Recursive solution of Maxwell's equations

Roger Haydock

Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403

(Received 25 January 1993)

The formal solution of Maxwell's equations may be written as the exponential of a linear operator, the Maxwellian, which generates the time evolution of the electromagnetic field. Given initial fields for a system which conserves electromagnetic energy, the Maxwellian can be transformed to a symmetric three-term recurrence relation or a symmetric tridiagonal matrix whose basis is a sequence of linearly independent fields. The power spectrum of this recurrence is the spectrum of a continued fraction, and the stationary electromagnetic waves, whose superposition gives the initial fields, are linear combinations of products of orthogonal polynomials in frequency with the basis fields. As an example, an initial field consisting of a Gaussian pulse from an electric dipole leads to an analytic three-term recurrence with a two-peaked power spectrum. The method can also be applied numerically to calculate the radiation patterns of antennas and, when generalized, to systems where the electromagnetic field exchanges energy with other degrees of freedom.

PACS number(s): 78.66.Sq

I. PROPAGATION OF LIGHT IN RANDOM MEDIA

The scattering of light by random media, for example, random arrays of dielectric spheres, produces such interference phenomena as coherent back scattering and speckle patterns. Although these phenomena are generally understood in terms of the interference of multiply scattered waves, the formation of structures such as optical dislocations [1-3] which depend on the vector nature of the electromagnetic fields are not so well understood because the solution of the vector wave equations in random media is so much more complicated than scalar wave equations such as the Schrödinger equation for electrons in random potentials. See, for example, Ref. [4].

The purpose of this paper is to show how Maxwell's equations can be solved for the evolution of electromagnetic waves from some initial field in three dimensions by reducing them to a three-term recurrence relation which is equivalent to scalar waves in one dimension. While such a transformation might seem to require some approximation, it does not because the recurrence only describes the evolution of a single initial field which may be resolved into a superposition of stationary waves, each with a different frequency. A dispersion relation for scalar waves in one dimension can be chosen to reproduce this nondegenerate spectrum.

Using this transformation, Maxwell's equations for any medium which conserves the electromagnetic energy can be solved either analytically, for simple media or small perturbations from simple media, or numerically, for any such medium. A summary of the method is that the evolution of the field is expanded in powers of a Maxwellian operator, the operator for the time derivative of the electromagnetic field, applied to the initial field. These powers of the Maxwellian on the initial field generate a sequence of linearly independent fields of which the Maxwellian couples only successive powers. When the fields are orthonormalized, the Maxwellian assumes the form of a symmetric three-term recurrence or a tridiagonal matrix. Once the Maxwellian is in tridiagonal form, the power spectrum may be expressed as a continued fraction, or the stationary waves may be expressed as linear combinations of the sequence of fields. Other quantities are similarly easy to calculate. In related work, Ratowsky, Fleck, and Feit [5] used the Lanczos method to solve the scalar Helmholtz equation.

The solution of the classical moment problem [6] is an early application of this method of finding the spectrum and other properties of a linear operator. It has been rediscovered and revived in many forms including the Lanczos method [7] for finding eigenfunctions of matrices, and the recursion method [8] for calculating the projected densities of states of the Schrödinger equation for electrons in noncrystalline potentials. This method has remarkable numerical stability for the calculation of spectra and invariants, despite numerical instability of other quantities [7,9,10].

The paper is organized into five further sections. The first describes the formal solution of Maxwell's equations using the Maxwellian operator. In the next section, the stationary solutions to the equations are expanded in the fields which tridiagonalize the Maxwellian, and the power spectrum is expanded as a continued fraction. In the fourth section, the recursion method is illustrated by its application to a Gaussian field to obtain its power spectrum. Section V contains a discussion of how the method may be applied numerically if the fields can be expanded in a basis such as the Gaussians in the example. In the last section, there are a few comments on how the method can be applied to systems with sources such as radiating antennas and to other more general systems.

II. FORMAL SOLUTIONS OF MAXWELL'S EQUATIONS

Maxwell's equations describe the evolution of the electromagnetic field in terms of the electric field E, the elec-

48 2172

tric displacement D, the magnetic field B, and the magnetic intensity H. In the absence of charge and current densities, Maxwell's equations in *Système International* (SI) units are

$$D_t = \operatorname{curl} H$$
, (2.1)

$$B_t = -\operatorname{curl} E , \qquad (2.2)$$

$$\operatorname{div} D = 0 , \qquad (2.3)$$

$$\operatorname{div} B = 0 , \qquad (2.4)$$

where the subscript t means the partial derivative with respect to time, keeping position fixed. In addition to Maxwell's equations, there are relations between the fields,

$$D = \epsilon E \tag{2.5}$$

and

$$B = \mu H , \qquad (2.6)$$

where ϵ and μ are, respectively, the permittivity and the permeability of the medium. When charges and currents are present, the current density must be subtracted from curlH in the first equation and the charge density subtracted from divD in the third equation. In general, the relationship between D and B on the one hand and E and H on the other is restricted only by causality and by the fact that the electromagnetic energy density must be non-negative.

The work which follows assumes for simplicity that there are no free charge or current densities, that the permeability always takes it vacuum value, and that the permittivity is isotropic and constant in time, but varies with position to describe an inhomogeneous dielectric medium. However, the methods presented here are general enough to deal with charge and current densities as well as any linear relationships between the fields which satisfy the physical constraints. The method may be applied to time-dependent densities, and even time-dependent media by techniques which are described in Sec. VI.

The above form of Maxwell's equations emphasizes the relation between the time and spacial derivatives of the fields. This can be written more simply in the form of a Maxwellian operator \mathbf{M} which acts on a field F having six components, the first three being E, the second three being H, and with all six varying in space and time. In this form, Maxwell's equations for F are

$$iF_t = \mathbf{M}F , \qquad (2.7)$$

where *i* is the positive square root of -1, and, in terms of *E*, and *H*, **M** is a 2×2 matrix operator whose diagonal elements are zero and whose off-diagonal elements are $i\epsilon^{-1}$ curl and $-i\mu^{-1}$ curl for the case under consideration. If the permittivity or permeability are nonlocal, then the above inverses are of their matrices or kernels.

Given a field F at time zero, then the formal solution to Maxwell's equations for a medium which is not explicitly time dependent is

$$F(t) = \exp\{-i\mathbf{M}t\}F, \qquad (2.8)$$

where the exponential of the Maxwellian is defined by its power series and $\mathbf{M}^n F$ grows no faster than n!. In what follows, the goal is to calculate F(t) efficiently and accurately given an arbitrary dielectric medium. The calculation begins by expressing F(t) in terms of the resolvent of the Maxwellian, the Fourier transform of its exponential,

$$F(t) = \int_C \exp(-i\omega t) (\omega - \mathbf{M})^{-1} F \, d\omega / (2\pi i) , \qquad (2.9)$$

where the integral is around a contour C which encloses all the angular velocities ω for which the Maxwellian has solutions. Submatrices of this resolvent can be conveniently calculated.

III. REPRESENTATION OF THE MAXWELLIAN AS A THREE-TERM RECURRENCE

When the Maxwellian is time independent, Maxwell's equations separate and their solutions can be written as the real part of $\psi_{\omega} \exp(-i\omega t)$ where ω is the angular velocity of the solution, and ψ_{ω} satisfies

$$\omega \psi_{\omega} = \mathbf{M} \psi_{\omega} . \tag{3.1}$$

For an initial field v_0 , solution of this time-independent equation proceeds by finding a sequence of bounded, linearly independent fields $v_1, v_2, \ldots, v_n, \ldots$ which reduce the Maxwellian to a symmetric three-term recurrence which in monic form is

$$\mathbf{M}v_n = v_{n+1} + a_n v_n + b_n^2 v_{n-1} . aga{3.2}$$

The sense in which this recurrence is symmetric is that a_n and b_n are real so that the fields can be normalized,

$$v_n = b_n b_{n-1} \cdots b_1 u_n , \qquad (3.3)$$

to put the recurrence in the explicitly symmetric form,

$$\mathbf{M}u_{n} = b_{n+1}u_{n+1} + a_{n}u_{n} + b_{n}u_{n-1} , \qquad (3.4)$$

where the coefficient of u_{n-1} in $\mathbf{M}u_n$ is the same as that of u_n in $\mathbf{M}u_{n-1}$.

The solutions ψ_{ω} of Eq. (3.1) can be expanded in either sequence of fields with coefficients which are polynomials in angular velocity,

$$\psi_{\omega} = \sum_{n} P_{n}(\omega) u_{n} , \qquad (3.5)$$

where the polynomials satisfy a three-term recurrence similar to the fields,

$$\omega P_{n}(\omega) = a_{n} P_{n}(\omega) + b_{n+1} P_{n+1}(\omega) + b_{n} P_{n-1}(\omega) , \qquad (3.6)$$

with the initial condition that $P_{-1}(\omega)$ is zero and the normalization condition that $P_0(\omega)$ is unity. Substituting Eq. (3.5) into Eq. (3.1), using properties of the fields in Eq. (3.4) and of the polynomials in Eq. (3.6) demonstrates this directly.

Since the fields can be normalized so that the recurrence is explicitly symmetric as in Eq. (3.4), these renormalized fields also serve as a basis in which the Maxwellian is a symmetric tridiagonal matrix whose invariant values, the angular velocities of the stationary fields, are real. Hence, the Maxwellian is Hermitian with The three-term recurrence distinguishes the initial field v_0 as the first of the sequence and so provides particularly simple expressions for this component as the field evolves. In terms of $R(\omega)$, the v_0 - v_0 element of the resolvent of the Maxwellian, the component of v_0 in F(t) is

$$v_0(t) = \int_C \exp(-i\omega t) R(\omega) d\omega / (2\pi i) , \qquad (3.7)$$

where $R(\omega)$ may be written as a continued fraction whose parameters are the coefficients of the three-term recurrence,

$$R(\omega) = \frac{1}{\omega - a_0 - \frac{b_1^2}{\omega - a_1 - \frac{b_2^2}{\omega - a_2 - \cdots}}}$$
(3.8)

and the contour C encloses the singularities of this continued fraction.

The sequence of fields $v_0, v_1, v_2, \ldots, v_n, \ldots$ spans only the electromagnetic fields which evolve from v_0 , which may be expressed as a superposition of stationary waves, each with a different frequency. The dispersion of these waves is exactly that of the scalar waves propagating on the one-dimensional chain described by the tridiagonalization of **M**. The choice of an initial field reduces the Maxwellian to the one-dimensional form of a three-term recurrence.

IV. A GAUSSIAN PULSE FROM A DIPOLE

As an example, consider the application of Maxwell's equations to the evolution of the fields arising from a sin-

gle pulse of a dipole in a homogeneous medium. A convenient form for the single pulse is as a Gaussian magnetic intensity so that

$$v_0 = \{0, H \exp[-\mathbf{r}^2/(2\mathbf{c}^2)]\mathbf{r} \times \mathbf{c}/\mathbf{c}^2\},$$
 (4.1)

where the curly brackets indicate the combination of electric and magnetic fields into a single vector, H is the magnetic intensity of the initial field, \mathbf{r} is the position vector, \mathbf{c} is a constant vector along the axis of the dipole, \times denotes the usual vector product in three dimensions, and the square of a vector is its magnitude squared. This initial field v_0 consists of a superposition of equal incoming and outgoing dipole waves whose electric vectors cancel making the electric part of v_0 equal to zero.

Applying the Maxwellian to v_0 gives the next basis field,

$$\mathbf{M}v_{0} = \{-i(1/\epsilon)(H/\mathbf{c}^{2})\exp[-\mathbf{r}^{2}/(2\mathbf{c}^{2})] \\ \times [\mathbf{r} \times (\mathbf{r} \times \mathbf{c})/\mathbf{c}^{2} + 2\mathbf{c}], 0\}, \qquad (4.2)$$

which is symmetric under inversion through the axis of c in contrast to v_0 which is antisymmetric. Since v_0 and $\mathbf{M}v_0$ have different symmetries a_0 is zero and

$$v_1 = \{-i(1/\epsilon)(H/c^2)\exp[-r^2/(2c^2)] \times [r \times (r \times c)/c^2 + 2c], 0\} .$$
(4.3)

The next step is to apply the Maxwellian to v_1 ,

$$\mathbf{M}v_{1} = \{\mathbf{0}, [1/(\epsilon\mu\mathbf{c}^{2})]H \exp[-\mathbf{r}^{2}/(2\mathbf{c}^{2})] \\ \times (\mathbf{r}^{2}/\mathbf{c}^{2}+5)\mathbf{r}\times\mathbf{c}/\mathbf{c}^{2}\}, \qquad (4.4)$$

so that b_1^2 is $5/(\epsilon \mu c^2)$, and

$$v_2 = \{0, [1/(\epsilon \mu c^2)]H \exp[-r^2/(2c^2)](r^2/c^2)r \times c\} .$$
(4.5)

Continuing the process,

$$\mathbf{M}v_{2} = \{-i(1/\epsilon)[1/(\epsilon\mu \mathbf{c}^{2})](H/\mathbf{c}^{2})\exp[-\mathbf{r}^{2}/(2\mathbf{c}^{2})][-(\mathbf{r}^{2}/\mathbf{c}^{2})\mathbf{r}\times(\mathbf{r}\times\mathbf{c})/\mathbf{c}^{2}+2\mathbf{r}\times(\mathbf{r}\times\mathbf{c})/\mathbf{c}^{2}-2(\mathbf{r}^{2}/\mathbf{c}^{2})\mathbf{c}],0\},$$
(4.6)

so that a_1 is zero by symmetry, and b_2^2 is $2/(\epsilon \mu c^2)$ leaving

$$v_{3} = \{-i(1/\epsilon)[1/(\epsilon\mu c^{2})]Hexp[-r^{2}/(2c^{2})][-(r^{2}/c^{2})r\times(r\times c)/c^{2}-2(r^{2}/c^{2})c-4c],0\}.$$
(4.7)

In general, the (2n)th field is

$$v_{2n} = \{0, [1/(\epsilon \mu c^2)]^n H \exp[-r^2/(2c^2)] (r^2/c^2)^n r \times c/c^2\}, \qquad (4.8)$$

and the (2n + 1)th field is

$$v_{2n+1} = \{ -i(1/\epsilon) [1/(\epsilon \mu c^{2})]^{n} (H/c^{2}) \exp[-r^{2}/(2c^{2})] \\ \times \{ (-r^{2}/c^{2})^{n} r \times (r \times c)/c^{2} + 2(-r^{2}/c^{2})^{n} c - 4n(-r^{2}/c^{2})^{n-1} c \\ + 8n(n-1)(-r^{2}/c^{2})^{n-2} c - \dots + 2(-2)^{m} [n!/(n-m)!] (-r^{2}/c^{2})^{n-m} c + \dots + 2(-2)^{n} c \}, 0 \}.$$
(4.9)

The diagonal coefficients of the recurrence a_n are all zero because v_0 has a definite symmetry and each application of the Maxwellian changes the symmetry of the field. The odd, off-diagonal elements are

$$b_{2n+1}^2 = (2n+5)/(\epsilon \mu c^2)$$
, (4.10)

while the even, off-diagonal elements are

$$b_{2n}^2 = 2n / (\epsilon \mu c^2)$$
 (4.11)

The spectrum of the continued fraction associated with the above recurrence gives the intensity of the wave of each frequency present in the initial field, so this is the power spectrum of the initial field. This spectrum is shown in Fig. 1 where the units of angular velocity are $(\epsilon\mu c^2)^{-1/2}$. The spectrum is symmetric with respect to the zero angular velocity because the initial field is real and so contains equal components of the positive and negative, complex angular velocities for each wave.

This power spectrum peaks at ± 2 in the above units, just as the power spectrum of a similar scalar pulse. A pulse described by a factor which is linear in displacement from the origin times a factor which is a Gaussian in displacement has a Fourier transform which is also a linear factor in wave number times a Gaussian factor in wave number. The power distribution is quadratic in wave number, and for nondispersive waves (angular velocity proportional to wave number) in three dimensions, the power distribution in angular velocity has a quartic factor multiplying the Gaussian which produces these maxima.

V. NUMERICAL SOLUTION OF MAXWELL'S EQUATIONS

The reduction of the Maxwellian to a three-term recurrence can also be done numerically with the help of an inner product for the fields, in which the Maxwellian is Hermitian. For a time-independent Maxwellian with nondissipative permeability and permittivity, the total electromagnetic energy is a conserved quantity. In the



FIG. 1. The power $P(\omega)$ radiated with angular velocity ω for a Gaussian pulse from an electric dipole.

case of a dielectric medium, this energy can be written as

$$W = \frac{1}{2} \int (E \cdot \epsilon E + H \cdot \mu H) d\Omega , \qquad (5.1)$$

where the integral is over the volume of the entire system, and the centerdot denotes the scalar product of vectors.

Since the total electromagnetic energy W is nonnegative, there is a positive, Hermitian inner product of fields u and v defined by

$$u^* v = \frac{1}{2} \int (u_E \cdot \epsilon v_E + u_H \cdot \mu v_H) d\Omega , \qquad (5.2)$$

where the electric part of each field has the subscript E, the magnetic part has the subscript H, and the u fields in the integral are conjugated if complex. Conservation of electromagnetic energy makes the Maxwellian Hermitian with respect to this inner product. There are other inner products which will serve just as well provided that the Maxwellian remains Hermitian, and for systems with nonlocal permittivity and permeability, the above expressions can be generalized.

Suppose at time zero, the fields are u, then the Maxwellian can be numerically tridiagonalized by the following recursion:

$$u_0 = u / b_0$$
, (5.3)

where

$$b_0^2 = u^* u$$
, (5.4)

to normalize u. The next step is to begin the recursion by calculating

$$a_0 = u_0^* \mathbf{M} u_0$$
, (5.5)

$$b_1^2 = (\mathbf{M}u_0 - a_0 u_0)^* (\mathbf{M}u_0 - a_0 u_0) , \qquad (5.6)$$

and taking

$$u_1 = (\mathbf{M}u_0 - a_0 u_0) / b_1 . (5.7)$$

In the general step of the recursion u_0, u_1, \ldots, u_n ; $a_0, a_1, \ldots, a_{n-1}$; and b_0, b_1, \ldots, b_n are known, with a_n , b_{n+1} , and u_{n+1} to be determined. These quantities are

$$a_n = u_n^* \mathbf{M} u_n \quad , \tag{5.8}$$

$$b_{n+1}^{2} = (\mathbf{M}u_{n} - a_{n}u_{n} - b_{n}u_{n-1})^{*} \times (\mathbf{M}u_{n} - a_{n}u_{n} - b_{n}u_{n-1}), \qquad (5.9)$$

and

$$u_{n+1} = (\mathbf{M}u_n - a_n u_n - b_n u_{n-1}) / b_{n+1} .$$
 (5.10)

The three-term recurrence is symmetric,

$$\mathbf{M}u_n = b_{n+1}u_{n+1} + a_nu_n + b_nu_{n-1} , \qquad (5.11)$$

with the initial conditions that u_{-1} is zero and u_0 is given.

In order to carry out the above recursion numerically, the fields $\{u_n\}$ must be expressed as linear combinations of some basis fields in terms of which the Maxwellian is a matrix with only a finite number of numerically significant elements in each row or column. Because the electromagnetic field has an infinite number of degrees of freedom, any matrix representation in terms of a basis must also be of infinite dimension, so in order to multiply numerically any element of the basis by the Maxwellian, there must only be a finite number of significant terms in the product. This is the property that the Maxwellian matrix must be sparse. An important consequence of the Maxwellian matrix being sparse is that the result of multiplying any finite combination of basis elements by the Maxwellian has only a finite number of significant terms, and so any finite power of the Maxwellian on any finite combination of basis elements is finite. As a result, each of the $\{u_n\}$ has only a finite number of significant terms and the tridiagonalization of the Maxwellian can be done to arbitrary accuracy on a finite computer.

One set of basis fields for which the Maxwellian is sparse is the set of vector Gaussians multiplied by vector polynomials used in the example, which can be augmented by Gaussians with other centers. This basis set has the advantage that, as shown above, it tridiagonalizes the free space Maxwellian, just as Gaussians tridiagonalize the free space Hamiltonian for electrons [11]. In terms of such a set $\{\Phi_{\alpha}\}$ of basis fields, each of which have an electric and magnetic part, the matrix elements of the Maxwellian **M** are

$$M_{\alpha,\beta} = \frac{i}{2} \int (\Phi_{H,\alpha} \cdot \operatorname{curl} \Phi_{E,\beta} - \Phi_{E,\alpha} \cdot \operatorname{curl} \Phi_{H,\beta}) d\Omega ,$$
(5.12)

where the subscripts E and H refer, respectively, to the electric and magnetic part of the basis fields, and the integral is over all space. Evaluation of these matrix elements involves only Gaussian integrals because the basis fields are Gaussians multiplied by polynomials, vector generalizations of isotropic oscillator wave functions, and the curls of these fields are also generalized isotropic oscillator functions.

The Gaussian fields defined above are not necessarily orthogonal with respect to the inner product, so the inner products or overlaps between the basis fields make up a matrix S whose elements are

$$S_{\alpha,\beta} = \frac{1}{2} \int (\Phi_{E,\alpha} \cdot \epsilon \Phi_{E,\beta} + \Phi_{H,\alpha} \cdot \mu \Phi_{H,\beta}) d\Omega \quad . \tag{5.13}$$

The matrix which produces the linear combination of basis fields which result from applying the Maxwellian is neither S nor M on its own, but $S^{-1}M$ which is also sparse and may be calculated by various methods [12]. By this means, the recursion is reduced to a set of operations in linear algebra for which there is a library of computer programs [13].

Once calculated, the coefficients $\{a_n\}$ and $\{b_n\}$ of the three-term recurrence can be used in the continued fraction, Eq. (3.8), to evaluate the power spectrum of the elec-

- [1] J. F. Nye and M. V. Berry, Proc. R. Soc. London, Ser. A 336, 165 (1974).
- [2] M. V. Berry, J. Phys. A 11, 27 (1978).
- [3] J. F. Nye, Proc. R. Soc. London, Ser. A 378, 219 (1981).

tromagnetic waves which evolve from u, or together with the $\{u_n\}$ and Eq. (3.5) to expand the waves themselves. The errors induced by finite precision arithmetic on these algorithms are understood and discussed in Ref. [8] and the references contained therein.

Briefly, the effect of finite precision is that the $\{u_n\}$ are not orthogonal with respect to the chosen inner product. This produces an error in the power spectrum of order the precision, as if the initial field differed from the actual one by an amount of order the root of the precision. Waves calculated using Eq. (3.5) have errors of order the root of the precision, provided that the coefficient of u_0 in Eq. (3.5) is no smaller, relative to the largest coefficient in the expansion, than the root of the precision.

VI. ANTENNAS AND OTHER SYSTEMS

The previous sections have emphasized the solution of Maxwell's equations for nondissipative, time-independent systems given some initial field. An important example of such a system is an antenna driven by an oscillator to which it is connected by a transmission line. The fields in the transmission line can be expanded in some convenient basis such as Gaussians, and the oscillator replaced by the initial condition that the transmission line carry an outward traveling wave. The zeroth diagonal element of the Maxwellian resolvent for this system has a spectrum which is the power reflected back down the transmission line by the antenna at each frequency. The calculation of the radiation pattern of the antenna is the same as calculating the transmittance of the antenna, a problem which has been solved for quantum-mechanical waves in Ref. [14]. Instead of just diagonal elements of the resolvent, the transmittance also depends on off-diagonal elements.

The recursion method can also be extended to systems with time dependence or dissipation provided that the sources or sinks of energy can be incorporated with the electromagnetic fields into a system which conserves its total energy and for which the equations of motion are linear. A simple example of such a system is an atom coupled to the electromagnetic field. The combined system conserves energy although its parts do not do so separately. The equations of motion include the states of the atom as well as the fields, and the coupling between the atomic transitions and the fields.

ACKNOWLEDGMENTS

The author is grateful to Moshe Kaveh, Isaac Freund (I.F.), and Michael Rosenbluh (M.R.) for suggesting this problem. Collaboration with I.F. and M.R. is supported by the U.S.-Israel Binational Science Foundation under Grant No. BSF 89-00150. This work was supported by National Science Foundation Materials Theory Grant No. DMR-9022525.

- [4] I. Freund, M. Kaveh, R. Berkovits, and M. Rosenbluh, Phys. Rev. B 42, 2613 (1991).
- [5] R. P. Ratowsky, J. A. Fleck, and M. D. Feit, Opt. Lett. 17, 10 (1992); J. Opt. Soc. Am. A 9, 265 (1992).

[6] J. A. Shohat and J. D. Tamarkin, The Problem of Moments (American Mathematical Society, New York, 1943). 1550 (1992).

- [12] Andrew Gibson, Roger Haydock, and John P. LaFemina, Phys. Rev. B 47, 9229 (1993).
- [13] C. M. M. Nex, *The Cambridge Recursion Library*, Theory by H. by New of Condensed Matter Group, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, England, revised 1992.
 - [14] T. J. Godin and Roger Haydock, Phys. Rev. B 38, 5237 (1988).
- ments (American Mathematical Society, New York, 1943).
 [7] B. N. Parlett, The Symmetric Eigenvalue Problem (Prentice-Hall, Englewood Cliffs, NJ, 1980).
- [8] Roger Haydock, in Solid State Physics, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1980), Vol. 35.
- [9] C. C. Paige, J. Inst. Math. Appl. 10, 373 (1972).
- [10] Roger Haydock, Comput. Phys. Commun. 53, 133 (1989).
- [11] Scott Blumberg and Roger Haydock, Phys. Rev. B 45,