Path-integral approach to electromagnetic phenomena in inhomogeneous systems

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We derive a path-integral expression for the time-evolution operator associated with the Maxwell's equations in an inhomogeneous medium and show that its asymptotic behavior for large light velocity corresponds to geometrical optics. We also describe a path-integral approach to the solution of the Laplace equation in an inhomogeneous medium. This approach leads to new numerical methods for the solution of Laplace and Poisson equations in inhomogeneous media of irregular shape. An expression for the image potential near a surface with continuously changing dielectric function is also derived.

INTRODUCTION

Optical properties of adsorbed molecules such as absorption line shapes, emission lifetimes and yields, and light-scattering cross sections are known to be strongly affected by the behavior of the local electromagnetic field near the surface. Evaluating the optical response of such molecules requires the ability to calculate the behavior of the electromagnetic field at such strongly inhomogeneous structures. The latter is a fundamental problem of electromagnetic theory that lies at the heart of many important physical phenomena (e.g., image potentials and solution energies).

Analytical solutions to this problem have been obtained for only very simple geometries characterized by high symmetry. Examples are the Fresnel equations of light reflection and transmission at a plane surface and the Mie theory of light scattering by a dielectric sphere and its extension to spheroids. For inhomogeneous media with less regular structure, solution of the problem requires large-scale numerical computations.

In this paper we describe two path-integral approaches to this problem. For the propagator of the Maxwell equations in an inhomogeneous medium we derive an exact path-integral representation, and we show that its $c \to \infty$ (c being the light velocity) limit corresponds to ray optics (Fermat principle). For electrostatic problems described by the Poisson equation we derive an exact path-integral representation of the corresponding Green's function. We show that the image potential of a charge near a dielectric surface and the related problem of the lifetime of an excited molecule near such a surface may be represented and solved with this formalism.

PATH-INTEGRAL FORMULATION OF THE MAXWELL EQUATIONS

We consider the Maxwell equations for a source-free medium:

$$\frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H}, \tag{1}$$

$$\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \tag{2}$$

$$\nabla \cdot \mathbf{D} = 0, \tag{3}$$

$$\nabla \cdot \mathbf{B} = 0. \tag{4}$$

We assume that the medium is linear and nondispersive; i.e.,

$$\mathbf{D} = \overleftrightarrow{\epsilon} \cdot \mathbf{E}, \tag{5}$$

$$\mathbf{B} = \overleftrightarrow{\mu} \cdot \mathbf{H}, \tag{6}$$

where $\overleftrightarrow{\epsilon}$ and $\overleftrightarrow{\mu}$ are the dielectric permittivity and the magnetic permeability dyadics, respectively. They are taken to be time-independent functions of space.

We start by transforming Eqs. (1)–(4) into a form similar to that of the Schrödinger equation. To this end we define the six-dimensional vector

$$\theta = (8\pi)^{-1/2}\mathcal{R}^{-1/2}\begin{bmatrix}\mathbf{E}\\ \mathbf{H}\end{bmatrix}, \tag{7}$$

where $\mathcal{R}$ is the six-dimensional matrix

$$\mathcal{R} = \begin{bmatrix}\overleftrightarrow{\epsilon} & 0\\ 0 & \overleftrightarrow{\mu}\end{bmatrix}. \tag{8}$$

We also introduce a set of three-dimensional matrices $\mathcal{L}_x$, $\mathcal{L}_y$, $\mathcal{L}_z$:

$$\mathcal{L}_x = \begin{bmatrix}0 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{bmatrix}, \tag{9a}$$

$$\mathcal{L}_y = \begin{bmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ -1 & 0 & 0\end{bmatrix}, \tag{9b}$$

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$$\mathcal{L}_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{9c}$$

These matrices satisfy the commutation rules

$$[\mathcal{L}_x, \mathcal{L}_y] = \mathcal{L}_z, \tag{10a}$$

$$[\mathcal{L}_z, \mathcal{L}_x] = \mathcal{L}_y, \tag{10b}$$

$$[\mathcal{L}_y, \mathcal{L}_z] = \mathcal{L}_x. \tag{10c}$$

By denoting $(\mathcal{L}_x, \mathcal{L}_y, \mathcal{L}_z)$ by $\mathcal{L}$, it is also easy to show that

$$\mathcal{L}^2 = -2\tilde{I}, \tag{11}$$

$$\mathbf{A} \cdot \mathcal{L}\mathbf{B} = \mathbf{A} \times \mathbf{B} \cdot \mathcal{L}, \tag{12}$$

and

$$[\mathbf{A} \cdot \mathcal{L}, \mathbf{B} \cdot \mathcal{L}] = \mathbf{A} \times \mathbf{B} \cdot \mathcal{L}. \tag{13}$$

On the left-hand side of Eq. (12), **B** should be taken as a three-component column vector. With these definitions it is easy to show that Eqs. (1) and (2) may be cast into the form

$$\frac{1}{c}\frac{\partial \theta}{\partial t} = \mathcal{R}^{-1/2} Q \mathcal{R}^{-1/2} \theta, \tag{14}$$

where

$$Q = \begin{bmatrix} 0 & \mathcal{L} \cdot \nabla \\ -\mathcal{L} \cdot \nabla & 0 \end{bmatrix}. \tag{15}$$

Note that a solution to Eqs. (1) and (2) will automatically satisfy Eqs. (3) and (4), provided that the initial conditions are taken to satisfy Eqs. (3) and (4). By choosing $\theta(0)$ accordingly, a complete solution to Eqs. (1)–(4) may be formally written in the form

$$|\theta(t)\rangle = U(t)|\theta(0)\rangle, \tag{16}$$

where the time-evolution operator is

$$U(t) = \exp(c\mathcal{R}^{-1/2} Q \mathcal{R}^{-1/2} t). \tag{17}$$

In Eq. (16) we have used a Dirac notation for θ. In this notation the value of θ at the space–time point $\mathbf{r}, t$ is $\theta(\mathbf{r}, t) = \langle \mathbf{r}|\theta(t)\rangle$. It is convenient to introduce, in addition to $\mathbf{r}$, another variable ψ to denote the six components ($\alpha = 1, 2, \ldots, 6$) of θ in the same way that $\mathbf{r}$ denotes any one of the continuum of components $\theta(\mathbf{r}, t)$. With this in mind we introduce a set of basis vectors

$$\chi_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \chi_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \ldots, \quad \chi_6 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \tag{18}$$

so that $\langle \chi_\alpha|\theta\rangle = \theta_\alpha$ ($\alpha = 1, 2, \ldots, 6$). More generally, we want to describe a particular linear combination $\sum a_\alpha \theta_\alpha$. This corresponds to the projection of θ on the vector

$$\psi = \sum_\alpha a_\alpha \chi_\alpha; \tag{19}$$

i.e., $\langle \psi|\theta\rangle = \sum a_\alpha \theta_\alpha$. Thus the most general projection of the state vector $|\theta\rangle$ can be written in the form

$$\langle \mathbf{r}, \psi|\theta(t)\rangle = \sum_\alpha a_\alpha \theta_\alpha(\mathbf{r}, t). \tag{20}$$

A reader familiar with quantum-mechanical notation should note the analogy between Eq. (20) and the following quantum-mechanical situation: Suppose that a quantum system (e.g., an atom) is characterized by position/momentum coordinates of its center of mass and by six internal states. Equation (20) then represents a general state of this system, where $\theta_\alpha(\mathbf{r}, t)$ is the wave function describing the system at state α. The probability of finding the system in this state is a_α^2, and we require here, as in the quantum-mechanical case, that the $\{a_\alpha\}$ be so normalized that

$$\sum_\alpha a_\alpha^2 = 1. \tag{21}$$

We next obtain a resolution of the identity operator in the ($\mathbf{r}$, ψ) space. We define a summation over the components of ψ by

$$\sum_\psi \equiv \frac{12}{\pi^3} \int \mathrm{d}^6 a \delta(a_1^2 + a_2^2 + \ldots + a_6^2 - 1). \tag{22}$$

With this definition it can be shown that

$$\sum_\psi a_i a_j = \delta_{ij}. \tag{23}$$

From Eq. (23) it can be easily shown that

$$\sum_\psi \psi\tilde{\psi} = I_6, \tag{24}$$

where I_6 is the six-dimensional unit matrix. Equation (24) thus describes the resolution of the identity in ψ space. The resolution of the identity in ($\mathbf{r}$, ψ) space is therefore

$$I = \sum_\psi \int \mathrm{d}\mathbf{r}|\mathbf{r}\psi\rangle\langle \mathbf{r}\psi|. \tag{25}$$

Given this resolution of the identity we can now derive a path-integral representation of the evolution operator in the usual way. First note that the evolution of θ may be written as

$$\langle \mathbf{r}\psi|\theta(t)\rangle = \sum_{\psi_0} \int \mathrm{d}\mathbf{r}_0 \langle \mathbf{r}\psi|U(t)|\mathbf{r}_0\psi_0\rangle\langle \mathbf{r}_0\psi_0|\theta(0)\rangle. \tag{26}$$

$U(t)$ is then written as a product $U(t) = \Pi_{j=1}{}^n U(\Delta t)$, with Δ[...] $= t/n$, and a resolution of the identity is inserted betwee[n] each consecutive term

$$\begin{aligned} \langle \mathbf{r}\psi|U(t)|\mathbf{r}_0\psi_0\rangle &= \sum_{\psi_{n-1}} \int \mathrm{d}\mathbf{r}_{n-1} \ldots \sum_{\psi_1} \int \mathrm{d}\mathbf{r}_1 \\ &\quad \times \langle \mathbf{r}\psi|U(\Delta t)|\mathbf{r}_{n-1}\psi_{n-1}\rangle \ldots \langle \mathbf{r}_1\psi_1|U(\Delta t)|\mathbf{r}_0\psi_0\rangle \\ &= \prod_{l=1}^{n-1} \sum_l \int \mathrm{d}\mathbf{r}_l \langle \mathbf{r}_l\psi_l|U(\Delta t)|\mathbf{r}_{l-1}\psi_{l-1}\rangle. \end{aligned} \tag{27}$$

In the second identity we have identified (r, ψ) with $(r_n, \psi$[...]

Consider now a typical term $\langle \mathbf{r}_l\psi_l|U(\Delta t)|\mathbf{r}_{l-1}\psi_{l-1}\rangle$. [...] evaluate it, we introduce intermediate eigenstates of $\mathbf{p}$[...] $-i\nabla$; then

$$\langle \mathbf{r}_l\psi_l|U(\Delta t)|\mathbf{r}_{l-1}\psi_{l-1}\rangle$$
$$= \langle \mathbf{r}_l\psi_l|[I_6 + c\Delta t\mathcal{R}^{-1/2}\mathcal{Q}\mathcal{R}^{-1/2} + \ldots]|\mathbf{r}_{l-1}\psi_{l-1}\rangle$$
$$= \left(\frac{1}{2\pi}\right)^3 \int \mathrm{d}\mathbf{p}_l(\langle \mathbf{r}_l|\mathbf{p}_l\rangle\langle \mathbf{p}_l|\mathbf{r}_{l-1}\rangle\langle\psi_l|\psi_{l-1}\rangle$$
$$+ c\Delta t\langle\psi_l|\langle\mathbf{r}_l|\mathcal{R}^{-1/2}(\mathbf{r})\mathcal{Q}|\mathbf{p}_l\rangle\langle\mathbf{p}_l|\mathcal{R}^{-1/2}(\mathbf{r})|\mathbf{r}_{l-1}\rangle|\psi_{l-1}\rangle + \ldots)$$
$$= \left(\frac{1}{2\pi}\right)^3 \int \mathrm{d}\mathbf{p}_l\langle \mathbf{r}_l|\mathbf{p}_l\rangle\langle \mathbf{p}_l|\mathbf{r}_{l-1}\rangle(\langle\psi_l|\psi_{l-1}\rangle$$
$$+ c\Delta t\langle\psi_l|\mathcal{R}_l^{-1/2}\mathcal{Q}_l\mathcal{R}_{l-1}^{-1/2}|\psi_{l-1}\rangle + \ldots), \tag{28}$$

where

$$\mathcal{R}_l = \mathcal{R}(\mathbf{r}_l) \tag{29}$$

and

$$\mathcal{Q}_l = \begin{bmatrix} 0 & +i\mathcal{L}\cdot\mathbf{p}_l \\ -i\mathcal{L}\cdot\mathbf{p}_l & 0\end{bmatrix}. \tag{30}$$

By also expanding ψ_{l-1} and $\mathbf{r}_{l-1}$ to first order in Δt:

$$\psi_{l-1} \doteq \psi_l - \Delta t\dot{\psi}_l, \tag{31}$$

$$\mathbf{r}_{l-1} \doteq \mathbf{r}_l - \Delta t\dot{\mathbf{r}}_l, \tag{32}$$

we find, to first order in Δt, that

$$\langle \mathbf{r}_l\psi_l|U(\Delta t)|\mathbf{r}_{l-1}\psi_{l-1}\rangle$$
$$= \frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}_l \exp[i\mathbf{p}_l\cdot(\mathbf{r}_l - \mathbf{r}_{l-1})](1 - \Delta t\langle\dot{\psi}_l|\psi_l\rangle$$
$$+ c\Delta t\langle\psi_l|\mathcal{R}_l^{-1/2}\mathcal{Q}_l\mathcal{R}_l^{-1/2}|\psi_l\rangle)$$
$$= \frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}_l \exp[\Delta t(i\mathbf{p}_l\cdot\dot{\mathbf{r}}_l - \langle\psi_l|\dot{\psi}_l\rangle$$
$$+ c\langle\psi_l|\mathcal{R}_l^{-1/2}\mathcal{Q}_l\mathcal{R}_l^{-1/2}|\psi_l\rangle)]. \tag{33}$$

Note that in the last term we have replaced $\mathcal{R}_{l-1}$ and ψ_{l-1} by $\mathcal{R}_l$ and ψ_l because this term is already of order Δt.

Equation (33) may now be used to write Eq. (27) in the limit $\Delta t \to 0$ as a path integral. We recall that in Eq. (27) the sum $\sum_{\psi_l}$ is restricted to such ψ_l's that satisfy $\langle\psi_l|\psi_l\rangle = 1$ (or $\sum_i a_{l_i}^2 = 1$). This restriction may be relaxed by multiplying the integral in Eq. (27) by $\delta(\langle\psi_l|\psi_l\rangle - 1) = [\Delta t/(2\pi)]\int_{-\infty}^{\infty}\mathrm{d}\omega_l \exp[-i\Delta t\omega_l(\langle\psi_l|\psi_l\rangle - 1)]$. We thus find that

$$\langle \mathbf{r}\psi|U(t)|\mathbf{r}_0\psi_0\rangle = \int D[\mathbf{r}(t)]\int D[\mathbf{p}(t)]\int D[\psi(t)]\int D[\omega(t)]$$
$$\times \exp\left\{\int_0^t \mathrm{d}t'[i\mathbf{p}\cdot\dot{\mathbf{r}} - \langle\psi|\dot{\psi}\rangle\right.$$
$$\left. + c\langle\psi|\mathcal{R}^{-1/2}\mathcal{Q}\mathcal{R}^{-1/2}|\psi\rangle - i\omega\langle\psi|\psi\rangle + i\omega]\right\}, \tag{34}$$

where

$$\int D[\mathbf{r}(t)] = \lim_{n\to\infty}\prod_{l=1}^{n-1}\int \mathrm{d}\mathbf{r}_l, \tag{35a}$$

$$\int D[\mathbf{p}(t)] = \lim_{n\to\infty}\prod_{l=1}^{n}\int \frac{\mathrm{d}\mathbf{p}_l}{(2\pi)^3}, \tag{35b}$$

$$\int D[\psi(t)] = \lim_{n\to\infty}\prod_{l=1}^{n-1}\frac{12}{\pi^3}\int \mathrm{d}^6 a_l, \tag{35c}$$

and

$$\int D[\omega(t)] = \lim_{\substack{n\to\infty \\ \Delta t\to 0}}\prod_{l=1}^{n-1}\int \frac{\mathrm{d}\omega_l}{2\pi}\Delta t. \tag{35d}$$

The $\mathbf{r}$ and ψ paths are restricted to satisfy

$$\mathbf{r}(0) = \mathbf{r}_0, \qquad \mathbf{r}(t) = \mathbf{r}; \tag{36a}$$

$$\psi(0) = \psi_0, \qquad \psi(t) = \psi. \tag{36b}$$

Some simplification of Eq. (34) may be achieved by noting that ψ (i.e., $|a_j|$) is real, so that $\langle\psi|\dot{\psi}\rangle = (\mathrm{d}/\mathrm{d}t)\langle\psi|\psi\rangle/2$. Therefore $\int_0^t\langle\psi|\dot{\psi}\rangle\mathrm{d}t = \frac{1}{2}[\langle\psi|\psi\rangle_t - \langle\psi|\psi\rangle_0] = 0$ because at the boundaries ψ is normalized to 1. Thus, finally,

$$\langle \mathbf{r}\psi|U(t)|\mathbf{r}_0\psi_0\rangle = \int D[\mathbf{r}]\int D(\mathbf{p})\int D[\psi]\int D[\omega]e^{iS}, \tag{37}$$

$$S = \int_0^t \mathrm{d}t'\mathfrak{L}(t'), \tag{38}$$

$$\mathfrak{L} = \mathbf{p}\cdot\dot{\mathbf{r}} - ic\langle\psi|\mathcal{R}^{-1/2}\mathcal{Q}\mathcal{R}^{-1/2}|\psi\rangle$$
$$- \omega\langle\psi|\psi\rangle + \omega. \tag{39}$$

Further simplification is obtained if the medium is isotropic, that is,

$$\vec{\epsilon} = \epsilon(\mathbf{r})\vec{I}, \tag{40}$$

$$\vec{\mu} = \mu(\mathbf{r})\vec{I}. \tag{41}$$

In this case

$$\mathcal{R}_l^{-1/2}\mathcal{Q}_l\mathcal{R}_l^{-1/2} = \frac{i}{n(\mathbf{r})}\Lambda\cdot\mathbf{p}_l, \tag{42}$$

where we have defined

$$\Lambda \equiv \begin{bmatrix} 0 & \mathcal{L} \\ -\mathcal{L} & 0\end{bmatrix} \tag{43}$$

and

$$\Lambda\cdot\mathbf{p}_l = \begin{bmatrix} 0 & \mathcal{L}\cdot\mathbf{p} \\ -\mathcal{L}\cdot\mathbf{p} & 0\end{bmatrix}. \tag{44}$$

Note that $\mathcal{L}\cdot\mathbf{p} = \mathcal{L}_x p_x + \mathcal{L}_y p_y + \mathcal{L}_z p_z$, so $\Lambda\cdot\mathbf{p}_l$ is a six-dimensional matrix. The Lagrangian, Eq. (39), now takes the form

$$\mathfrak{L} = \mathbf{p}\cdot\dot{\mathbf{r}} + \frac{c}{n(\mathbf{r})}\tilde{\mathbf{a}}(\mathbf{p}\cdot\Lambda)\,\mathbf{a} - \omega(\tilde{\mathbf{a}}\cdot\mathbf{a}) + \omega. \tag{45}$$

Here we have represented ψ by the corresponding six-dimensional vector coefficient $\mathbf{a}$ so that, e.g., $\langle\psi|\psi\rangle = \tilde{\mathbf{a}}\cdot\mathbf{a}$ ($\tilde{\mathbf{a}}$ is the transpose of the column vector $\mathbf{a}$).

The following comments should be made at this point:

(a) The derivation presented above for the path integral associated with the Maxwell equations follows essentially similar derivations for the Schrödinger equation. This derivation rests on some mathematical steps whose validity is not strongly established [e.g., Eq. (31)], and the same doubts

Table 1. Eigenvectors and Eigenvalues of $(c/n)\Lambda \cdot \mathbf{T}$

Index	Eigenvector	Eigenvalue
1	$\begin{bmatrix} \hat{p} \\ 0 \end{bmatrix}$	0
2	$\begin{bmatrix} 0 \\ \hat{p} \end{bmatrix}$	0
3	$\frac{1}{\sqrt{2}}\begin{bmatrix} \hat{s} \\ \hat{q} \end{bmatrix}$	$\frac{cp}{n}$
4	$\frac{1}{\sqrt{2}}\begin{bmatrix} \hat{q} \\ -\hat{s} \end{bmatrix}$	$\frac{cp}{n}$
5	$\frac{1}{\sqrt{2}}\begin{bmatrix} \hat{s} \\ -\hat{q} \end{bmatrix}$	$-\frac{cp}{n}$
6	$\frac{1}{\sqrt{2}}\begin{bmatrix} \hat{q} \\ \hat{s} \end{bmatrix}$	$-\frac{cp}{n}$

expressed with regard to the quantum-mechanical derivation[1] are also relevant here.

(b) In many interesting situations ϵ and μ are functions of ω, a fact not taken into account by Eqs. (1)–(4). For problems involving a monochromatic field we can still use the present formalism by putting the corresponding values for ϵ and μ in Eqs. (1)–(4).

(c) The speed of light c is seen here to play a role similar to that of $1/\hbar$ in quantum mechanics. It is of interest to examine the "classical limit," which is the asymptotic expansion of the path integral for $c \to \infty$. In particular, the maximal path should have some physical significance. We examine this path next.

For large c, most of the contribution to the path integral [Eq. (37)] should come from the vicinity of the path for which $\delta S = 0$ (classical). The Lagrange equations associated with this problem yield

$$\dot{\mathbf{p}} = \frac{c}{n}\,\tilde{\mathbf{a}}(\mathbf{p}\cdot\Lambda)\mathbf{a}n\nabla\left(\frac{1}{n}\right), \tag{46}$$

$$\dot{\mathbf{r}} = -\frac{c}{n}\,\tilde{\mathbf{a}}\cdot\Lambda\cdot\mathbf{a}, \tag{47}$$

$$0 = 1 - \tilde{\mathbf{a}}\cdot\mathbf{a}, \tag{48}$$

$$0 = \frac{c}{n}\,\mathbf{p}\cdot\Lambda\mathbf{a} - \omega\mathbf{a}. \tag{49}$$

Equations (48) and (49) restrict the vectors $\mathbf{a}$ to being normalized eigenvectors of the six-dimensional matrix $(c/n)\mathbf{p}\cdot\Lambda$ and restrict ω to being the corresponding eigenvalue. These eigenvectors and eigenvalues are easily found and are listed in Table 1. In this table $\hat{p}$ is a unit vector in the direction of $\mathbf{p}$, while $\hat{q}$ and $\hat{s}$ are unit three-dimensional vectors chosen so that $(\hat{q}, \hat{p}, \hat{s})$ constitutes a right-handed mutually perpendicular set of vectors.

We observe that there are four propagating modes and two nonpropagating modes and that for the propagating modes each three-dimensional subvector of $\mathbf{a}$ is perpendicular to $\hat{p}$. For all these modes Eqs. (46) and (47) may be written as

$$\dot{\mathbf{p}} = \omega n\nabla\frac{1}{n}, \tag{50}$$

$$\dot{\mathbf{r}} = -\omega\frac{\hat{p}}{p}, \tag{51}$$

where $\omega = 0$ for the nonpropagating modes and $\omega = \pm cp/n(\mathbf{r})$ is the local speed of light for the propagating modes.

Equation (51) is very suggestive, as it describes the motion of a particle in the direction $\hat{p}$ with the local speed of light c/n. In what follows we show that Eqs. (50) and (51) lead to the Fermat principle.

The Fermat principle of geometrical optics states that a ray of light propagating in an inhomogeneous medium characterized by an isotropic refractive index $n(\mathbf{r})$ follows a path for which

$$\delta = \int \mathrm{d}\tau\,\frac{n}{c} = 0, \tag{52}$$

where $\mathrm{d}\tau$ is an element of path length. By rewriting Eq. (52) in the form

$$\delta\int_0^t \mathrm{d}t n(\mathbf{r})\sqrt{\left(\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right)^2} = 0, \tag{53}$$

we get the corresponding Lagrange equation in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}(n\hat{v}) = v\nabla n, \tag{54}$$

where $v = |\mathrm{d}\mathbf{r}/\mathrm{d}t|$ and $\hat{v} = \mathbf{v}/v$. It is not difficult to show that Eqs. (50) and (51) also imply Eq. (54). Thus the external path associated with the Lagrangian [Eq. (45)] satisfies the laws of geometrical optics. A possible interpretation of the trajectory defined by Eqs. (50) and (51) is that it describes the motion of the wave front or of the ray. The vector $\mathbf{a}$ seems to be related to the polarization.

Further advances in this direction may be expected along lines similar to those taken in the corresponding quantum-mechanical problem, namely, "semiclassical" evaluation of the path integral or numerical calculations based on methods developed for quantum-mechanical path integrals. This goal has not yet been achieved for the general electrodynamical problem. We next turn to the electrostatic problem, where another path-integral formulation leads to numerically tractable expressions.

PATH-INTEGRAL FORMULATION OF THE POISSON EQUATION

When the characteristic distances of the physical system are much smaller than the electromagnetic wavelength, the solution to the electromagnetic problem can be found in the electrostatic approximation. In this case the time dependence of the field is given by, e.g., $\mathbf{E}(\mathbf{r})\exp(i\omega t)$, where the amplitude $\mathbf{E}(\mathbf{r})$ is derived from a potential that satisfies the Poisson equation

$$-\nabla\cdot[\epsilon(\mathbf{r})\nabla\Phi(\mathbf{r})] = 4\pi\rho(\mathbf{r}), \tag{55}$$

where $\rho(\mathbf{r})$ is the source charge distribution. Equation (55) may be rewritten in the form

$$\nabla^2\Phi(\mathbf{r}) + \mathbf{F}(\mathbf{r})\cdot\nabla\Phi(\mathbf{r}) = -\frac{4\pi}{\epsilon(\mathbf{r})}\rho(\mathbf{r}), \tag{56}$$

where

$$\mathbf{F}(\mathbf{r}) = \nabla \ln \epsilon(\mathbf{r}). \qquad (57)$$

It is sufficient to solve Eq. (56) for the Green's function $G(\vec{r}, \vec{r}')$:

$$[\nabla^2 + \mathbf{F}(\mathbf{r}) \cdot \nabla] G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \qquad (58)$$

in terms of which $\Phi(\mathbf{r})$ is given by

$$\Phi(\mathbf{r}) = -4\pi \int \mathrm{d}\mathbf{r}' \frac{\rho(\mathbf{r}')}{\epsilon(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}'). \qquad (59)$$

We recently showed that $G(\mathbf{r}, \mathbf{r}')$ can be represented as

$$G(\mathbf{r}, \mathbf{r}') = -\int_0^\infty \mathrm{d}t K(\mathbf{r}, \mathbf{r}'; t), \qquad (60)$$

where $K(\mathbf{r}, \mathbf{r}'; t)$, which satisfies the equation

$$\frac{\partial K(\mathbf{r}, \mathbf{r}'; t)}{\partial t} = [\nabla_r^2 + \mathbf{F}(\mathbf{r}) \cdot \nabla_r] K(\mathbf{r}, \mathbf{r}'; t) \qquad (61)$$

with the initial condition

$$K(\mathbf{r}, \mathbf{r}'; 0) = \delta(\mathbf{r} - \mathbf{r}'), \qquad (62)$$

has the path-integral representation

$$K(\mathbf{r}, \mathbf{r}'; t) = \int D[\mathbf{r}(t)] e^{-S}, \qquad (63)$$

$$S = \int_0^t \mathfrak{L}\left(\mathbf{r}, \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right) \mathrm{d}t, \qquad (64)$$

$$\mathfrak{L} = \frac{1}{4}\left[\mathbf{F}(\mathbf{r}) + \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right]^2 + \frac{1}{2} \nabla \cdot \mathbf{F}. \qquad (65)$$

The paths contributing to Eq. (63) are restricted by $\mathbf{r}(0) = \mathbf{r}'$ and $\mathbf{r}(t) = \mathbf{r}$.

An approximate numerical evaluation of the path integral of Eq. (63) may be achieved by using the (approximate) discretized form

$$K(\mathbf{r}, \mathbf{r}'; t) = (4\pi\Delta t)^{-3N/2} \int \mathrm{d}\mathbf{r}_1 \ldots \int \mathrm{d}\mathbf{r}_{N-1} \times \exp\left\{-\frac{\Delta t}{4} \sum_{n=0}^{N-1} \left[\mathbf{F}(\mathbf{r}_n) + \frac{\mathbf{r}_n - \mathbf{r}_{n+1}}{\Delta t}\right]^2\right\} \qquad (66)$$

and calculating Eq. (66) by the Monte Carlo method. We have shown by comparing numerical and analytical solutions for an analytically solvable model that this method is indeed reliable.

For problems of low dimensionality (mainly one-dimensional problems) K may be evaluated also by direct matrix multiplication:

$$K(x, x'; t) = \frac{1}{\Delta x} \sum_{l_1=-\infty}^{\infty} \cdots \sum_{l_{N-1}=-\infty}^{\infty} \mathcal{M}_{l_N, l_{N-1}} \cdots \mathcal{M}_{l_1, l_0}, \qquad (67)$$

where $\mathcal{M}$ is the non-Hermitian matrix

$$\mathcal{M}_{l_{n+1}, l_n} = \frac{\Delta x}{\sqrt{4\pi\Delta t}} \exp\left\{-\frac{\Delta t}{4}\left[F(l_n \Delta x) + \frac{\Delta x}{\Delta t}(l_n - l_{n+1})\right]^2\right\} \qquad (68)$$

and where Δx is the spatial discretization step. In Eq. (67) $l_0 \Delta x = x'$ and $l_N \Delta x = x$. In actual calculation the infinite l summations are truncated:

$$\sum_{l=-\infty}^{\infty} \rightarrow \sum_{l=-L}^{L}. \qquad (69)$$

The fact [Eq. (60)] that what we actually require is the time integral over K may in some cases lead to a simplification of the problem. Consider, for example, the problem of calculating the image potential experienced by a point charge at location x near a flat surface (the surface is in the yz plane) where the dielectric function depends on x in some specified manner. [In the regular textbook problem $\epsilon(x)$ is a step function.] Even though the problem is of one-dimensional symmetry, we have to consider the three-dimensional propagator, given by an equation similar to Eq. (67):

$$K(\mathbf{r}, \mathbf{r}'; t) = \frac{1}{(\Delta x)^3} \sum_{\mathbf{l}_1} \cdots \sum_{\mathbf{l}_{N-1}} \mathcal{M}_{\mathbf{l}_N, \mathbf{l}_{N-1}} \cdots \mathcal{M}_{\mathbf{l}_1, \mathbf{l}_0}, \qquad (70)$$

where

$$\sum_{\mathbf{l}_j} \equiv \sum_{l_{jx}} \sum_{l_{jy}} \sum_{l_{jz}}$$

and where

$$\mathcal{M}_{\mathbf{l}_j, \mathbf{l}_{j-1}} = \mathcal{M}_{l_{jx}, l_{(j-1)x}}{}^{(x)} \mathcal{M}_{l_{jy}, l_{j-1y}}{}^{(y)} \mathcal{M}_{l_{jz}, l_{(j-1)z}}{}^{(z)}, \qquad (71)$$

$$\mathcal{M}_{ll'}{}^{(x)} = \frac{\Delta x}{\sqrt{4\pi\Delta t}} \exp\left\{-\frac{\Delta t}{4}\left[F(\Delta x l') + \frac{\Delta x}{\Delta t}(l' - l)\right]^2\right\}, \qquad (72)$$

$$\mathcal{M}_{ll'}{}^{(y)} = \frac{\Delta y}{\sqrt{4\pi\Delta t}} \exp\left[-\frac{(\Delta y)^2}{4\Delta t}(l' - l)^2\right], \qquad (73)$$

$$\mathcal{M}_{ll'}{}^{(z)} = \frac{\Delta z}{\sqrt{4\pi\Delta t}} \exp\left[-\frac{(\Delta z)^2}{4\Delta t}(l' - l)^2\right]. \qquad (74)$$

The summations over the free propagators in the y and z directions can be carried out exactly, leading to [for $\mathbf{r} = (l\Delta x, 0, 0)$ and $\mathbf{r}' = (l'\Delta x, 0, 0)$]

$$K(\mathbf{r}, \mathbf{r}'; N\Delta t) = \frac{1}{4\pi N\Delta t} \frac{1}{\Delta x} [(\mathcal{M}^{(x)})^N]_{ll'}, \qquad N \geq 1 \qquad (75)$$

or

$$K(l\Delta x, l'\Delta x; N\Delta t) = \frac{1}{\Delta x}\left[I + \frac{1}{4\pi N\Delta t}(1 - \delta_{N,0})(\mathcal{M}^{(x)})^N\right]_{ll'} \qquad (76)$$

Inserting into Eq. (60), we get

$$\mathcal{G} = -\Delta t \sum_{N=0}^{\infty} \mathcal{K}(N\Delta t)$$

$$= -\frac{\Delta t}{\Delta x}\left[I + \frac{1}{4\pi\Delta t} \sum_{N=1}^{\infty} (\mathcal{M}^{(x)})^N / N\right] \qquad (77)$$

or

$$\mathcal{G} = -\frac{\Delta t}{\Delta x}\left[I - \frac{1}{4\pi\Delta t} \ln(I - I^{(x)})\right]. \qquad (78)$$

Thus, to evaluate $\mathcal{G}$, we need the evaluation of $\ln(I - \mathcal{M}^{(x)})$, which requires diagonalization of the matrix $I - \mathcal{M}^{(x)}$. The image potential felt by a charge Q at location $\Delta x l'$ is

$$\Phi^{\text{image}} = -\frac{4\pi Q}{\epsilon(l'\Delta x)} [\mathcal{G} - \mathcal{G}^{(0)}]_{l l'}. \tag{79}$$

CONCLUSION

We have derived a path-integral expression for the time-evolution operator associated with the Maxwell equations in inhomogeneous media and have shown that its asymptotic behavior yields geometrical optics. We have also obtained a path-integral expression for the Green's function of the Laplace equation and reduced it to a form that can be evaluated numerically. Application of this method to surface electromagnetic phenomena will be described in a future paper.

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REFERENCE

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