Path Integrals for Photonic Crystals.

Yair Dimant and Shimon Levit* ,

Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

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We develop a path integrals approach for analyzing stationary light propagation appropriate for photonic crystals. The hermitian form of the stationary Maxwell equations is transformed into a quantum mechanical problem of a spin 1 particle with spin-orbit coupling and position dependent mass. After appropriate ordering several path integral representations of a solution are constructed. One leaves the propagation of polarization degrees of freedom in an operator form integrated over paths in coordinate space. The use of spin 1 coherent states allows to represent this part as a path integral over such states. Finally a path integral in transversal momentum space with explicit transversality enforced at every time slice is also given. As an example the geometrical optics limit is discussed and the ray equation is recovered together with the Rytov rotation of the polarization vector.

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Introduction. Description of stationary light fields in photonic crystals can be formulated, cf. [1, 2], as solutions of an eigenvalue equation,

$$\nabla \times \frac{1}{\varepsilon(x)} \nabla \times H = \left(\frac{\omega}{c}\right)^2 H$$

(1)

where $H$ is the magnetic field and $\varepsilon(x)$ is the space dependent dielectric constant. This equation is sometimes referred to in the literature as the master equation. The operator $\hat{\Theta} = \nabla \times \frac{1}{\varepsilon(x)} \nabla \times$ is hermitian and positive definite. This formulation allows direct applications to photonic crystals of many powerful techniques developed in quantum mechanics.

Our goal is to follow on this development and formulate the path integral representation of solutions of this equation. Within the scalar approximation

$$\frac{1}{\varepsilon(x)} \nabla^2 u(x) = \left(\frac{\omega}{c}\right)^2 \cdot u(x)$$

(2)

works in this spirit have already been presented in the past [3, 4, 5, 6, 7], but here we deal with the full vector version. To the best of our knowledge this have not yet been done.

Let us consider an auxiliary time dependent Schrodinger like equation

$$i\partial_\tau C(x, \tau) = \hat{\Theta} C(x, \tau)$$

(3)

with fictitious time parameter $\tau$. This equation has the formal solution

$$C(x, \tau) = \exp \left[ -i\tau \hat{\Theta} \right] C(x, 0)$$

(4)

from which we can recover a solution of the original master equation by using

$$H(x) = \lim_{\eta \to 0} \int_{-\infty}^{\infty} d\tau \left[ e^{i(\pm)^2 \tau - n|x|} C(x, \tau) \right]$$

(5)

Note that for any $\omega \neq 0$ the solutions $H(x)$ of Eq. (1) are transversal, $\nabla \cdot H = 0$. The solutions $C(x, \tau)$ of (3) are not. However since $\partial_\tau [\nabla \cdot C(x, \tau)] = 0$ we have that the above transversality condition is satisfied also by $H(x)$ given by (5).

The Dirac notations. The Hilbert space of all complex vector functions $H(x)$ is equivalent to the Hilbert space of a spin 1 particle in quantum mechanics. The spin operators are hidden in the vector product signs which we make explicit by using the antisymmetric tensor (and the summation over repeated indices convention)

$$\left[ \hat{\Theta} H \right]_i = \left[ \nabla \times \left( \frac{1}{\varepsilon(x)} \nabla \times H \right) \right]_i = \epsilon_{ijk} \epsilon_{klm} \theta_j \frac{1}{\varepsilon(x)} \partial_l H_m =$$

$$= \left( -i \epsilon_{ijk} \right) \left( -i \epsilon_{klm} \right) \left( -i \partial_j \right) \frac{1}{\varepsilon(x)} \left( -i \partial_l \right) H_m ,$$

The operator $\hat{\Theta}$ is therefore

$$\hat{\Theta} = (\hat{p} \cdot \hat{S}) v(x)(\hat{p} \cdot \hat{S})$$

(7)

with $\hat{p} = -i\nabla$, $v(x) = 1/\varepsilon(x)$ and $\hat{S}$ – the spin 1 matrix vector with components $[S_j]_{ik} = -i \epsilon_{ikj}$.

It is convenient to introduce the Dirac notations

$$\hat{\Theta} |H\rangle = \left( \frac{\omega}{c} \right)^2 |H\rangle$$

$$H_i(x) = \langle x, i | H \rangle , \quad i = 1, 2, 3$$

$$\langle x, i | \hat{\Theta} | H \rangle = \left[ \nabla \times \frac{1}{\varepsilon(x)} \nabla \times H(x) \right]_i$$

*The Harry and Kathleen Kweller Professor of Condensed Matter Physics.
In this notation equation (11) is

\[ \langle x, i | C(\tau) \rangle = \sum_{j=1}^{3} \int d\mathbf{x}' \langle x, i | e^{-it\hat{\Theta}} | x', j \rangle \langle x', j | C(0) \rangle \] (9)

**Ordering the "Hamiltonian".** We intend to write the path integral expression for the propagator \( \langle x, i | e^{-it\hat{\Theta}} | x', j \rangle \). Following the usual procedure we rewrite \( \hat{\Theta} \) in the ordered form placing the \( \hat{p} \) operators to the right of \( x \)’s,

\[ \hat{\Theta} = -i(\nabla v \cdot \hat{S})(\hat{p} \cdot \hat{S}) + v(x)\hat{p}^2\hat{P}_T \] (10)

with \( \hat{P}_T \) - the transversal projection operator

\[ [\hat{P}_T]_{ij} = i\delta_{ij} - \nabla_i \nabla_j \] (11)

where we used \((\hat{S}_i\hat{S}_j)_{mn} = \epsilon_{km}\epsilon_{knj} = \delta_{ij}\delta_{mn} - \delta_{mj}\delta_{ni}\)

We are interested only in how the transverse functions \( C(x, \tau) \) propagate for which \( \hat{P}_T | C \rangle = | C \rangle \). Accordingly we can drop \( \hat{P}_T \) in Eq. (10) and define a reduced operator

\[ \hat{\theta}_R = v(x)\hat{p}^2 - i(\nabla v \cdot \hat{S})(\hat{p} \cdot \hat{S}) \] (12)

Note that the operators (4) and (12) are equivalent when acting on transversal functions. In general one can show that \( \hat{\Theta} = \hat{\Theta}_R\hat{P}_T \). Note that \( \hat{\Theta}_R \) is hermitian in the transverse subspace.

**Path Integral - The Operator Version.** We are now in a position to use the standard time slicing process to construct the path integral. In this we first choose to keep the vector part of the evolution at the operator level inserting complete (coordinate and momentum) states only for the spatial part. As a result we obtain a functional integral over the positions and momenta of spatial paths with the integrand containing the evolution operator of the vectorial part of the field for each path

\[ \langle x | e^{-i\hat{\Theta}} | x' \rangle = \lim_{\Delta \tau \to 0} \int \frac{d\mathbf{x}_1 dp_1 \ldots dp_N}{(2\pi)^N} \prod_{j=1}^{N} e^{ip_j(x_j - x_{j-1})} [1 - i\Delta v_j p_j^2] \left[ 1 - \Delta \tau (\nabla v_j \cdot \hat{S})(\hat{p}_j \cdot \hat{S}) \right] \]

where \( T \) stands for time ordering, \( \Delta \tau = \tau / N \), \( x(0) = x' \), \( x(\tau) = x \). This functional integral has position dependent mass \( m(x) = 1/2v(x) = c(x)/2 \) and spin orbit coupling terms which enter the time ordered exponential.

**The Spin Coherent States Version.** The operator part of the above path integral, i.e. the time ordered exponential can be further developed using the spin coherent states. These states are generated, cf. (14), by rotations of one of the eigenstates of \( \hat{S}_z \), i.e. \( |1, \mu \rangle \), \( \mu = 1, 0, -1 \). In the cartesian basis used above these states are

\[ \begin{pmatrix} 1, 1 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \begin{pmatrix} 0, 0 \rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1, -1 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} +1 \\ -i \\ 0 \end{pmatrix} \]

The most common spin coherent states are given by

\[ |\Omega \rangle = |\theta, \phi \rangle = e^{-i\phi \hat{S}_x} e^{-i\theta \hat{S}_y} |1, 1 \rangle \] (14)

They are eigenstates of the spin component in the appropriate direction, \( \hat{\Omega} \cdot \hat{\hat{S}} |\Omega \rangle = |\Omega \rangle \), and form an over complete set which has a useful “resolution of unity” property

\[ \hat{I} = \frac{3}{4\pi} \int d\Omega |\Omega \rangle \langle \Omega |, d\Omega = \sin \theta d\theta d\phi \] (15)

Going again through the time slicing process and inserting (13) between the slices one finds the propagator between two spin coherent states

\[ \langle x, \Omega | e^{-i\hat{\Theta}_R} | x', \Omega \rangle = \int D[x, p] \int D[\Omega] \exp \left[ i \int_0^\tau \left( p \cdot d_r x + \cos \theta d_r \phi - v p^2 + i|\Omega| (\nabla v \cdot \hat{S})(\hat{p} \cdot \hat{S})|\Omega \rangle \right) d\tau \right] \] (16)

All that is left is to evaluate the matrix element

\[ \langle \Omega | (\nabla v \cdot \hat{S})(\hat{p} \cdot \hat{S}) |\Omega \rangle = \sum_{i,j} (\nabla_i v) p_j \langle \Omega | \hat{S}_i \hat{S}_j |\Omega \rangle \]

Using \( \hat{S}_i \hat{S}_j = \frac{1}{2} (|\hat{S}_i \hat{S}_j \rangle + \{\hat{S}_i, \hat{S}_j \}) \) together with the com-
mutation relations of spin operators, the identity
\[ \hat{S}_l \hat{S}_m \hat{S}_n + \hat{S}_n \hat{S}_m \hat{S}_l = \delta_{l,m} \hat{S}_n + \delta_{n,m} \hat{S}_l \]
valid for spin 1 matrices, as well as
\[ \langle \Omega | \hat{S}_l | \Omega \rangle = \Omega_i \]
cf. [17], we obtain
\[ \langle \Omega | \hat{S}_l \hat{S}_j | \Omega \rangle = \frac{i}{2} \epsilon_{ijk} \Omega_k + \frac{1}{2} (\Omega_i \Omega_j + \delta_{ij}) \]
and finally
\[ \langle \Omega | (\nabla v \cdot \hat{S})(p \cdot \hat{S}) | \Omega \rangle = \frac{i}{2} \Omega \cdot (\nabla v \times p) + \]
\[ + \frac{1}{2} \left[ (\nabla v \cdot \Omega)(p \cdot \Omega) + \nabla v \cdot p \right] . \] (19)

Explicit Transversal Projection. The above path integral expressions for the exact propagator will propagate only transverse vector functions despite unrestricted integrations at every time slice. It may be desirable however, especially in making approximations, to have path integral expressions with explicit transversal projection enforced at every time step. This can be achieved by inserting the projection operator (11) at every time slice. Moreover one must start with a transverse state, the simplest of which is \( \lambda \exp(ip \cdot x) \) with \( \lambda \cdot p = 0 \). It is natural then to take also the final state to be a transversal plane wave. Using the spin coherent states this means working with \( \langle pf, \Omega f | e^{-ir \hat{B}_R} | pi, \Omega i \rangle \) and imposing the transversality conditions
\[ \Omega_{i,f} = \pm \frac{|pi,f|}{|pf,i|} \] (20)
under which \( P_T |pi,f, \Omega_{i,f}\rangle = |pi,f, \Omega_{i,f}\rangle \). Once one uses such transversal initial and final states and due to the fact that the transversality is conserved by the infinitesimal transformations in between infinitesimal time slices, the projection operator insertion will not alter the propagation. Expression [13] will then become (in the limit \( \Delta \tau \to 0 \))
\[ \langle pf | e^{-ir \hat{B}_R} | pi \rangle = \int D [p, \nabla v \cdot \hat{S}](p \cdot \hat{S}) \] \[ \times \] \[ \prod_{\tau} \left[ 1 - \delta_{\tau} \left( \nabla v \cdot \hat{S} \right) \left( p_{\tau} \cdot \hat{S} \right) \right] \frac{p \cdot \hat{S}}{p_{\tau}^2} \]

The Saddle Point Approximation - The Geometrical Optics Limit. Geometrical optics is a short wavelength expansion. The vacuum wavelength of light must be short with respect to the scale \( v/|\nabla v| \) over which the dielectric function is changing. Accordingly we treat the spin dependent part of Eqs. [13] and [10] as slowly varying and evaluate it on the saddle point of the functional \( S_0 = \int_0^\tau (p \cdot d_v x - v p^2) d\tau \). The corresponding Euler-Lagrange equations are
\[ d_v x = 2v p \quad ; \quad d_v p = -p^2 \nabla v . \] (21)
The conserved "energy" is \( E = v p^2 \) which we will use in order to reparametrize
\[ d_v = 2v \sqrt{E} d_t \] (22)
and obtain the standard differential equation of the ray
\[ \frac{d^2 x}{d t^2} = \nabla \left( \frac{n^2}{2} \right) \] (23)
Once the geometrical ray (or rays) satisfying the appropriate boundary conditions (e.g. \( x(0) = x', x(\tau) = x \)) is found the propagator along each ray is given
\[ K = T \left\{ e^{-\int_0^\tau (\nabla v \cdot \hat{S})(p \cdot \hat{S}) d\tau} \right\} e^{iS_0(x,x')} \int D [x, p] e^{i\hat{S}S_0/2} \] (24)
where the subscript \( r \) means evaluation at the ray values which also applies for \( S_0 \) and \( \delta^2 S_0 \). The Gaussian integral over \( \exp i \hat{S} \) is evaluated in a standard way, giving the Van-Vleck determinant factor \( \sqrt{(1/2\pi)^d \det \{ \partial x_{\tau}^2 S_0(x, x') \}} \). The evolution of the vector degrees of freedom along a geometrical ray is given by the equation
\[ \frac{d |\lambda\rangle}{d \tau} = - \left( \nabla v_{\tau} \cdot \hat{S} \right) \left( p_{\tau} \cdot \hat{S} \right) |\lambda\rangle \] (25)
as follows from the time ordered operator in [21]. In the usual vector representation this is just an evolution of a vector \( \lambda \)
\[ \frac{d \lambda}{d \tau} = \nabla v_{\tau} \times (p_{\tau} \times \lambda) \] (26)
with time dependent \( \nabla v_{\tau} \equiv \nabla v(x_{\tau}) \) and \( p_{\tau}(\tau) \) determined by the ray trajectory \( x_{\tau}(\tau), p_{\tau}(\tau) \). We will now show that the orientation of \( \lambda \) relative to the ray is governed by the Rytov equation for the polarization while its magnitude fits one of the components of the energy flow equation along the ray, cf. [19, 20].
It is convenient to switch from "time" \( \tau \) to the length parameter \( s \) and write [21] as
\[ \frac{d \lambda}{d s} = - \frac{\nabla n}{n} \times (T(s) \times \lambda) \] (27)
where \( T(s) = d x/d s \) is the tangent to the curve. Considering also the normal and the binormal vectors
\[ N(s) = \frac{dT(s)}{d s} \mid \frac{dT(s)}{d s} \mid , \quad B(s) = T(s) \times N(s) \]
one can expand
\[ \lambda = \lambda_T T + \lambda_N N + \lambda_B B. \] (28)

We transform the equation \[23\] of the ray from \( \tau \) to \( s \)
\[ \frac{d}{ds} \left( n \frac{d\kappa}{ds} \right) = \nabla n \] (29)
and use the Frenet equations, describing the differential geometry of curves, \[22\]
\[ \frac{d}{ds} \begin{pmatrix} T \\ N \\ B \end{pmatrix} = \begin{pmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} T \\ N \\ B \end{pmatrix} \] (30)
where \( \kappa (s) = |dT/ds| \) is the curvature and \( \tau (s) = B \cdot dN/ds \) is the torsion (not to be confused with the time parameter \( \tau \)). We can rewrite Eq. \[27\] as
\[ \frac{d}{ds} \begin{pmatrix} \lambda_T \\ \lambda_N \\ \lambda_B \end{pmatrix} = \begin{pmatrix} 0 \\ -\kappa \lambda_T + \tau \lambda_B + \frac{d \ln n}{ds} \lambda_N \\ -\tau \lambda_N + \frac{d \ln n}{ds} \lambda_B \end{pmatrix} \] (31)
The \( \lambda_T (s) \) component is conserved along the curve and we will take it to be zero (a transversal solution). We will rewrite the remaining two equations as equations for \( \varphi \) – the angle between \( \lambda \) and \( N \) and \( \lambda^2 = \lambda_N^2 + \lambda_B^2 \) – the square length of \( \lambda \). We obtain
\[ \frac{d\varphi}{ds} = \tau , \quad \frac{d\lambda^2}{ds} = \frac{d\ln |n^2|}{ds} \lambda^2 \] (32)
The first equation is the Rytov equation from geometrical optics governing the rotation of polarization along an optical ray, cf., Fig. 1. The solution of the second equation is simply \( \lambda = n(s) \lambda_0 \).

The Van-Vleck determinant contained in the last term in Eq. \[23\]. The second term is identical with what we obtained for \( \lambda^2 \) in Eq. \[22\].

**FIG. 1:** Rytov rotation of the field relative to the ray. \( T, \, N \) and \( B \) are respectively tangent, normal and binormal vectors. \( H \) is the magnetic field vector. \( x \) is the geometrical ray.

In the standard derivations of the geometrical optics from the Maxwell equations, cf., \[19\] \[20\], one finds the following equation for the change with respect to the length parameter of the field amplitude square along a geometrical ray
\[ \frac{d}{ds} |A|^2 = - \left( \frac{\nabla^2 S_0}{n} - \frac{d}{ds} \ln |n^2| \right) |A|^2 \] (33)
The two terms in the right hand side are clearly associated with the two contributions which we derived in the geometrical optics approximation to the amplitude of the propagator. The first term, which involves the second spatial derivatives of the action, is related to the Van-Vleck determinant contained in the last term in Eq. \[23\]. The second term is identical with what we obtained for \( \lambda^2 \) in Eq. \[22\].

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