Structural Contribution to the Anisotropic Reflection from the Si(110) Surface*

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Abstract

For a single plane of dipoles of arbitrary configuration the optical reflection has been calculated, using the screened discrete dipole model. Results differ from continuum approaches. Further the results show that the experimentally observed reflection anisotropy has besides the dominating intrinsic contribution, also a structural one.

1. Introduction

The influence of the very outmost layer of a semiinfinite solid on the optical reflectivity is still not well understood. It is this region where one has to locate the surface states, but the problem gets its current interest from the observation of surface induced optical anisotropy. This article offers a contribution to the understanding of this phenomenon.

First we give some historical background. During the fifties a link was established between bulk optical experiments and quantummechanics of solids. Shortly after, with the same aim, experimentalists developed a surface sensitive optical spectroscopy. This sensitivity was obtained through explicit modification of the surface if gas molecules were absorbed on top of it. The resulting difference in reflectivity turned out to be easily detectable. This type of differential spectroscopies has been described in Refs [2, 3, 4] dating from the late sixties. Despite their technological importance, those spectroscopies could not rival their bulk like equivalents as far as scientific impact was concerned, for two reasons. First, a workable theoretical model, as e.g., Bassani [1] developed for the bulk, was not there. Secondly, a forceful breakthrough towards the underlying quantummechanical microscopy contained in the surface joint density of states [3, 5], required unjustifiable assumptions and was of limited applicability. Certainly one of the blocking factors was the necessity to extract the difference signal from systems with different composition (surfaces with and without gas coverage).

A possible way out to this problem however almost passed unnoticed after its first observation. This was the case with the discovery of anisotropic reflection from Ag (110) surfaces by Furtak [6], an interesting phenomenon, since bulk silver is isotropic, leaving only the surface as its possible cause. The progress was that if difference signals were obtained from anisotropy measurements, only a single system having a single composition was involved (e.g., the clean surface). Practically this means a drastic reduction of the number of unknown model parameters, the impediment if one wants to use descriptions developed by McIntyre and Aspnes [3]. Anisotropy measurements were done later also for the semi-

conductors Si and Ge [7]. Only the Italians managed to connect theory and experiment in the case of the anisotropy caused by the (2×1) reconstruction of the Si(111) surface [8, 9]. Their theoretical model has been developed by Del Sole and coworkers [9]. Del Sole derived his anisotropies mainly from momentum matrix elements, i.e., quantummechanically, and local fields play no explicit role. Local field contributions as such have been treated recently by Mochán and Barrera [10]. Their approach differs from ours in that they treat a semiinfinite case, but with neglect of retardation and screening. The present article shows that the rigorous solution of the local field problem for a (110) oriented single plane of dipoles, causes anisotropic reflectivity in a systematic and transparent way. Then one may most naturally distinguish between the structural and intrinsic contribution to it. Like in Del Sole's approach tedious algebra has to be overcome, but the difference is that the basic principles upon which the method is based, are only a few.

2. Experimental environment and surface structure

For the calculation proper introduction of the variables to be used, is indispensable. Figure 1 shows a configuration which may be considered to be characteristic for most optical experiments using specular reflection. A monocrystalline piece of silicon (or any other material which may be treated in the dielectric limit) cleaved in a well defined crystallographic direction (100, 111 or 110) is mounted on top of an axis which allows for a rotation around the surface normal. This is the fundamental motion for anisotropic measurements. While doing so, the anisotropic azimuth Ω , defined in the (110) case as the angle with respect to the $(1\bar{1}0)$ surface direction (x -axis),

Fig. 1. Experimental configuration, see text.

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Fig. 2. Top view of the three main cleavage planes of monocrystalline silicon.

changes. The other parameters are the traditional ones. Thus $\hat{\mathbf{z}}$ indicates the surface normal, the electromagnetic plane wave impinging upon the surface is characterized by a wavevector $\mathbf{k}$, which changes upon reflection into $\mathbf{k}$. Stated explicitly we get:

$$\mathbf{k} = (\mathbf{k}_{\parallel}, k_z) = (k_x, k_y, k_z)$$

$$\mathbf{k} = (\mathbf{k}_{\parallel}, -k_z) = (k_x, k_y, -k_z) \quad (1)$$

The angle of incidence or reflection is defined by means of the polar angle ϑ . Since polarized light beams should be preferred, the two transverse polarization directions $\hat{\mathbf{s}}$ and $\hat{\mathbf{p}}$ are shown as well. These conventions are in agreement with the ones used by Born and Wolf [11], where also more background information may be found.

Figure 2 shows in a pictorial way the location of the nuclei of the silicon atoms in the surface plane which is assumed to be unreconstructed in the rest of this article. The surface Bravais lattice is spanned by two vectors $\mathbf{s}_1, \mathbf{s}_2$ being in the three cases:

$$\begin{aligned} \text{100} \quad \mathbf{s}_1 &= (a^c/\sqrt{2}, 0, 0) \\ \mathbf{s}_2 &= (0, a^c/\sqrt{2}, 0) \\ \text{111} \quad \mathbf{s}_1 &= (a^c/\sqrt{2}, 0, 0) \\ \mathbf{s}_2 &= (-a^c/\sqrt{8}, a^c\sqrt{3}/8, 0) \\ \text{110} \quad \mathbf{s}_1 &= (a^c\sqrt{2}, 0, 0) \\ \mathbf{s}_2 &= (0, a^c, 0) \end{aligned} \quad (2)$$

where a^c means the lattice constant for the conventional unit cell of silicon. This description is incomplete, as far as the (110) plane is considered. In this plane the surface unit cell contains two atoms. The second atom indicated by the filled circle in Fig. 2 is located at the coordinate τ given by:

$$\text{110} \quad \tau = (a^c/\sqrt{8}, a^c/4, 0) \quad (3)$$

Using this geometrical information we treat the (mathematically) simplest configuration, which already shows anisotropic reflection, within the induced dipole approach. This case is a (110) oriented single plane of dipoles. For completeness also the (100) and (111) oriented planes are given. In contrast an equivalent (equivalent to be defined later on) homogeneous dielectric thin layer will be treated simultaneously. For the farguing theoretical approaches as for instance given in [9] such a comparison is almost trivial. However one has to keep in mind that the majority of the experimentalists working in the field still relies in one way or the other upon the simple homogeneous dielectric approach. For them this simple comparison might be revealing as well.

3. The thin dielectric layer

Reflection and transmission from thin dielectric layers

Fig. 3. The dielectric film model and its parameters.

belongs to the realm of classical optics. So what follows is a direct quotation from Born and Wolf [11]. Take a look at Fig. 3. The layer is supposed to be nonabsorbing, so $\tilde{\epsilon}_r$ is real. Small r 's symbolize field reflection coefficients and capital R 's symbolize intensity reflection coefficients. Now define the auxiliary quantities:

$$\sin(\vartheta_i) = \sqrt{\tilde{\epsilon}_r} \sin(\vartheta_t) \quad (4)$$

$$\alpha = \cos(\vartheta_i)/\cos(\vartheta_t) \quad (5)$$

$$\beta' = \left[\frac{2\pi d}{\lambda} \right] \sqrt{\tilde{\epsilon}_r} \cos(\vartheta_t) \quad (6)$$

With these abbreviations, we may for the case of a single boundary write the reflection coefficients as:

$$r_{12}^s = \frac{1 - \sqrt{\tilde{\epsilon}_r} \alpha}{1 + \sqrt{\tilde{\epsilon}_r} \alpha} \quad (7a)$$

$$r_{12}^p = \frac{\sqrt{\tilde{\epsilon}_r} - \alpha}{\sqrt{\tilde{\epsilon}_r} + \alpha} \quad (7b)$$

Symbols s, p denote the state of polarization involved. Using (6) and (7) the reflection coefficient for a thin homogeneous dielectric film is given by:

$$\tilde{r} = r_{12} \left[\frac{1 - \exp(i2\beta')}{1 - r_{12}^2 \exp(i2\beta')} \right] \quad (8)$$

This expression has become famous, especially for the calculation of anti-reflective coatings for lenses etc., but the thickness's we are interested in, are a few orders of magnitude smaller. This means that $\tilde{r}$ in eq. (8) will become almost completely imaginary, whereas the r 's in eqs. (7a, b) are always real in the nonabsorbing case.

4. Dipole calculations: the principles

A system of atoms or molecules may be described by dipoles if it can be subdivided into cells not exchanging charge during interaction with e.m. waves. Formally the solution of sources and fields for such systems can be found using only four principles. To each cell i one assigns a dipole strength $\mathbf{p}_i$, using the *principle of induction*:

$$\mathbf{p}_i = \hat{\alpha}_i \cdot \mathbf{E}_{\text{LOC},i} \quad (9)$$

$\hat{\alpha}_i$, the polarizability tensor characterizes the material system. $\mathbf{E}_{\text{LOC},i}$ is the electric field strength in cell i if its own dipole is not taken into account. This is the process illustrated in Fig. 4 if the incoming wave hits the filled circle. The dipoles, induced in such a way, start to emit spherical waves, best

Fig. 4. Reflection of e.m. radiation from a regular lattice of dipoles.

described by *Hertz-potentials* [12] (dipole in the origin):

$$\mathbf{Z}_i(\mathbf{r}, t) = \frac{\mathbf{p}_i}{4\pi\epsilon_0} \frac{\exp(i[kr - \omega t])}{r} \quad (10a)$$

$$\mathbf{E}_i(\mathbf{r}, t) = \nabla(\nabla \cdot \mathbf{Z}_i) - \frac{1}{c^2} \frac{\partial^2 \mathbf{Z}_i}{\partial t^2} \quad (10b)$$

Magnetic fields are generally ignored in optics. The spherical waves as given by [12] are indicated by circles in fig. 4. If more of them meet, they have to be combined by means of the *principle of superposition*:

$$\mathbf{E}_{\text{TOT}}(\mathbf{r}, t) = \mathbf{E}_{\text{EXT}}(\mathbf{r}, t) + \sum_i \mathbf{E}_i(\mathbf{r}, t) \quad (11)$$

Remote and local fields shown e.g., in Fig. 4, are obtained in this way. These three principles govern a truly general system of induced dipoles. The specific geometry of a regular surface of a monocrystalline solid enters through a fourth condition, the *principle of parallel translational symmetry*:

$$\mathbf{p}_{\text{qr}} = \exp(i\mathbf{k} \cdot \mathbf{s}_{\text{qr}}) \mathbf{p}_{00} \quad (12)$$

Valid for all dipoles located in the same plane, $\mathbf{s}_{\text{qr}}$ belongs to the surface lattice. From these four principles the interaction equations may be obtained, which are presented in three equivalent forms:

$$\mathbf{p}_i = \tilde{\alpha}_i \left[\mathbf{E}_{\text{EXT}} + \sum_{j \neq i} \frac{1}{\epsilon} \tilde{\mathbf{T}}_{ij} \cdot \mathbf{p}_j \right] \quad (13)$$

It is necessary to remark that superposition has been modified in such a way that all internal fields were screened, a common habit in solid state physics. The fact that a single symbol ϵ was used to indicate this screening, does not mean that it is a pure constant. It might as well depend on the relative coordinates, a point we will elucidate later on. Without screening unphysical, or no results at all will be obtained. $\tilde{\mathbf{T}}_{ij}$ governs the electromagnetic interaction between two dipoles labelled i and j [13]. The mathematically preferable form of (13) becomes:

$$\mathbf{p}_N = [\tilde{\alpha}_N^{-1} - \tilde{\mathbf{F}}_N]^{-1} \mathbf{E}_{0,N} \quad (14)$$

The expression between brackets represents the interaction matrix, a form of the Green's function. Equation (14) can best be seen as a $(N \times N)$ matrix with (3×3) tensors as its elements and (N) vectors with (3) -vectors as their elements. After use of (12) each (3) -vector represents exactly one plane. The larger the matrix (14), the more interesting optical problems may be studied. But therefore the matrix elements of $\mathbf{F}_N$ are required and obtaining these is already a tedious problem by itself. So we confine ourselves to a single plane and (14) becomes:

$$\mathbf{p} = (\alpha_0 E_0) [\alpha_0 \tilde{\alpha}^{-1} - \tilde{\mathbf{c}}]^{-1} \hat{\mathbf{e}}_E \quad (15a)$$

$$\alpha_0 = 4\pi\epsilon_0 a^3$$

$$s_1 = a\hat{\mathbf{x}} \quad s_2 = a(\alpha\hat{\mathbf{x}} + \beta\hat{\mathbf{y}})$$

$$\mathbf{E}_{\text{EXT}}(\mathbf{r}, t) = E_0 \hat{\mathbf{e}}_E \exp(i[\mathbf{k} \cdot \mathbf{r} - \omega t]) \quad (15b)$$

Here we have changed to dimensionless coordinates. The only matrix element left out from $\mathbf{F}_N$ is renamed $\tilde{\mathbf{c}}$ in its dimensionless form. It was the object of a number of mathematical investigations for a few decades.

5. Some remarks about lattice sums

By confining ourselves to a single plane of dipoles, the effort for solution is greatly reduced. Suppose we know $\tilde{\mathbf{c}}$ in eq. (15), the $\mathbf{p}$ follows immediately for any given $\hat{\mathbf{e}}_E$. In turn $\mathbf{p}$ will produce immediately the remote fields, from which r , the reflection coefficient, can be found. So the problem is to find $\tilde{\mathbf{c}}$. $\tilde{\mathbf{c}}$ consists of 9 numbers, 3 of them being nonzero. Each of these 3 numbers is a so-called lattice sum. Calculation of lattice sums is a large mathematical problem, which we reduced by using Vlieger's [13] quasistatic approach:

$$\tilde{\mathbf{c}} = \epsilon^{-1} \tilde{\mathbf{c}}_{\text{STAT}} + i \frac{N_c 2\pi a}{\beta |k_z|} [k^2 \tilde{\mathbf{I}} - \mathbf{k}_{\parallel}^T \mathbf{k}_{\parallel} - k_z^2 \hat{\mathbf{z}}\hat{\mathbf{z}}] \quad (16)$$

Here N_c means the number of dipoles per surface unit cell, so it will be 1 for the 100 and 111 cases and 2 for the 110 case. Equation (16) offers the possibility to use the easier static lattice sums, for dynamic calculations, provided that k is small (e.g., $\lambda \gg a$). Van der Hoff and Benson [14] used a Jacobi transformation to solve the static problem for square and hexagonal lattices. We have generalized this to truly arbitrary cases, where (α, β) are arbitrary and the planes may be centered and non-centered. Screening was applied to the real part of $\tilde{\mathbf{c}}$, which contains the short range interaction. If screening is applied to the imaginary part as well reflection coefficients exceeding 1 may be obtained. Rather than discussing details, we immediately give the results for the three cleavage planes:

$$100 \quad \tilde{\mathbf{c}}_{\text{STAT}} = \begin{pmatrix} 4.517 & 0 & 0 \\ 0 & 4.517 & 0 \\ 0 & 0 & -9.0336 \end{pmatrix} \quad (17a)$$

$$111 \quad \tilde{\mathbf{c}}_{\text{STAT}} = \begin{pmatrix} 5.517 & 0 & 0 \\ 0 & 5.517 & 0 \\ 0 & 0 & -11.034 \end{pmatrix} \quad (17b)$$

$$110 \quad \tilde{\mathbf{c}}_{\text{STAT}} = \begin{pmatrix} 15.056 & 0 & 0 \\ 0 & 3.851 & 0 \\ 0 & 0 & -18.907 \end{pmatrix} \quad (17c)$$

The poor convergence of the lattice sums makes it difficult to perform a direct test of the results shown above. Instead we use a simple trick to produce independent results. For a point outside the plane the lattice sum may be transformed by means of the first Ewald transformation [11, 13]. Since this requires the full lattice, we subtract the spherical wave emanating from the origin. The closer one gets to the origin, the poorer the method converges, but the lattice sum itself is well defined at the origin. Now a three dimensional Taylor series is fitted to the results. The coefficients belonging to second order are the components of $\vec{c}$. In this way both (16) and (17) could be tested. It is important in this test to approach the origin as close as possible. For the required excessively long summations a Cyber 205 was used.

6. The reflection coefficients

As a first step one needs to know the dipole strength $\mathbf{p}_0$ induced in the plane by the external field. For this we need (15) and (17):

$$\mathbf{p}_0 = (\alpha_0 E_0) [\alpha_0 \vec{\alpha}^{-1} - \vec{c}]^{-1} \hat{\mathbf{e}}_E \quad (18)$$

As can be seen from eq. (17) $\vec{c}$ is diagonal. For the (110) case however the xx - and yy -components are different. This is vital, since this causes anisotropy. Because $\vec{c}$ depends on the lattice positions only, so on the crystallographic structure, one may say that $\vec{c}$ yields the structural contribution to the anisotropy. The polarizability $\vec{\alpha}$ is intentionally chosen to be isotropic. If here also xx - and yy -components are different, the anisotropy has an intrinsic contribution. Now inversion of eq. (18) is trivial. Using again the first Ewald transformation the remote fields can be found from:

$$E(\mathbf{r}, t) = \frac{iN_c \exp(i[\mathbf{k} \cdot \mathbf{r} - \omega t])}{2\epsilon_0 a^2 \beta |k_z|} [\mathbf{k}^2 \vec{\mathbf{I}} - \mathbf{k}^T \mathbf{k}] \mathbf{p}_0 \quad (19)$$

Combining eqs. (17–19) readily produces the reflection coefficients. If one makes use of the abbreviations:

$$\kappa = (2\pi a)/\lambda \quad (20a)$$

$$A_{\alpha\alpha} = \left[\frac{2\epsilon_0 a^3}{\alpha} - \frac{c_{\alpha\alpha, \text{STAT}}}{2\pi\epsilon} \right] \quad (\alpha = x, y, z) \quad (20b)$$

one obtains for those reflection coefficients ($\Omega = 0$):

$$\tilde{r}_s = \left[\frac{iN_c \kappa}{A_{yy} \beta \cos \vartheta - iN_c \kappa} \right] \quad (21a)$$

$$\tilde{r}_p = \left[\frac{iN_c \kappa \sin^2 \vartheta}{(A_{zz} \beta \cos \vartheta - iN_c \kappa \sin^2 \vartheta)} - \frac{iN_c \kappa \cos \vartheta}{(A_{xx} \beta - iN_c \kappa \cos \vartheta)} \right] \quad (21b)$$

Using those mathematical tools, we will show some numerical results. We start with a simple comparison of the results obtained from a dielectric continuum approach and from a discrete dipole approach. After that the intriguing anisotropic optical properties of a 110 oriented plane of dipoles are discussed.

7. Continuum versus discrete approach

To compare the two approaches we need a consistent set of input parameters, such as α , $\tilde{\epsilon}_r$, d or a^c . Those data were

Fig. 5. Reflection from a 1.36 Å thin layer of silicon in the continuum approach (Note: the indication $\times 10^{-9}$ for the axis's in the figures means that division indication has to be multiplied with 10^9)

systematically taken from bulk measurements. This yields $\tilde{\epsilon}_r = 15.5 + i 0.0$ for bulk silicon if $\lambda = 6200 \text{ Å}$ and $a^c = 5.43 \text{ Å}$, the lattice parameter of the same material. The dipole calculations were performed first unscreened, using $\epsilon = 1.0$. Next they were repeated using $\epsilon = 11.7$, in agreement with most band bending calculations. The thickness d of the dielectric film was derived from the condition that $d \times$ the surface of the 100 surface unit cell has to equal the volume occupied by one silicon atom in the bulk. The polarizability $\tilde{\alpha}$ for the 100 dipole lattice has been calculated by means of the conventional Clausius–Mossotti equation:

$$\tilde{\alpha} = \frac{3\epsilon_0 a^3}{8} \left[\frac{\tilde{\epsilon}_r - 1}{\tilde{\epsilon}_r + 2} \right] \quad (22)$$

The results are shown in Figs. 5, 6 and 7. Since only for angles ϑ close to 90° , the reflection changes significantly, only the area close to $\vartheta = 90^\circ$ is displayed. The $\vartheta = 0^\circ$ data are given separately:

$$\begin{aligned} \text{Im } \tilde{r}_s &= 9.9911 \times 10^{-9} \quad (\text{dielectric}) \\ \text{Im } \tilde{r}_s &= 2.4993 \times 10^{-9} \quad (\text{dipole, } \epsilon = 1.0) \\ \text{Im } \tilde{r}_s &= 1.7573 \times 10^{-9} \quad (\text{dipole, } \epsilon = 11.7) \end{aligned} \quad (23)$$

The real part of $\tilde{r}_s$ goes smoothly to -1 if ϑ approaches 90° . Close to $\vartheta = 90^\circ$ the imaginary component shows a maximum of exactly 0.5 in all cases. So all models yield a qualitatively similar result. But the quantitative results are definitely different. The width of the imaginary peak in the dielectric case exceeds largely the width in the unscreened dipole case.

Fig. 6. Reflection from a 100 lattice plane of dipoles, unscreened.

Fig. 7. Reflection from a 100 lattice plane of dipoles, screened.

Fig. 9. Anisotropic differential reflection from a 110 lattice plane of dipoles, screened.

Increasing ε causes a decrement of this width in the screened dipole case. This illustrates clearly that no simple equivalency between dielectric constants and polarizabilities, such as given by Clausius–Mossotti, exists for thin films.

8. The anisotropic results

In order to find anisotropic reflection, one has to enter the crystallographic data for the 110 plane. This means that the factor β first introduced in eq. (15) has to be taken as $\beta = \sqrt{2}$. Further only eq. (21a) has to be considered, since it is easy to show that p-type reflection is only weakly structure sensitive. Only field-components in the plane are affected by surface structure. Next one should realize that a s-polarized light beam hitting the surface at near grazing incidence conditions (so ϑ close to 90°), if it enters along the $\hat{x}$ -axis, where $\Omega = 0^\circ$, has a field component in the $\hat{y}$ -direction. This means that A_{yy} should be used. Converse arguments have to be used for the $\Omega = 90^\circ$ direction. The difference in reflection for those two Ω -directions is shown in Fig. 9 for the case of screened dipoles. Again the response is predominantly imaginary. At maximum the difference signal reaches 2% in this case. The unscreened case shows extrema of about 25%. Considering what is known experimentally, such values have to be considered unrealistic. More relevant however is the ratio of difference and average signal, as shown in Fig. 10 (screened case only). Almost up to 90° this is a perfect con-

stant of about 8%. For $\vartheta = 0^\circ$ we find for the two cases:

$$\begin{aligned} \text{Im } \tilde{r}_s &= 1.6546 \times 10^{-3} \quad (\Omega = 0^\circ) \quad (\varepsilon = 1.0) \\ \text{Im } \tilde{r}_s &= -2.2822 \times 10^{-2} \quad (\Omega = 90^\circ) \end{aligned} \quad (24a)$$

$$\begin{aligned} \text{Im } \tilde{r}_s &= 1.2375 \times 10^{-3} \quad (\Omega = 0^\circ) \quad (\varepsilon = 11.7) \\ \text{Im } \tilde{r}_s &= 1.3286 \times 10^{-3} \quad (\Omega = 90^\circ) \end{aligned} \quad (24b)$$

The screened s-polarized reflection in the 110 case is weaker than for the screened 100 case despite the denser packing of the 110 lattice. Only for p-type polarized light reflection from 110 planes is stronger than from 100 planes. Figures 8, 9 and 10 show what should be observed. Under isotropic assumptions both for the polarizability and for the dielectric constant, the discrete dipole approach will and the continuum approach will not yield anisotropic results. Nevertheless the occurring reflection coefficients for the more realistic screened case are very small and if one tries to extrapolate tentatively those results to the case of reflection from a semi-infinite bulk, the theoretically predicted intensity roughly coincides with the usual noise level. In practice for Ag, Cu and Si (111) in its (2×1) reconstruction, results were found considerably larger (about five times). In this context this means that the intrinsic contribution to the effect has to be the dominant one. This in turn means that anisotropic reflection from surfaces of cubic crystals is mainly a quantummechanical effect.

Fig. 8. Anisotropic differential reflection from a 110 lattice plane of dipoles, unscreened.

Fig. 10. Relative anisotropic differential reflection (difference in reflection/average reflection) from a 110 lattice plane of dipoles, screened.

9. Conclusions

The simple examples given, clearly show that dielectric models apparently differ from dipole models, though it requires the help of a computer to show this. Nevertheless publications related to reflection problems almost exclusively use the first model. Highly unclear reasonings are necessary then, to explain phenomena like anisotropy. However it is not necessary to use a dielectric constant at all. Equation (14) shows the corner stone of an approach, in which measurable quantities follow directly from the polarizability. This has the following advantages, as far as theory is concerned. One starts from only four clearcut principles (9–12), from which just one has to be modified to produce physically acceptable results. The rest is heavy, but absolutely transparent mathematics. This makes the approach ideally suited for computer implementation.

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