PRA-HEP 93/13

PHOTONIC BAND GAP CALCULATIONS : INWARD AND OUTWARD INTEGRAL EQUATIONS AND THE KKR METHOD[1]

Alexander Moroz[2]

Institute of Physics CAS, Na Slovance 2
CZ-180 40 Prague 8, Czech Republic

1. INTRODUCTION

Our main goals have been to calculate photonic bands on various periodic dielectric lattices, to clarify some controversy regarding existence of a photonic band gap for fcc lattice of dielectric spheres [1], and finally treat impurities in a photonic crystal [2]. Motivated by the search for a photonic band gap [3] we have tried to adapt one of the standard methods of electron band theory - namely the scalar bulk Kohn-Korringa-Rostocker (KKR) method [4, 5] to the form appropriate for photons [2, 6, 7]. We recall that in the case of photons the role of a (periodic) potential plays $v(\mathbf{r}) = \epsilon(\mathbf{r}) - \epsilon_o$. Here $\epsilon(\mathbf{r})$ is the dielectricity of a medium and ϵ_o is its host value which is assumed to be uniform and *homogeneous* [3, 6]. A dielectric "*atom*" V_s is called a connected region where $v(\mathbf{r}) \neq 0$. The reason of our choice was that the KKR method proceeds *analytically* as far as possible and enables to go beyond nearly-free photon and plane wave approximations. The latter were cast into doubts for discontinuous potentials [1], and by a rigorous proof on the existence of finite number of gaps in two and higher dimensions for the periodic Schrödinger operator [8]. The KKR starts with an integral equation which is after expansion in a suitable basis transformed into an *algebraic* one. A band structure then follows from the conditions of solvability of the algebraic equation which is vanishing of a determinant of a matrix (see below) which determines dispersion relation and eventually photonic bands. The electronic KKR method is known to lead to a very compact scheme if the perturbing periodic potential $v(\mathbf{r})$ is *spherically symmetric* within inscribed spheres and zero (constant) elsewhere [4, 5]. In the case of electrons already p-wave approximation gives agreement within 2% with experiment.

Another distinguished feature of the method is a separation of *pure geometrical* and

[1]To appear in: "Confined Electrons and Photons : New Physics and Applications", ed. by E. Burstein and C. Weisbuch, Plenum Press, New York (1993).

[2]Address after September 1, 1993: Div. of Theor. Physics, IPN, Univ. Paris-Sud, F-91 406 Orsay Cedex, France.

scattering properties of a medium. Geometrical properties are encoded in *geometrical structure constants* $A_{lm;l'm'}$, $A_{l'm';lm} = A_{lm;l'm'}{}^*$, characteristic for the lattice under consideration. They are functions of energy σ (for photons $\sigma = \omega\sqrt{\epsilon_o}$, where ω is frequency) and the Bloch momentum $\mathbf{k}$. Once the structure constants are known then all that is needed in the case of lattice of identical scatterers is to know scattering properties (*phase shifts*) of a *single* scatterer.

We shall try to elucidate you a derivation of the photonic KKR along the lines of [4] and from the multiple-scattering theory (MST) [9]. The latter is a formal method for calculation of the spectrum in a (photonic) crystal under the presence of impurities. In fact it gives a formal solution to the problem of finding the spectrum in the case of a collection of *arbitrary* distributed scatterers of *different* shape and of *different* scattering properties. In order to simplify our discussion dielectric medium is assumed to be *magnetically isotropic* and from now on we shall set $\mu(\mathbf{r}) = 1$ as well as $c = 1$. On discontinuities Σ of $\epsilon(\mathbf{r})$ side limits of $\epsilon(\mathbf{r})$ and its derivatives as well as limiting values of fields and their derivatives are assumed to be well defined, too.

2. INTEGRAL EQUATIONS

In course of their derivation we have found that there still persists some confusion. This originates from the fact that unlike the scalar case in the case of photons fields can change *discontinuously* across *discontinuities* of electric and magnetic permeabilities and fields are *different* on *different* sides of discontinuities. This is the *essential* difference between the Schödinger and the Maxwell equations[3]. Therefore, in the latter case one has to carefully distinguish between "*inward*" and "*outward*" formulations, i. e., whether in a given surface integral inward or outward limits of fields and their derivatives at the atom boundary are taken [2, 6, 7]. The inward formalism is basically that of KKR [4] while outward formalism is originally due to Morse [5]. In particular we have found that the photonic KKR method proposed in [10] does not serve the purpose. There fields in integral equations are *outward* limits of fields with respect to the atom boundary while a scalar product with *inward* limits of fields is taken.

The outward integral equation for $\mathbf{E}(\mathbf{r})$ can be written as follows [6],

$$\mathbf{E}(\mathbf{r}) = \oint_{\partial V_{s+}} [\mathbf{E}(\mathbf{r}')\,(d\mathbf{S}'\cdot\boldsymbol{\nabla}')G_\sigma(\mathbf{r},\mathbf{r}') - G_\sigma(\mathbf{r},\mathbf{r}')\,(d\mathbf{S}'\cdot\boldsymbol{\nabla}')\mathbf{E}(\mathbf{r}')]. \tag{1}$$

Here $G_\sigma(\mathbf{r},\mathbf{r}')$ is the Green function of the Helmholtz equation in a region Ω with suitable boundary conditions imposed, defined by

$$(\boldsymbol{\nabla}^2 + \sigma^2)G_\sigma(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{2}$$

The same equation also holds for $\mathbf{B}(\mathbf{r})$. Thus, formally both $\mathbf{B}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$ satisfy the same integral equation (1) outside a dielectric atom V_s. What makes the difference between them are matching conditions across a boundary of the atom.

Corresponding inward integral equation for $\mathbf{E}(\mathbf{r})$ is [6]

$$\begin{aligned}\mathbf{E}(\mathbf{r}) = \chi_{V_s}(\mathbf{r})\,\mathbf{E}(\mathbf{r}) + \oint_{\partial V_{s-}} [G_\sigma(\mathbf{r},\mathbf{r}')\,(d\mathbf{S}'\cdot\boldsymbol{\nabla}')\mathbf{E}(\mathbf{r}') - \mathbf{E}(\mathbf{r}')(d\mathbf{S}'\cdot\boldsymbol{\nabla}')\,G_\sigma(\mathbf{r},\mathbf{r}')]\\ -\frac{1}{\epsilon_o}\oint_{\partial V_{s-}} [\boldsymbol{\nabla}'G_\sigma(\mathbf{r},\mathbf{r}')]v(\mathbf{r}')\,(\mathbf{E}(\mathbf{r}')\cdot d\mathbf{S}') - \oint_{\partial V_{s-}} G_\sigma(\mathbf{r},\mathbf{r}')[\boldsymbol{\nabla}'\cdot\mathbf{E}(\mathbf{r}')]\,d\mathbf{S}',\end{aligned} \tag{3}$$

[3]Another principle difference is that the Maxwell equations *do not* seperate even if $\epsilon(\mathbf{r})$ is a sum of functions of a single coordinate.

$\chi_{V_s}(\mathbf{r})$ being the characteristic function of V_s [6].

The equivalence of the two expressions can be established either by taking different limits in integral equations for the vector potential $\mathbf{A}(\mathbf{r})$ [6] or directly by looking at the matching rules of fields and their derivatives on different sides of Σ. It can be found in almost any textbook that

$$(E_n^+ - E_n^-)\Big|_\Sigma = \frac{\epsilon_- - \epsilon_+}{\epsilon_+} E_n^- = \frac{v(\mathbf{r})}{\epsilon_o} E_n^-, \qquad E_t^+ = E_t^-. \tag{4}$$

However, none of the standard textbooks (as far as we know) tells you how derivatives of fields behave on a discontinuity of permeabilities. Our results are that normal derivative $\partial_n \mathbf{E}_t(\mathbf{r})$ of tangential component of $\mathbf{E}(\mathbf{r})$ changes *discontinously* across Σ,

$$(\partial_n \mathbf{E}_t^+ - \partial_n \mathbf{E}_t^-)\Big|_\Sigma = \left(\frac{1}{\epsilon_+} - \frac{1}{\epsilon_-}\right) \boldsymbol{\nabla}_t D_n = \frac{v}{\epsilon_o} \boldsymbol{\nabla}_t E_n^-, \tag{5}$$

$\boldsymbol{\nabla}_t D_n(\mathbf{r})$ is continuous and $\partial_n \mathbf{E}_t^- = \boldsymbol{\nabla}_t E_n^-$. Rather surprisingly, albeit normal component $E_n(\mathbf{r})$ of $\mathbf{E}(\mathbf{r})$ is discontinuous,

$$(\partial_n E_n^+ - \partial_n E_n^-)\Big|_\Sigma = -\left(\frac{1}{\epsilon_+^2}(\partial_n \epsilon)_+ - \frac{1}{\epsilon_-^2}(\partial_n \epsilon)_-\right), \tag{6}$$

and provided $(\partial_n \epsilon)_+ = (\partial_n \epsilon)_- = 0$ the derivative changes *continously* [6]. In this manner singularities appearing due to discontinuities of permeabilities are *safely* treated. These relations explain why the Gauss theorem which requires at least continuous functions can be applied to electromagnetic fields despite that fields change discontinuosly.

3. PHOTONIC KKR METHOD

In the case of photons the KKR method has been only used within the scalar approximation to the Maxwell equations [11]. Following the lines of [4] we have formulated a general variational principle for the Maxwell equations which holds for an *arbitrary shape* of the basic "atom" of a dielectric lattice. The photonic analogue of the scalar KKR functional is defined to be

$$\Lambda = \omega^2 \int_{V_s} d^3\mathbf{r}\, v(\mathbf{r})\, \mathbf{E}^*(\mathbf{r}) \cdot \Big\{ \mathbf{E}(\mathbf{r}) + \omega^2 \int_{V_s} G_\sigma(\mathbf{r},\mathbf{r}')\, v(\mathbf{r}')\, \mathbf{E}(\mathbf{r}') d^3\mathbf{r}' + \\ + \int_{V_{s+}} \boldsymbol{\nabla}' G_\sigma(\mathbf{r},\mathbf{r}') [\boldsymbol{\nabla}' \cdot \mathbf{E}(\mathbf{r}')] d^3\mathbf{r}' \Big\}. \tag{7}$$

The integral over $\mathbf{r}$ is well defined and does exist as a *bothside* limit. Provided $\epsilon(\mathbf{r})$ is *real* (no absorbtion), and using well-known hermitian properties of Green's functions, $\partial_\mathbf{r} G_\sigma(\mathbf{r},\mathbf{r}') = -\partial_{\mathbf{r}'} G_\sigma(\mathbf{r},\mathbf{r}')$ and $G_\sigma^*(\mathbf{r},\mathbf{r}') = G_\sigma(\mathbf{r}',\mathbf{r})$ one can check that variations of Λ with respect to $\mathbf{E}(\mathbf{r})$ or $\mathbf{E}^*(\mathbf{r})$ reproduce correctly the equation for electric field $\mathbf{E}(\mathbf{r})$ or its complex conjugate $\mathbf{E}^*(\mathbf{r})$ within V_s, respectively. Rather surprisingly, unless $\epsilon(\mathbf{r})$ is piecewise constant, i. e., the classical *muffin-tin potential*, there is *impossible* (at least for our variational principle) to write (7) in terms of surface integrals only. Thus, when working with the variational KKR functional it is necesary to confine ourselves to the case when $\epsilon(\mathbf{r})$ is nothing but a *real muffin-tin potential.* Then in the case of spherically symmetric dielectric atoms general formula (7) can be simplified further as follows,

$$\Lambda := \lim_{\epsilon\to 0} \oint_{r=r_s-2\epsilon} dS\; [\partial_r \mathbf{E}^*(\mathbf{r}) - \mathbf{E}^*(\mathbf{r})\partial_r] \cdot \Big\{ \oint_{r'=r_s-\epsilon} dS'\; [\partial_{r'} \mathbf{E}(\mathbf{r}') - \mathbf{E}(\mathbf{r}')\, \partial_{r'}]\, G_\sigma(\mathbf{r},\mathbf{r}') \\ - \frac{1}{\epsilon_o} \oint_{\partial V_{s-}} [\boldsymbol{\nabla}' G_\sigma(\mathbf{r},\mathbf{r}')]\, v(\mathbf{r}')\, (\mathbf{E}(\mathbf{r}') \cdot d\mathbf{S}') \Big\}. \tag{8}$$

The final expression (8) resembles the scalar case [4], the only difference being the last term. The formula (7) is called *off-shell* while the later (8) is *on-shell.* The reason behind this is that the latter formula is derived from (7) by using field equations which for a (relativistic) free particle means that it is on its mass-shell. Therefore in looking for an extremum of (7) one is allowed to use "*arbitrary*" test functions while in the case of (8) one has to ensure that the test functions are *local solutions* to the Maxwell equations. In the latter case the variational principle selects among the local solutions that which satisfies prescribed (Bloch) boundary conditions.

To find the local solutions is rather difficult. Usually only inward solutions can be found. From now on the further treatment along lines in [4] is straightforward, albeit more involved [2]. To proceed further analytically $\mathbf{E}(\mathbf{r})$ and $G_\sigma(\mathbf{r},\mathbf{r}')$ are expanded into spherical harmonics [12, 13] after which the integral equations are transformed into matrix equations for expansion coefficients. If it is done in (3) one obtains (in our notation) *direct* KKR method while starting from (8) *variational* KKR method [2, 6]. The "direct" photonic KKR method has a wider region of applications : complex and nonconstant $\epsilon(\mathbf{r})$ within atoms, while the variational KKR method has a rather limited range of applications. However, being variational it is expected to converge more rapidly within its range of application.

4. MULTIPLE-SCATTERING THEORY

Standard assumption of MST is that a given medium can be divided into *non-overlapping* spheres $V_n{}'^s$ each of which contains *one and only one* scatterer. MST implicitely assumes that the t-matrix (*transition factor* [9]) or phase shifts for a single scatterer are known. Once they are known it is convenient to use the *outward* integral equation which is simpler than the inward one. However, one must not forget that the problem of finding inward local solutions still remains - they are necessary to determine just the t-matrix! Following a standard derivation [9] one starts with the $on-shell$ Lippmann-Schwinger equation for $\mathbf{E}(\mathbf{r})$ [6],

$$\mathbf{E}_o(\mathbf{r}) = \sum_n \oint_{\partial V_{n+}} dS'[\partial_{r'}G_\sigma(\mathbf{r},\mathbf{r}') - G_\sigma(\mathbf{r},\mathbf{r}')\,\partial_{r'}]\mathbf{E}(\mathbf{r}'), \tag{9}$$

which holds provided $\mathbf{r}$ stays inside spheres. $\mathbf{E}_o(\mathbf{r})$ is an *incident* wave and n labels scatterers (or spheres containing single scatterers, as you want). After expanding fields and the Green function into spherical harmonics one arrives at the *basic photonic MST equations* [7],

$$C^o_{iAL} = \sum_{jA'L'} \left[\delta_{ij}\delta_{LL'}\delta_{AA'} + \sum_{A"L"} G^{ij}_{AL,A"L"} t^j_{A"L",A'L'}\right] C_{jA'L'}. \tag{10}$$

Here indices i, j label different scatterers, $G^{ii} \equiv 0$, and C^o_{jAL} or C_{jAL} are expansion constants of $\mathbf{E}_o(\mathbf{r})$ or $\mathbf{E}(\mathbf{r})$ into spherical harmonics around j-th sphere, respectively. In contrast to the scalar case the expansion is more involved due to vectorial nature of fields. This is reason for additional index A which labels magnetic ($A = M$) and electric ($A = E$) multipoles [13]. As a result the order of matrix (10) in a given (s-, p-,...-wave approximation) is doubled with regard to the scalar case. $G^{ij}_{AL,A"L"}$ is the vector (propagator) Green function. Physically it describes what amount of a particular multipole field *scattered* from the i-th site contributes to the particular multipole field *incident* on the j-th site.

To write the *vector* Green function $G^{ij}_{AL,A'L'}$ explicitely we have defined quantities $\bar{C}^\alpha$ in terms of $3j$-*symbols* $C^\alpha(l'm'lm)$ [13],

$$\begin{aligned}\bar{C}^\alpha(l-1,m+\alpha) &= \sqrt{l+1}\,C^\alpha(l-1,m+\alpha,l,m),\\ \bar{C}^\alpha(l+1,m+\alpha) &= -\sqrt{l}\,C^\alpha(l+1,m+\alpha,l,m),\end{aligned} \tag{11}$$

and

$$\bar{T}^\alpha_{lm+\alpha} = \frac{1}{\sqrt{l(l+1)}}T^\alpha_{lm+\alpha}, \tag{12}$$

where T^α_L are defined by action of spherical components $\mathbf{L}^\alpha$ of orbital angular momentum on spherical harmonics Y_L, $\mathbf{L}^\alpha Y_L = T^\alpha_{lm+\alpha}Y_{lm+\alpha}$ [2, 7]. Radial functions which are proportional to $j_l(\sigma r_i)'^s$ (the spherical Bessel functions) are normalized to unity on the boundary of the i-th sphere. This simply amounts to *redefinition* of C^o_{iML} and C_{iML}. We also *redefine* $G^{ij}_{EL,EL'}$ by dividing factor σ^2 to which $\mathbf{J}_{EL}{}'^s$ are normalized (they have different dimension than $\mathbf{J}_{ML}{}'^s$ because of rotation operation applied). Afterwords the resulting expresions can be written in the following compact form

$$G^{ij}_{ML,ML'} = i\sum_{\alpha=-1}^{1} g^{ij}_{l'm'+\alpha;lm+\alpha}\bar{T}^\alpha_{lm+\alpha}\bar{T}^\alpha_{l'm'+\alpha}, \tag{13}$$

$$G^{ij}_{ML,EL'} = \sigma\sum_{\substack{p'=-1\\ p'\neq 0}}^{1}\sum_{\alpha=-1}^{1} g^{ij}_{l'+p',m'+\alpha,lm+\alpha}\bar{C}^\alpha(l'+p',m'+\alpha)\bar{T}^\alpha_{lm+\alpha}, \tag{14}$$

$$G^{ij}_{EL,ML'} = -\sigma\sum_{\substack{p=-1\\ p\neq 0}}^{1}\sum_{\alpha=-1}^{1} g^{ij}_{l',m'+\alpha,l+p,m+\alpha}\bar{C}^\alpha(l+p,m+\alpha)\bar{T}^\alpha_{l'm'+\alpha}, \tag{15}$$

$$G^{ij}_{EL,EL'} = i\sum_{\alpha=-1}^{1}\sum_{\substack{p=-1\\ p\neq 0}}^{1}\sum_{\substack{p'=-1\\ p'\neq 0}}^{1} g^{ij}_{l'+p',m'+\alpha,l+p,m+\alpha}\bar{C}^\alpha(l+p,m+\alpha)\bar{C}^\alpha(l'+p',m'+\alpha). \tag{16}$$

Note that $G^{ij}_{AL,A'L'}$ *is not* Hermitian. This is a consequence of using the t-matrix which also is not Hermitian [4, 9]. For spherically symmetric scatterers the t-matrix is *diagonal* and for homogeneous spheres it is explicitely known as the *Mie solution* [14].

Provided scatterers are identical and arranged in a *periodic* way one can take Fourier transform with regard to the Bloch momentum $\mathbf{k}$. The condition of existence of a solution to (10) for $C^o_{iAL} = 0$,

$$\det\left|\delta_{LL'}\delta_{AA'} + \sum_{A"L"} G_{AL,A"L"}(\mathbf{k})t_{A"L",A'L'}\right| = 0, \tag{17}$$

then gives the *photonic KKR equation.*

We have noted an attempt to derive MST for photons [15]. However one can find obvious difference : our expression is much more symmetric while in [15] there is no summation over p, p' which is necessary here since electric multipoles of order l have nonzero matrix elements with $Y_{L'}$ only for $l' = l \pm 1$. Moreover, in our case vector structure constant are determined via $3j$-symbols and T^α_L coefficients in contrast to the Gaunt numbers in [15].

Presented results use as much as possible existing electron structure constants and hence allow for a direct numerical application. They allow to calculate photonic bands and to treat impurities as well. Despite that a photonic band calculation is more involved due to its vectorial nature there is one small advantage with regard to the

Schrödinger equation : the Maxwell equations are *conformally invariant* and therefore a scale of a dielectric lattice can be chosen arbitrary. By taking the scale identical to that of electrons the scalar structure constants can be used without any changes. For more complete treatment of the above problems together with numerical results see [2].

Last but not least some new phenomenon in a photonic crystal which has not been discussed yet and which may be of some importance : particles propagating through such medium can emit Tcherenkov radiation at rather small velocity.

ACKNOWLEDGEMENTS

Financial support of the Swiss National Foundation in the early stage of this work as well as a partial support by the CAS grant No. 11086 are gratefully acknowledged. My thanks is also to the organizers of the School for preparing very friendly and stimulating enviroment.

References

[1] H. S. Sözüer, J.W. Haus, and R. Inguva, Photonic bands : convergence problem with the plane-wave method, *Phys. Rev.* B 45:13962 (1992).

[2] A. Moroz *et. al.*, in preparation.

[3] E. Yablonovitch, Inhibited spontaneous emission in solid-state physics and electronics, *Phys. Rev. Lett.* 58:2059 (1987).

[4] W. Kohn and N. Rostoker, Solution of the Schrödinger equation in periodic lattices with an application to methalic lithium, *Phys. Rev.* 94:1111 (1954); J. Korringa, *Physica* **13**:392 (1947).

[5] P.M. Morse, Waves in a lattice of spherical scatters, *Proc. Nat. Acad. Sci. U.S.A.* 42:276 (1956).

[6] A. Moroz, Inward and outward integral equations and the KKR method for photons, Prague preprint PRA-HEP 93/10.

[7] A. Moroz, Multiple-scattering theory for photons, Prague preprint PRA-HEP 93/11.

[8] M. M. Skriganov, *Invent. Math.* **80**, 107 (1985).

[9] P. Lloyd and P.V. Smith, Multiple-scattering theory in condensed materials, *Adv. Phys.* 21:69 (1972); P. Weinberger, "Electron Scattering Theory for Ordered and Disordered Matter", Clarendon Press, Oxford (1990).

[10] W. Lamb, D.M. Wood, and N.W. Ashcroft, Long-wavelength propagation in heterogeneous media, *Phys. Rev.* B 21:2248 (1980).

[11] S. John and R. Rangarajan, Optimal structures for classical wave localization : an alternative to the Ioffe-Regel criterion, *Phys. Rev.* B 38:10101 (1988).

[12] J.D. Jackson, "Classical Electrodynamics", 2nd. ed., J. Wiley & Sons, Inc., New York (1962).

[13] A.R. Edmonds, "Angular momentum in quantum mechanics", 2nd ed., Princeton University Press, Princeton (1960).

[14] R.G. Newton, "Scattering Theory of Waves and Particles", McGraw-Hill Inc., New York (1982), ch. 2.

[15] X. Wang, X.-G. Zhang, Q. Yu, and B.N. Harmon, Multiple-scattering theory for electromagnetic waves, *Phys. Rev.* B 47:4161 (1993).