Hamiltonian

It is seen above that the Hamiltonians for the scalar, vector, and electromagnetics cases are time independent both for the traveling wave case as well as the standing wave case, albeit for quite different reasons. In the traveling wave case, $P_k(t)$ and $Q_k(t)$ are complex functions with $e^{-i\Omega_k t}$ time dependence, but $|P_k|^2$ and $|Q_k|^2$ are real, time independent, and equal to each other, or $\frac{1}{2}(|P_k|^2 + |Q_k|^2) = |B_k|^2$. Therefore, the Hamiltonian can be written as

$$H = \sum_k B_k(t)B_k^*(t) \quad (3.49)$$

where $B_k(t) \sim e^{-i\Omega_k t}$ is a rotating wave.

For the standing wave case, since $P_k(t)$ and $Q_k(t)$ are real sinusoidal functions similar to the case in (3.48). One can define $B_k(t) = \frac{1}{\sqrt{2}} [iP_k(t) + Q_k(t)]$ which naturally become a rotating wave with $e^{-i\Omega_k t}$ time dependence. Then the Hamiltonian defined by (3.49) is manifestly a constant of time. For the electromagnetic field case, since B_k is a linear superposition of the \mathbf{E} and \mathbf{H} fields in quadrature phase, it is related to the Beltrami field [15].

4 Quantization via Mode Decomposition

The mode decomposition approach gives a lucidly clear picture of the coupled harmonic oscillators as a sum of individual harmonic oscillators each of which is a natural or resonant mode. It is also given in most text books. Equations (3.29) and (3.49) give the physical picture that when the coupled harmonic oscillators are expressed in terms of the natural modes of the equations of motion, be it traveling wave modes or standing wave modes, one can clearly see that the Hamiltonian of spatially coupled harmonic oscillators is the sum of the individual Hamiltonians of the harmonic oscillators corresponding to the natural modes of the system: each of them is a lone harmonic oscillator. So when the system is elevated to a quantum system, each of the harmonic oscillators is elevated to be a quantum harmonic oscillator individually with a resonant frequency of Ω_k as in the case of the lone harmonic oscillator.

4.1 Factorized Schrödinger Equation for Lone Quantum Harmonic Oscillator

At this juncture, it is prudent to revisit the lone harmonic oscillator case. One needs to connect quantum Hamiltonian of

$$\hat{H}\psi_n(q) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2}m\Omega^2 q^2 \right) \psi_n(q) = E_n\psi_n(q) \quad (4.1)$$

with classical Hamiltonian defined by

$$H = \frac{1}{2} [P^2(t) + Q^2(t)] = \frac{1}{2} [iP(t) + Q(t)] [-iP(t) + Q(t)] = B(t)B^*(t) = \frac{1}{2} (B(t)B^*(t) + B^*(t)B(t)) \quad (4.2)$$

To this end, it is necessary to cast the quantum Hamiltonian into a similar form. On defining a new variable $\xi = \sqrt{\frac{m\Omega}{\hbar}}q$, and then defining

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} \left(-\frac{d}{d\xi} + \xi \right), \quad (4.3)$$

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\frac{d}{d\xi} + \xi \right), \quad (4.4)$$

The above are actually the sloppy notation of these operators in coordinate representation. It can be shown that (4.1) becomes [16, 17]

$$\hat{H}\psi_n(q) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2}m\Omega^2 q^2 \right) \psi_n(q) = \frac{1}{2}\hbar\Omega (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \psi_n(\xi) = E_n\psi_n(\xi) \quad (4.5)$$

where with the abuse of notation, the new wave function is $\psi_n(\xi)$. In the above, \hat{a}^\dagger is called the creation (raising) operator, and \hat{a} is the annihilation (lowering) operator. Furthermore, it can be easily shown that the commutator ¹

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \hat{I} \quad (4.6)$$

The Hamiltonian can then be defined as

$$\hat{H} = \frac{1}{2}\hbar\Omega (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \hbar\Omega \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right) \quad (4.7)$$

¹Sometimes, this is used as the quantum postulate, rather than the commutation $[\hat{p}, \hat{q}]$.

The above Hamiltonian is in the Schrödinger picture. The corresponding Hamiltonian in the Heisenberg picture can be easily derived using (6.3) in Part I, or as in the Appendix C.

$$\hat{H} = \frac{1}{2}\hbar\Omega [\hat{a}(t)\hat{a}^\dagger(t) + \hat{a}^\dagger(t)\hat{a}(t)] \quad (4.8)$$

Previously, the quantum Hamiltonian has been obtained by elevating the conjugate variables p and q to their quantum operator forms. By the same token, comparing the above with (4.2), one can infer that the quantum Hamiltonian can be obtained from the above equations by the following inference or elevations:

$$B(t) \rightarrow \sqrt{\hbar\Omega}\hat{a}(t), \quad B^*(t) \rightarrow \sqrt{\hbar\Omega}\hat{a}^\dagger(t) \quad (4.9)$$

One can further define that

$$\hat{\pi} = \frac{-i}{\sqrt{2}} \frac{d}{d\xi}, \quad \hat{\zeta} = \frac{\xi}{\sqrt{2}} \quad (4.10)$$

then

$$\hat{a} = i\hat{\pi} + \hat{\zeta}, \quad \hat{a}^\dagger = -i\hat{\pi} + \hat{\zeta} \quad (4.11)$$

and the Hamiltonian can further be written as

$$\hat{H} = \frac{1}{2}\hbar\Omega (\hat{\pi}^2 + \hat{\zeta}^2) = \frac{1}{2}\hbar\Omega (\hat{\pi}^2(t) + \hat{\zeta}^2(t)) \quad (4.12)$$

where the latter form can be easily shown to be in the Heisenberg picture. By comparing the above with (4.2), one can infer that the above quantum Hamiltonian can also be obtained by the following elevations:

$$P(t) \rightarrow \sqrt{\hbar\Omega}\hat{\pi}(t), \quad Q(t) \rightarrow \sqrt{\hbar\Omega}\hat{\zeta}(t) \quad (4.13)$$

In the above, \hat{a} is a non-Hermitian operator, while $\hat{\pi}$ and $\hat{\zeta}$ are Hermitian operators [16,17]. Also, these operators have been expressed in their coordinate representation of the basis $|\xi\rangle$.

4.2 Connecting Classical Hamiltonian to Quantum Hamiltonian–Mode Decomposition Approach

As a result, by writing the classical Hamiltonian in (3.49) more suggestively as

$$H = \frac{1}{2} \sum_k [B_k(t)B_k^*(t) + B_k^*(t)B_k(t)] \quad (4.14)$$

each term of the above now becomes similar to the Hamiltonian of a lone quantum harmonic oscillator. Therefore, by letting

$$B_k(t) \rightarrow \sqrt{\hbar\Omega_k}\hat{a}_k(t), \quad B_k^*(t) \rightarrow \sqrt{\hbar\Omega_k}\hat{a}_k^\dagger(t) \quad (4.15)$$

the classical Hamiltonian can thus be elevated to be a quantum Hamiltonian as

$$\hat{H} = \frac{1}{2} \sum_k \hbar\Omega_k (\hat{a}_k(t)\hat{a}_k^\dagger(t) + \hat{a}_k^\dagger(t)\hat{a}_k(t)) \quad (4.16)$$

Similarly, by letting

$$P_k(t) \rightarrow \sqrt{\hbar\Omega_k}\hat{\pi}_k(t), \quad Q_k(t) \rightarrow \sqrt{\hbar\Omega_k}\hat{\zeta}_k(t) \quad (4.17)$$

the classical Hamiltonian for each mode can be elevated to become

$$\hat{H} = \frac{1}{2} \sum_k \hbar \Omega_k \left(\hat{\pi}_k^2(t) + \hat{\zeta}_k^2(t) \right) \quad (4.18)$$

In this manner, the quantum version of the Hamiltonian can be arrived at.

Alternatively, one can elevate the field to be quantum operators in the classical Hamiltonian by the procedure of letting

$$\hat{\Phi}(\mathbf{r}, t) = \sum_k \hat{s}_k(t) \Phi_k(\mathbf{r}) = \sum_k \hat{s}_k^\dagger(t) \Phi_k^*(\mathbf{r}) = \frac{1}{2} \sum_k \left[\hat{s}_k(t) \Phi_k(\mathbf{r}) + \hat{s}_k^\dagger(t) \Phi_k^*(\mathbf{r}) \right] \quad (4.19)$$

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \sum_k \hat{\alpha}_k(t) \mathbf{A}_k(\mathbf{r}) = \sum_k \hat{\alpha}_k^\dagger(t) \mathbf{A}_k^*(\mathbf{r}) = \frac{1}{2} \sum_k \left[\hat{\alpha}_k(t) \mathbf{A}_k(\mathbf{r}) + \hat{\alpha}_k^\dagger(t) \mathbf{A}_k^*(\mathbf{r}) \right] \quad (4.20)$$

where $\hat{s}_k(t)$ and $\hat{\alpha}_k(t)$ are now quantum operators. The last forms above are preferred as they keep the field operator for each mode to be Hermitian, especially for the traveling wave case. The above equalities are based only on mathematical logic, and that $\hat{\Phi}(\mathbf{r}, t)$ and $\hat{\mathbf{A}}(\mathbf{r}, t)$ are Hermitian operators.

Going through the same mode decomposition algebra as before, one can arrive at the aforementioned quantum Hamiltonians. If the modes are traveling wave modes as in the free space case, then the field operators can be written as

$$\hat{\mathbf{E}}(\mathbf{r}, t) = \frac{1}{2} \sum_k \sqrt{\hbar \Omega_k} \left[\hat{a}_k e^{-i\Omega_k t} \mathbf{E}_k(\mathbf{r}) + \hat{a}_k^\dagger e^{i\Omega_k t} \mathbf{E}_k^*(\mathbf{r}) \right] \quad (4.21)$$

$$\hat{\mathbf{H}}(\mathbf{r}, t) = \frac{1}{2} \sum_k \sqrt{\hbar \Omega_k} \left[\hat{a}_k e^{-i\Omega_k t} \mathbf{H}_k(\mathbf{r}) + \hat{a}_k^\dagger e^{i\Omega_k t} \mathbf{H}_k^*(\mathbf{r}) \right] \quad (4.22)$$

where the sum over k is over all traveling wave modes. In the index k above, the polarizations of the modes are also incorporated.

4.3 Circuit View of the Mode Decomposition Picture

The fact that a mode can be viewed as a quantum simple harmonic oscillator is because a mode is due to the coupling of infinitely many quantum simple harmonic oscillators made from electron-positron (e-p) pairs. As long as these oscillators are coupled to form a mode, and remain in quantum coherence, the macroscopic oscillator thus formed are in quantum coherence, and hence, is still a quantum harmonic oscillator, even though the mode involves the coherent coupling of many quantum simple harmonic oscillators spread over space.

One can think likewise of the LC tank circuit [19]. Even though it is a macroscopic oscillator spread over space, it is due to the coupling of the many quantum simple harmonic oscillators formed by e-p pairs at the fundamental level. The equations of motion for a tank circuit can be easily written and derived in classical as well as quantum forms. Alternatively, one can draw an analogue of each mode to a LC tank resonator, and write down its equations of motion. This picture is shown in Figure 2.

Figure 2 shows that the total Hamiltonian of the electromagnetic field can be expressed as a superposition of energy stored in each independent eigenmode. Each eigenmode behaves like a LC resonator or harmonic oscillator, where the electric energy ($\frac{1}{2} \frac{Q^2}{C}$ or $\frac{1}{2} m \Omega^2 q^2$) is stored in capacitors, and magnetic energy ($\frac{1}{2} L \phi^2$ or $\frac{1}{2} m p^2$) is stored in inductors, and $\Omega = 1/(LC)$ is the resonant frequency of the tank circuit. Here, ϕ and Q denote magnetic flux and electric charge, and p and q denote momentum and coordinate. Analogous to the classical harmonic oscillator, the quantum harmonic oscillator obeys the same Hamilton equations of motion (see the right side of Figure 2).

The momentum and coordinate operators satisfy the commutation relation if the de Broglie and Schrödinger postulates are made. The energy level (eigen-energy) of each quantum harmonic oscillator is $(n + \frac{1}{2}) \hbar \Omega$. The lowest energy $\frac{1}{2} \hbar \Omega$ of the quantum harmonic oscillator is called the zero-point energy, which is responsible for many quantum electrodynamic effects including spontaneous emission, Casimir force, etc. Due to the zero-point energy, the vacuum electromagnetic field still fluctuates even when the Kelvin temperature is equal to zero [36].

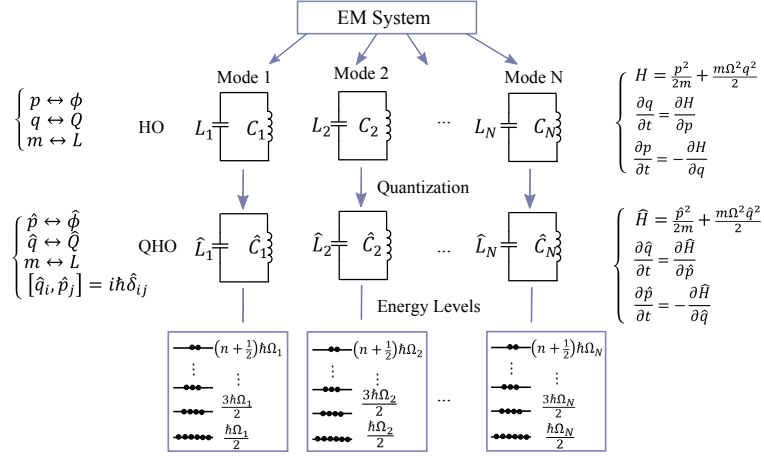


Figure 2: It is shown here that the mode decomposition picture for quantization of Maxwell's equations can be related to the resonance of many LC resonators (tank circuits). Each mode can be represented by a single LC tank circuit.

5 Impressed Sources in the Hamiltonians

If the term [18]

$$\mathbf{A}(\mathbf{r}, t) \cdot \mathbf{J}_{\text{ext}}(\mathbf{r}, t) \quad (5.1)$$

is added to the Hamiltonian density of the vector potential part, and

$$\Phi(\mathbf{r}, t)\varrho_{\text{ext}}(\mathbf{r}, t) \quad (5.2)$$

is added to the Hamiltonian density of the scalar potential part, upon taking the functional derivatives, the equations of motion with a source term result. For instance, the classical Hamiltonian can be modified to be

$$H_{\Phi} = \frac{1}{2} \int d\mathbf{r} \left[(\Pi_s(\mathbf{r}, t))^2 + (\nabla\Phi(\mathbf{r}, t))^2 - 2\Phi(\mathbf{r}, t)\varrho_{\text{ext}}(\mathbf{r}, t) \right] \quad (5.3)$$

These sources are external sources that do not vary when the variation with respect to the fields is taken. Hence, they are immutable with respect to the change of the conjugate variables, Π_s and Φ . In classical electromagnetics, these are called impressed sources [20].

By taking the variation of the above Hamiltonian with respect to the conjugate variables Π_s and Φ , the resultant equation of motion for the scalar potential becomes

$$\partial_t^2 \Phi(\mathbf{r}, t) - \nabla^2 \Phi(\mathbf{r}, t) = \varrho_{\text{ext}}(\mathbf{r}, t) \quad (5.4)$$

Similarly, if the Hamiltonian for the vector potential is modified to be

$$H_A = \frac{1}{2} \int d\mathbf{r} \left[(\mathbf{\Pi}(\mathbf{r}, t))^2 + (\nabla \times \mathbf{A}(\mathbf{r}, t))^2 + (\nabla \cdot \mathbf{A}(\mathbf{r}, t))^2 - 2\mathbf{A}(\mathbf{r}, t) \cdot \mathbf{J}_{\text{ext}}(\mathbf{r}, t) \right] \quad (5.5)$$

then the resultant equation of motion for the vector potential is

$$\nabla \times \nabla \times \mathbf{A}(\mathbf{r}, t) - \nabla(\nabla \cdot \mathbf{A}(\mathbf{r}, t)) + \partial_t^2 \mathbf{A}(\mathbf{r}, t) = \mathbf{J}_{\text{ext}}(\mathbf{r}, t) \quad (5.6)$$

The external current sources are impressed sources in this case. The above can be extended to the anisotropic inhomogeneous medium case yielding the classical equations of motion as

$$\nabla \cdot \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}, t) - \partial_t^2 \chi(\mathbf{r}) \Phi(\mathbf{r}, t) = -\varrho_{\text{ext}}(\mathbf{r}, t) \quad (5.7)$$

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{A}(\mathbf{r}, t) - \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \nabla (\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t)) + \partial_t^2 \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t) = \mathbf{J}_{\text{ext}}(\mathbf{r}, t) \quad (5.8)$$

5.1 Green's Functions

Since we have two kinds of source-driven equations, one for the scalar potential, and one for the vector potential, two kinds of Green's functions can be derived. Since their derivations are similar, the Green's function for the vector potential will be discussed first.

The Green's function for vector potential can be expressed in terms of a dyadic Green's function that relates two field quantities:

$$\mathbf{A}(\mathbf{r}, t) = \int d\mathbf{r}' \overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', t) \circledast \mathbf{J}_{\text{ext}}(\mathbf{r}', t) \quad (5.9)$$

where the ‘‘circled asterisk’’ means ‘‘convolution’’ in time, whereas the $d\mathbf{r}'$ integral is a convolution in space. To avoid the use of the convolution notation, it is best that the above relationship is expressed in the frequency domain, namely,

$$\mathbf{A}(\mathbf{r}, \omega) = \int d\mathbf{r}' \overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) \cdot \mathbf{J}_{\text{ext}}(\mathbf{r}', \omega) \quad (5.10)$$

The source driven equations for inhomogeneous anisotropic medium are given in (5.7) and (5.8). One can expand the solution in terms of the auxiliary eigenmodes of the above. To this end, one lets

$$\mathbf{A}(\mathbf{r}, \omega) = \sum_m \mathbf{A}_k(\mathbf{r}) a_k(\omega) \quad (5.11)$$

Substituting this into (3.15), and making use of the fact that the eigenmodes satisfy the eigenequation, one arrives at

$$\sum_k (\Omega_k^2 - \omega^2) \overline{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \mathbf{A}_k(\mathbf{r}) a_k(\omega) = \mathbf{J}_{\text{ext}}(\mathbf{r}, \omega) \quad (5.12)$$

Using the orthonormality relationship of the eigenmodes yields

$$(\Omega_k^2 - \omega^2) a_k(\omega) = \int d\mathbf{r}' \mathbf{A}_k^*(\mathbf{r}') \cdot \mathbf{J}_{\text{ext}}(\mathbf{r}', \omega) \quad (5.13)$$

Accordingly,

$$\mathbf{A}(\mathbf{r}, \omega) = \sum_k \frac{1}{\Omega_k^2 - \omega^2} \mathbf{A}_k(\mathbf{r}) \int d\mathbf{r}' \mathbf{A}_k^*(\mathbf{r}') \cdot \mathbf{J}_{\text{ext}}(\mathbf{r}', \omega) \quad (5.14)$$

One can subsequently identify the dyadic Green's function to be [13]

$$\overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) = \sum_k \frac{\mathbf{A}_k(\mathbf{r}) \mathbf{A}_k^*(\mathbf{r}')}{\Omega_k^2 - \omega^2} \quad (5.15)$$

The dyadic Green's function in the time domain is related to that in the frequency domain by the Fourier inverse integral, namely,

$$\overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) \quad (5.16)$$

In order to ensure causality, the Fourier inversion contour in the complex ω plane has to be above the poles in (5.15).

Defining similar Green's function for the scalar potential case, one arrives at

$$\Phi(\mathbf{r}, t) = \int d\mathbf{r}' g(\mathbf{r}, \mathbf{r}', t) \circledast \varrho_{\text{ext}}(\mathbf{r}', t) \quad (5.17)$$

and

$$\Phi(\mathbf{r}, \omega) = \int d\mathbf{r}' g(\mathbf{r}, \mathbf{r}', \omega) \varrho_{\text{ext}}(\mathbf{r}', \omega) \quad (5.18)$$

where

$$g(\mathbf{r}, \mathbf{r}', \omega) = \sum_k \frac{\Phi_k(\mathbf{r}) \Phi_k^*(\mathbf{r}')}{\Omega_k^2 - \omega^2} \quad (5.19)$$

and its time domain version can be obtained by a Fourier inverse transform.

5.2 The Quantum Case

When sources are introduced, the Hamiltonians in the quantum case are elevated from that for classical case in (5.3). For the scalar potential case, it is

$$\hat{H}_\Phi = \frac{1}{2} \int d\mathbf{r} \left[\left(\hat{\Pi}_s(\mathbf{r}, t) \right)^2 + \left(\nabla \hat{\Phi}(\mathbf{r}, t) \right)^2 - 2\hat{\Phi}(\mathbf{r}, t) \hat{\varrho}_{\text{ext}}(\mathbf{r}, t) \right] \quad (5.20)$$

Both the fields and the sources are elevated to be quantum operators. Since the source $\hat{\varrho}_{\text{ext}}(\mathbf{r}, t)$ is external, it should be an operator that operates on the state vector of another quantum system that is independent of the change in the primary quantum system. The state of the quantum system should be described by the product of $|\psi_{\text{field}}\rangle|\psi_{\text{source}}\rangle$. Since the operators are in the Heisenberg picture, these state vectors should be their initial value at $t = 0$.

In the above, since the field operator $\hat{\Phi}(\mathbf{r}, t)$ and the source operator $\hat{\varrho}_{\text{ext}}(\mathbf{r}, t)$ operate on different independent Hilbert space vectors, if each of them is a Hermitian operator, the matrix representation of the product of these two matrices remain Hermitian. They are like direct product of two matrices. The above scenario can occur when one considers the atom-field interaction system [18] where the atom produces a source that feeds into the field system, but there is no back-action of the field onto the atom system.

Then the resultant equation of motion for the scalar potential operator becomes

$$\partial_t^2 \hat{\Phi}(\mathbf{r}, t) - \nabla^2 \hat{\Phi}(\mathbf{r}, t) = \hat{\varrho}_{\text{ext}}(\mathbf{r}, t) \quad (5.21)$$

Similarly, if the classical Hamiltonian for the vector potential is elevated to be quantum, the corresponding quantum Hamiltonian is

$$\hat{H}_A = \frac{1}{2} \int d\mathbf{r} \left[\left(\hat{\Pi}(\mathbf{r}, t) \right)^2 + \left(\nabla \times \hat{\mathbf{A}}(\mathbf{r}, t) \right)^2 + \left(\nabla \cdot \hat{\mathbf{A}}(\mathbf{r}, t) \right)^2 - 2 \hat{\mathbf{A}}(\mathbf{r}, t) \cdot \hat{\mathbf{J}}_{\text{ext}}(\mathbf{r}, t) \right] \quad (5.22)$$

The same remark applies to the product of two operators that act on two independent Hilbert vector spaces as that in (5.20). By taking the variation of the above, then the resultant equation of motion for the vector potential is

$$\nabla \times \nabla \times \hat{\mathbf{A}}(\mathbf{r}, t) - \nabla(\nabla \cdot \hat{\mathbf{A}}(\mathbf{r}, t)) + \partial_t^2 \hat{\mathbf{A}}(\mathbf{r}, t) = \hat{\mathbf{J}}_{\text{ext}}(\mathbf{r}, t) \quad (5.23)$$

The external current sources are impressed sources in this case. The source-driven quantum equations of motion for the anisotropic inhomogeneous media can be similarly derived yielding

$$\nabla \cdot \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \nabla \hat{\Phi}(\mathbf{r}, t) - \partial_t^2 \chi(\mathbf{r}) \hat{\Phi}(\mathbf{r}, t) = -\hat{\varrho}_{\text{ext}}(\mathbf{r}, t) \quad (5.24)$$

$$\nabla \times \bar{\boldsymbol{\mu}}^{-1}(\mathbf{r}) \cdot \nabla \times \hat{\mathbf{A}}(\mathbf{r}, t) - \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \nabla \left(\chi^{-1}(\mathbf{r}) \nabla \cdot \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \hat{\mathbf{A}}(\mathbf{r}, t) \right) + \partial_t^2 \bar{\boldsymbol{\epsilon}}(\mathbf{r}) \cdot \hat{\mathbf{A}}(\mathbf{r}, t) = \hat{\mathbf{J}}_{\text{ext}}(\mathbf{r}, t) \quad (5.25)$$

The Green's function relation can be similarly derived for the quantum case as follows:

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \int d\mathbf{r}' \bar{\mathbf{G}}(\mathbf{r}, \mathbf{r}', t) \otimes \hat{\mathbf{J}}_{\text{ext}}(\mathbf{r}', t) \quad (5.26)$$

$$\hat{\Phi}(\mathbf{r}, t) = \int d\mathbf{r}' g(\mathbf{r}, \mathbf{r}', t) \otimes \hat{\varrho}_{\text{ext}}(\mathbf{r}', t) \quad (5.27)$$

Hence, the Green's function technique is still very useful for quantum effects calculations.

From (5.24) and (5.25) above, by defining that $\hat{\mathbf{B}}(\mathbf{r}, t) = \nabla \times \hat{\mathbf{A}}(\mathbf{r}, t)$, $\hat{\mathbf{E}}(\mathbf{r}, t) = -\partial_t \hat{\mathbf{A}}(\mathbf{r}, t) - \nabla \hat{\Phi}(\mathbf{r}, t)$, $\hat{\mathbf{D}}(\mathbf{r}, t) = \bar{\epsilon} \cdot \hat{\mathbf{E}}(\mathbf{r}, t)$, one can show that the quantum Maxwell's equations of motion for the anisotropic inhomogeneous medium case are

$$\nabla \times \hat{\mathbf{H}}(\mathbf{r}, t) - \partial_t \hat{\mathbf{D}}(\mathbf{r}, t) = \hat{\mathbf{J}}_{\text{ext}}(\mathbf{r}, t), \quad \nabla \times \hat{\mathbf{E}}(\mathbf{r}, t) + \partial_t \hat{\mathbf{B}}(\mathbf{r}, t) = 0, \quad (5.28)$$

$$\nabla \cdot \hat{\mathbf{D}}(\mathbf{r}, t) = \hat{\varrho}_{\text{ext}}(\mathbf{r}, t), \quad \nabla \cdot \hat{\mathbf{B}}(\mathbf{r}, t) = 0. \quad (5.29)$$

These quantum operators need to act on a quantum state vector, to generate a state vector that is representative of the fields. Hence, a classical field, which can be described by a three component vector, now needs to replace each of its component by a state vector with infinite dimension. The potential for encoding quantum information in these fields is greatly increased!

The above external current formulation can be used to couple free field to simple harmonic oscillators formed by Drude-Lorentz-Sommerfeld model. They can also be used to couple free field to the particle current in an atom in a field-atom calculation. These cases will be shown in our future works. In the next section we outline the very rudiments of field-atom interactions considered using the fully quantized Maxwell's equations.

6 Field-Atom Interactions

The quantized Maxwell's equations presented above is essential to the fully quantum mechanical description of field-atom interactions. With the invention of artificial atoms in recent decades [42], this field is becoming increasingly important and will benefit greatly from the active participation of the electrical engineering community. To include atoms in the description, one may wish to extend the quantized Maxwell's equations to include quantum sources, resulting in the quantized Maxwell-Lorentz equations. However, the resulting equations are too cumbersome for descriptions of atoms. Hence, considerable simplification is typically made on the atomic part.

The goal is to solve the atom-field dynamics governed by some Hamiltonian, which in simple scenarios, can be the electric dipole Hamiltonian. For a single two level atom coupled to the electric field, we have [18]

$$\hat{H}_{ed} = \frac{1}{2} \hbar \omega_0 \hat{\sigma}_z + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \hbar \left(g(\mathbf{k}, \mathbf{r}_0) \hat{a}_{\mathbf{k}} \hat{\sigma}_+ + g^*(\mathbf{k}, \mathbf{r}_0) \hat{a}_{\mathbf{k}}^\dagger \hat{\sigma}_- \right) \quad (6.1)$$

Here the first term represents the quantized two level atom, with a transition frequency of ω_0 . The second represents the quantized electromagnetic fields in mode decomposed picture. The summation over the field modes typically runs through three wavenumber indices, and a polarization index. Here we choose to denote everything generically by \mathbf{k} . The last term represents the dipole interaction between the two level atom and the electric field. We may identify the term with $\hat{a}_{\mathbf{k}}$ as representing absorption of a photon by the atom, while the other term, emission. The coupling coefficient $g(\mathbf{k}, \mathbf{r}_0)$ are dependent on the dipole moment of the particular atomic transition, as well as the \mathbf{k} -th mode of the electric field local to the position of the atom. Note that it is a function of both the position of the atom and the wavenumber of the field modes.

The above electric dipole Hamiltonian is highly simplified. To derive it, one would start from a first principle minimal coupling Hamiltonian, which corresponds with the quantized Maxwell-Lorentz equations [18]. Then the long wavelength and rotating wave approximations are applied. Simplification made to the atomic part may include the neglect of diamagnetic interactions (interactions of the currents internal to the atom with the magnetic field) and few level approximation of the atom. The fully quantized Maxwell's equations play an essential role in the understanding of the above approximations. For cases where the electric dipole Hamiltonian is inadequate and more elaborate atom-field interactions desired, the full force of the quantized Maxwell's equations are needed.

Going back to the electric dipole Hamiltonian, a striking feature of the solution to the atom-field dynamics is the appearance and usefulness of the classical dyadic Green's function. For example, the decay rate and radiative shift of the atom are related to the imaginary and real parts of the classical dyadic Green's function, evaluated at

the position of the atom. This relates the important modification of spontaneous emission for atoms, sometimes termed the Purcell effect [41], to the classical dyadic Green's function. This type of modification has been shown in our previous work, which utilized the dyadic Green's function in a semi-classical setting [43]. With the quantized Maxwell's equations, scattering from a single two level atom can be studied fully quantum mechanically. However, the classical dyadic Green's function still plays an essential role in the scattering dynamics, as well as the in the electromagnetic field associated with the scattered photon. This will be shown in a future work. When multiple atoms are involved, the dyadic Green's function linking the positions of the atoms becomes important with the advent of multiple scattering [38].

Another important feature of the quantized Maxwell's equations is the prediction of vacuum fluctuations of the electromagnetic field. The spontaneous emission of atoms mentioned above can be explained as a consequence of coupling to the fluctuating electromagnetic vacuum. The Casimir force between closely spaced objects is understood to be another such consequence. Due to the close analogy between the quantum mechanical and classical Maxwell's equations, the classical dyadic Green's function is still important in the calculation of the Casimir force [44].

7 Conclusion

In this work, the quantization of electromagnetic fields has been presented from a different viewpoint. The vector and scalar potential formulation is used with a generalized Lorenz gauge [5]. The view of electromagnetic field propagation through space is presented as the coupling of harmonic oscillators via Maxwell's equations.

To enhance our understanding of a quantum Maxwellian system, we look at the classical and quantum mechanics of a lone harmonic oscillator. A new simple way to look at Hamiltonian mechanics is introduced that avoids the ceremony of Lagrangian mechanics followed by Legendre transform. Furthermore, classical electromagnetic theory from classical Hamiltonian mechanics is presented. For the quantum case, a new set of quantum Hamilton equations of motion is derived, with striking similarities to the classical Hamilton equations. In this manner, quantized forms of the equations of motion for scalar and vector potential fields are easily obtained once their classical Hamiltonians are derived. The equations of motion are in the coordinate (\mathbf{r}, t) space without having to go through the mode-decomposition approach. Furthermore, the mode decomposition approach is presented to show its connection and equivalence to these quantized equations. The Green's function approach in solving these equations is also discussed.

A lucid understanding of these quantum equations of motion can potentially open a new area of research in allowing the combination of electromagnetics with quantum electromagnetics (QEM). They could be important in the future development of quantum technologies. Examples are quantum information, quantum cryptography, computing, communication, etc.

Moreover, this work shows that the concept of Green's function is equally important in quantum effects as in classical effects. Hence, the host of knowledge developed in computational electromagnetics in solving classical Maxwell's equations are still useful in quantum technologies of the future [21–35]. It is also explained why the quantum Maxwell's equations of motion can greatly increase the potential for encoding quantum information.

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Appendix A Dirac Notation

The Dirac notation for the inner product between two vectors (also called functions) is

$$\langle f|g\rangle = \int d\mathbf{r} f^*(\mathbf{r})g(\mathbf{r}) \quad (\text{A.1})$$

This notation is in line with that of the mathematics community, where a complex conjugation is always used on one of the functions. The corresponding inner product is defined as in the mathematics community

$$\langle f, g\rangle = \int d\mathbf{r} f^*(\mathbf{r})g(\mathbf{r}) \quad (\text{A.2})$$

But in the electromagnetics community, two kinds of inner products are used, the energy inner product such as the above, and the reaction inner product where the functions are complex, but a complex conjugation is not taken on one of the functions. The reaction inner product is expressed as [26]

$$\langle f, g\rangle = \int d\mathbf{r} f(\mathbf{r})g(\mathbf{r}) \quad (\text{A.3})$$

When $f = g$ in the Dirac, or the energy inner product, (A.1) or (A.2) gives rise to a positive definite number, making it a useful measure for length of a vector, called the metric or the norm. The norm is proportional to the energy of the function, and Hilbert spaces correspond to infinite dimensional vector spaces where the vectors or functions have finite norm or energy.

In Dirac notation, the expectation value of an operator \hat{q} which is an observable is

$$\bar{q}(t) = \langle \hat{q} \rangle = \langle \psi | \hat{q} | \psi \rangle = \int_{-\infty}^{\infty} dq |\psi(q, t)|^2 q \quad (\text{A.4})$$

For a general operator, its expectation value is

$$\bar{O}(t) = \langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle \quad (\text{A.5})$$

For a quantum operator representing an observable, the expectation value of the quantum operator yields a measurable or observable quantity in the real world implying that $\bar{O}(t)$ is real valued. As a result, \hat{O} has to be a Hermitian operator with real eigenvalues [16, 17].

Appendix B Identity Operators and Matrix Representations

There is a close relationship between operations in Hilbert space in Dirac notation and operations in finite dimensional vector space in linear algebraic notation. A one-to-one map can be established between the vector operations in Hilbert space and the vector operations in linear algebra, as shown below

$$|f\rangle \leftrightarrow \mathbf{f}, \quad \langle g| \leftrightarrow \mathbf{g}^\dagger, \quad \langle g|f\rangle \leftrightarrow \mathbf{g}^\dagger \cdot \mathbf{f}, \quad (\text{B.1})$$

$$\langle q|q'\rangle = \delta(q - q') \leftrightarrow \mathbf{q}_i^\dagger \cdot \mathbf{q}_j = \delta_{ij} \quad (\text{B.2})$$

One can define an identity operator in a finite dimensional vector space spanned by a complete, orthonormal set of vectors \mathbf{q}_i , $i = 1, \dots, N$. This set is also called a basis set. An identity matrix operator is then

$$\bar{\mathbf{I}}_d = \sum_{j=1}^N \mathbf{q}_j \cdot \mathbf{q}_j^\dagger \quad (\text{B.3})$$

where the above is an outer product. The above can be verified as follows. First, assume that the set of orthonormal vectors \mathbf{q}_j , $j = 1, \dots, N$ or its complex conjugate is complete. Then given an arbitrary vector \mathbf{V} , it can be expanded in terms of these vectors as:

$$\mathbf{V} = \sum_j a_j \mathbf{q}_j = \sum_j \mathbf{q}_j \cdot \mathbf{q}_j^\dagger \cdot \mathbf{V} = \bar{\mathbf{I}}_d \cdot \mathbf{V} \quad (\text{B.4})$$

where the expansion coefficients a_j have been found by invoking the orthonormality of the vectors. By the same token,

$$\mathbf{V} = \sum_j b_j \mathbf{q}_j^\dagger = \sum_j \mathbf{V} \cdot \mathbf{q}_j \cdot \mathbf{q}_j^\dagger = \mathbf{V} \cdot \bar{\mathbf{I}}_d \quad (\text{B.5})$$

Therefore, it can be shown that for any vector \mathbf{V} in a finite dimensional vector space, $\mathbf{V} \cdot \bar{\mathbf{I}}_d = \bar{\mathbf{I}}_d \cdot \mathbf{V} = \mathbf{V}$, where $\bar{\mathbf{I}}_d$ as defined above behaves like a matrix identity operator.

Using the analogy in (B.1), the definition of an identity operator in an infinite dimensional Hilbert space becomes

$$\hat{I} = \int dq |f_q\rangle \langle f_q| \quad \text{or} \quad \hat{I} = \sum_{j=1}^{\infty} |f_j\rangle \langle f_j| \quad (\text{B.6})$$

The first case is for indenumerable (uncountably infinite) Hilbert space, while the second case is for denumerable (countably infinite) Hilbert space.

The Hilbert space operator \hat{O} acting on a state vector $|\psi\rangle$ is analogous to a matrix operator $\bar{\mathbf{O}}$ acting on a vector \mathbf{x} , namely,

$$\hat{O}|\psi\rangle \leftrightarrow \bar{\mathbf{O}} \cdot \mathbf{x} \quad (\text{B.7})$$

Given an operator equation $\hat{O}|\psi\rangle = |b\rangle$, one can insert an identity operator into this Hilbert space equation and obtain

$$\sum_{j=1}^{\infty} \hat{O}|f_j\rangle \langle f_j|\psi\rangle = |b\rangle \quad (\text{B.8})$$

Further testing or multiplying the above by $\langle f_i|$ leads to

$$\sum_{j=1}^{\infty} \langle f_i|\hat{O}|f_j\rangle \langle f_j|\psi\rangle = \langle f_i|b\rangle, \quad i = 1, \dots, \infty \quad (\text{B.9})$$

The above is similar to

$$\sum_{j=1}^{\infty} O_{ij} x_j = b_i, \quad i = 1, \dots, \infty \quad (\text{B.10})$$

where $O_{ij} = \langle f_i|\hat{O}|f_j\rangle$, $x_j = \langle f_j|\psi\rangle$, and $b_i = \langle f_i|b\rangle$. Here, O_{ij} is the matrix representation of \hat{O} , and x_j and b_i are the vector representations of $|\psi\rangle$ and $|b\rangle$, respectively. The above corresponds to an infinite dimensional matrix equation. One way to compute its solution is to truncate it into a finite dimensional matrix equation.

Repeating the exercise with the set of indenumerable basis, $|f_q\rangle$, one arrives at

$$\int dq \langle f_{q'}|\hat{O}|f_q\rangle \langle f_q|\psi\rangle = \langle f_{q'}|b\rangle, \quad \forall q' \quad (\text{B.11})$$

In this case, the matrix and vector representations in this basis are $\langle f_{q'}|\hat{O}|f_q\rangle$, $\langle f_q|\psi\rangle$, and $\langle f_{q'}|b\rangle$. The above is still an integral equation. There are many ways to convert the above into a matrix equation. One way is to use quadrature rules to replace the integral with summation.

Appendix C Time Evolution of Raising and Lowering Operators

In the Heisenberg picture, the Hamiltonian of the harmonic oscillator can be easily derived from (4.7), after using (6.3) from Part I, to be

$$\hat{H} = \frac{1}{2} \hbar \Omega [\hat{a}(t) \hat{a}^\dagger(t) + \hat{a}^\dagger(t) \hat{a}(t)] \quad (\text{C.1})$$

Since the raising and lowering operators have very similar commutator as the \hat{p} and \hat{q} operators, one can show that

$$\frac{d}{dt}\hat{a}(t) = -\frac{i}{\hbar} [\hat{a}, \hat{H}] = -\frac{i}{\hbar} \frac{\partial}{\partial \hat{a}^\dagger} \hat{H} = -i\Omega\hat{a}(t), \quad \frac{d}{dt}\hat{a}^\dagger(t) = -\frac{i}{\hbar} [\hat{a}^\dagger, \hat{H}] = \frac{i}{\hbar} \frac{\partial}{\partial \hat{a}} \hat{H} = i\Omega\hat{a}^\dagger(t) \quad (\text{C.2})$$

The above Heisenberg operators evolve with time as

$$\hat{a}(t) = \hat{a}(0)e^{-i\Omega t}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{i\Omega t} \quad (\text{C.3})$$

Furthermore, one can define that for an operator,

$$\hat{a} = \frac{1}{2} (\hat{a} + \hat{a}^\dagger) + \frac{1}{2} (\hat{a} - \hat{a}^\dagger) = \hat{a}_R + i\hat{a}_I \quad (\text{C.4})$$

where $\hat{a}_R = \frac{1}{2} (\hat{a} + \hat{a}^\dagger)$ and $\hat{a}_I = \frac{1}{2i} (\hat{a} - \hat{a}^\dagger)$ are Hermitian operators. Then

$$\hat{a}_R(t) = \hat{a}_R(0) \cos(\Omega t) + \hat{a}_I(0) \sin(\Omega t), \quad \hat{a}_I(t) = -\hat{a}_R(0) \sin(\Omega t) + \hat{a}_I(0) \cos(\Omega t), \quad (\text{C.5})$$

Consequently,

$$\hat{\zeta}(t) = \frac{1}{2} (\hat{a}(t) + \hat{a}^\dagger(t)) = \hat{a}_R(t), \quad \hat{\pi}(t) = \frac{1}{2i} (\hat{a}(t) - \hat{a}^\dagger(t)) = \hat{a}_I(t) \quad (\text{C.6})$$

Then one can show that

$$\hat{\zeta}(t) = \hat{a}_R(0) \cos(\Omega t) + \hat{a}_I(0) \sin(\Omega t), \quad \hat{\pi}(t) = -\hat{a}_R(0) \sin(\Omega t) + \hat{a}_I(0) \cos(\Omega t) \quad (\text{C.7})$$

The above can be used to connect the classical Hamiltonian to the quantum Hamiltonian.

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