Relation between the surface impedance and the extinction theorem on a rough surface

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The surface-impedance (SI) expression that was recently obtained for a corrugated metal surface, up to second order in the penetration depth, is reconsidered in connection with the extinction-theorem equations for the electromagnetic field. Instead of using a coordinate transformation, which stretches the corrugated surface, we obtain here the same SI expression from Green's theorem in a more natural and easy way. In addition, this method allows us to evaluate SI corrections of the third order in the penetration depth. We also show that for a one-dimensional corrugation our result reduces to the SI expression given recently by Maradudin.

I. INTRODUCTION

The problem of the scattering of light from a rough surface has received recently new theoretical interest in the framework of the surface-impedance (SI) approximation,[1–4] which yields a relation between the electric and magnetic fields parallel to the surface, $\mathbf{E}_\parallel$ and $\mathbf{B}_\parallel$. The advantage of having a relation of this type is remarkable, since the solution for the field in vacuum is greatly simplified.[5] The number of equations is in this case reduced by a factor of two, and the field in the interior of the medium is eliminated, making it easier to obtain both the analytical solution (for small roughness) and the numerical simulation, especially for a two-dimensional (2D) surface corrugation.[6]

The main points in the SI formulation can be summarized as follows. The SI approximation postulates a local relation between the fields $\mathbf{E}_\parallel$ and $\mathbf{B}_\parallel$ on the surface, while the exact boundary condition includes nonlocal terms, i.e., terms that involve these fields at neighboring points on the surface, or, equivalently, both the fields and their derivatives. Such nonlocal terms are actually to be expected, since they are present even in a perfectly flat geometry,[2] and it is important to estimate them. The relation between $\mathbf{E}_\parallel$ and $\mathbf{B}_\parallel$ on the surface can be obtained as a formal series expansion in the penetration depth d, defined by

$$d^{-1} = \frac{\omega}{c}\sqrt{-\epsilon}\,, \tag{1.1}$$

where ϵ is the dielectric constant of the medium at angular frequency ω. This expansion is formally valid for a general complex ϵ, although it is primarily of interest to us for metals at infrared and optical frequencies, where the real part of ϵ is large and negative. It has been carried out to second order in d for any surface,[2,3] and up to third order for a one-dimensional surface profile,[4] with the following results.

First, the dimensionless expansion parameter for the local terms, up to second order, is Δd, where

$$\Delta = \frac{1}{2}(K_1 - K_2)\,, \tag{1.2}$$

$K_{1,2}$ being the principal curvatures of the surface, i.e., the inverse of the principal radii of curvature $R_{\min}, R_{\max}$. Second, the relation between $\mathbf{E}_\parallel$ and $\mathbf{B}_\parallel$ turns out to be local to first order in d, and the second-order nonlocal terms are very similar to those present on a flat surface, i.e., they vanish for normal incidence but are nonnegligible when the fields vary rapidly along the surface. In summary, then, the (local) SI approximation is exact to order Δd and the second-order nonlocal corrections can be explicitly estimated.

The d expansion is certainly suited to treat problems of antenna radiowaves, and the inclusion of linear terms only suffices with a quite good approximation to treat problems up to the infrared range of frequencies. In optics however, second-order and higher-order terms become relevant since in this range of frequencies the penetration depth of many metals increases.

Full second-order terms have been recently calculated by Ong *et al.*[2,3] using a coordinate transformation, thus generalizing the 1D result of Ref. 1. Local contributions up to third order in the penetration depth have been recently calculated by Maradudin for a 1D grating.[4] Here we generalize this last result to a 2D (rough) surface, and furthermore, as in Ref. 2, we do include nonlocal terms. We go in this way beyond the SI approximation which forces from the start a local relation between the fields at the surface. These results are one of the two main points of the paper, the other being the method by which they are obtained. Our method is based on the *extinction theorem* formalism: it not only allows us to proceed more easily with the expansion, but it also clarifies the relation between the SI approach and other treatments of the boundary value problem.

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What we are doing in this paper can be summarized as follows. Green's theorem furnishes two vector equations for the fields. The first is obtained working with the Green function in vacuum, the second with that appropriate to the medium.[7] It is known that using these equations within the Rayleigh hypothesis for the fields in vacuum, the first of the two is identically satisfied,[8] while the second gives a true equation for the fields in vacuum.[9,10] It is precisely this last equation, where the Green function of the medium appears, that furnishes the wanted SI relation between the fields, in the penetration depth. Nonlocal terms, i.e., those involving field derivatives at the surface, are also obtained. When compared to the coordinate transformation method used previously,[2,3] the present method seems more appropriate, since it is algebraically simpler.

In Sec. II, we present the starting equations gotten from the extinction theorem, while in Sec. III, we show how they are used to recover the relation between the fields to linear order in d. In Sec. IV, we set up the general expansion procedure and we obtain the terms of $o(d^2)$. In Sec. V, we consider terms of $o(d^3)$, thus extending previous results.

II. THE STARTING EQUATIONS

We consider a dielectric medium bounded by the surface

$$z = \zeta(\mathbf{R}) , \tag{2.1}$$

where $\mathbf{R} \equiv (x, y)$. In the medium placed at $z < \zeta$ the magnetic field $\mathbf{B}$ satisfies the wave equation

$$\left\{\nabla^2 + \epsilon\left(\frac{\omega}{c}\right)^2\right\}\mathbf{B} = 0 . \tag{2.2}$$

With the appropriate Green function of the medium $G(\mathbf{r}, \mathbf{r}')$ satisfying

$$\left\{\nabla'^2 + \epsilon\left(\frac{\omega}{c}\right)^2\right\} G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') , \tag{2.3}$$

we get

$$\int \{\mathbf{B}\partial_n' G - G\partial_n' \mathbf{B}\}\, dS' = 0 , \tag{2.4}$$

where the observation point $\mathbf{r}$ is taken in vacuum, i.e., $z > \zeta$, and the $\mathbf{r}'$ variable runs over the surface of separation. The ∂_n' denotes normal derivative at the surface with respect to the primed variable $\mathbf{r}'$ and $\partial_n = \hat{\mathbf{n}} \cdot \nabla$, where $\hat{\mathbf{n}}$ is the unit vector normal the surface and pointing into the vacuum

$$\hat{\mathbf{n}} = \phi(\hat{\mathbf{z}} - \nabla\zeta) , \tag{2.5}$$

with

$$\phi = \left[1 + (\nabla\zeta)^2\right]^{-1/2} . \tag{2.6}$$

The differential surface area is $dS = dx\, dy/\phi$. As shown by Jackson,[7] Eq. (2.4) can be transformed into the equivalent expression

$$\int \Big\{(\hat{\mathbf{n}}' \times \mathrm{curl}\mathbf{B})\, G(\mathbf{r}, \mathbf{r}') + (\hat{\mathbf{n}}' \cdot \mathbf{B})\, \nabla' G(\mathbf{r}, \mathbf{r}') + (\hat{\mathbf{n}}' \times \mathbf{B}) \times \nabla' G(\mathbf{r}, \mathbf{r}')\Big\} dS' = 0 , \tag{2.7}$$

where still the observation point $\mathbf{r}$ is taken in vacuum, and $\mathbf{r}'$ runs over the surface of separation. One can equally well work with the Green function and fields in vacuum and *not* in the medium as done presently. In this second case, to the surface integral (2.4) one has to add the contribution of the incident wave coming from the integration at infinity on the vacuum side. The sum of both terms is equal to zero if the observation point is taken outside the volume of integration, i.e., if one is looking now *into* the medium. That result is known as *"extinction theorem,"*[8] where the name comes from the fact that the incident field in vacuum is totally *"extinguished"* by the field at the surface. Equation (2.7), which could be called the *"extinction-theorem boundary condition,"* is the one appropriate for the present purposes.

To proceed, we use the Green function representation

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{L^2}\sum_{\mathbf{K}} \frac{1}{2iq} e^{iq|z - z'|} e^{i\mathbf{K}\cdot(\mathbf{R} - \mathbf{R}')} , \tag{2.8}$$

where L^2 is the area of the sample, and

$$q = \left[\epsilon\left(\frac{\omega}{c}\right)^2 - K^2\right]^{1/2} , \quad \mathrm{Im}\, q > 0. \tag{2.9}$$

Inserting (2.8) in (2.7), then using from Maxwell's equations the relation

$$\begin{aligned} \hat{\mathbf{n}} \times \mathrm{curl}\mathbf{B} &= -i(\omega/c)\epsilon\hat{\mathbf{n}} \times \mathbf{E} \\ &= (\sqrt{\epsilon}/d)\hat{\mathbf{n}} \times \mathbf{E} , \end{aligned} \tag{2.10}$$

with d defined in (1.1), we get

$$\int \left(\hat{\mathbf{n}} \times \mathbf{E} - \frac{d}{\sqrt{\epsilon}}\Big\{i(\mathbf{K} + q\hat{\mathbf{z}})(\hat{\mathbf{n}} \cdot \mathbf{B}) - i\,(\mathbf{K} + q\hat{\mathbf{z}}) \times (\hat{\mathbf{n}} \times \mathbf{B})\Big\}\right) \frac{1}{\phi} e^{-iq\zeta} e^{-i\mathbf{K}\cdot\mathbf{R}}\, d\mathbf{R} = 0 . \tag{2.11}$$

In going from (2.7) to (2.11), we have taken the observation point $\mathbf{r}$ such that

$$z > \zeta_{\max} > \zeta(\mathbf{R}') , \tag{2.12}$$

then changed the integration variable from $\mathbf{r}'$ to $\mathbf{r} = (\mathbf{R}, \zeta)$ and dropped the sum over the parallel momentum $\mathbf{K}$ in the x, y plane. Since the quantities appearing in (2.11) are continuous across the surface, we have in effect obtained a boundary condition on the fields *outside* the medium.

At this point, it is convenient to take a partial integration for terms proportional to $\mathbf{K}$ using

$$\int i\mathbf{K} e^{-i\mathbf{K}\cdot\mathbf{R}} F d\mathbf{R} = \int e^{-i\mathbf{K}\cdot\mathbf{R}} (\nabla_{\mathbf{R}} F) d\mathbf{R} , \tag{2.13}$$

where F is a generic function of $\mathbf{R}$. We note explicitly that $\nabla_{\mathbf{R}}$ is a surface derivative: for instance, the x component of $\nabla_{\mathbf{R}} B_y$ is $\partial B_y/\partial x + (\partial B_y/\partial z)(\partial\zeta/\partial x)$ at $z = \zeta(\mathbf{R})$, where $B_y(x, y, z)$ is the y component of the $\mathbf{B}$ field in space. With this understanding, we can drop the $\mathbf{R}$ subscript on ∇, but we shall reintroduce it in the text when confusion may arise. With a change of nomenclature, we put $q = is/d$, with

$$s = \sqrt{1 + K^2 d^2} \tag{2.14}$$

in agreement with (2.9). From (2.10), we get the equivalent relation

$$\int \left(\frac{1}{\phi}(\hat{\mathbf{n}} \times \mathbf{E}) - \frac{1}{\sqrt{\epsilon}} \Big\{ -s\mathbf{B}/\phi^2 + d[\nabla_{\mathbf{R}}(\hat{\mathbf{n}} \cdot \mathbf{B}/\phi) - \nabla_{\mathbf{R}} \times (\hat{\mathbf{n}} \times \mathbf{B}/\phi)] \Big\} \right) e^{\zeta s/d} e^{-i\mathbf{K}\cdot\mathbf{R}} d\mathbf{R} = 0 , \tag{2.15}$$

where we have used the vector identity

$$-\hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \mathbf{v}) = \mathbf{v} - \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{v}) , \tag{2.16}$$

with $\mathbf{v} = \mathbf{B}$. Equation (2.15) is the starting equation of our calculation. The wanted relation, between $\mathbf{E}_{\parallel}$ and $\mathbf{B}_{\parallel}$ on the boundary, can be obtained once the large bracket in (2.15), or an equivalent relation that follows from it, can be equated to zero by itself. A necessary and sufficient condition to do this is to render this expression K independent. How this is done is shown in the next sections.

III. FIRST-ORDER SOLUTION

In order to replace s by an equivalent K-independent operator in Eq. (2.14), we start from the identity, valid for an arbitrary scalar or vector $F \equiv F(\mathbf{R})$:

$$\int K^2 d^2 F e^{\zeta s d} e^{-i\mathbf{K}\cdot\mathbf{R}} d\mathbf{R} = \int \Big\{ -s^2 (\nabla\zeta)^2 F - d\, s \left[\nabla^2\zeta + 2\nabla\zeta \cdot \nabla \right] F - d^2 \nabla^2 F \Big\} e^{\zeta s/d} e^{-i\mathbf{K}\cdot\mathbf{R}} d\mathbf{R} . \tag{3.1}$$

This is obtained by replacing $K^2 \exp(-i\mathbf{K}\cdot\mathbf{R})$ with $-\nabla^2 \exp(-i\mathbf{K}\cdot\mathbf{R})$ and integrating by parts twice. Substituting $s^2 = 1 + K^2 d^2$ on the left hand side and using Eq. (2.6), we obtain

$$\int s^2 (F/\phi^2) e^{\zeta s/d} e^{-i\mathbf{K}\cdot\mathbf{R}} d\mathbf{R} = \int \left\{ F - d\, s\tilde{a}F - d^2 \nabla^2 F \right\} e^{\zeta s/d} e^{-i\mathbf{K}\cdot\mathbf{R}} d\mathbf{R}, \tag{3.2}$$

where for future use we have introduced the linear operator

$$\tilde{a} = \nabla^2\zeta + 2\nabla\zeta\cdot\nabla . \tag{3.3}$$

In compact notation, we write this result as

$$\left\{ s^2 F/\phi^2 \right\} = \left\{ F - d\, s\tilde{a}F - d^2 \nabla^2 F \right\} \tag{3.4}$$

and we make the convention that for the two terms enclosed in curly brackets equality applies under the integral sign, once both sides are first multiplied by the common factor

$$e^{\zeta s/d} e^{-i\mathbf{K}\cdot\mathbf{R}} . \tag{3.5}$$

For brevity we shall use this convention, unless specified differently, in the equations that follow. We now proceed to find an equivalent K-independent operator $\hat{s}$ that still satisfies Eq. (3.4) regarded as a true equation, thus dropping the curly brackets and preserving the order.

To lowest order, we obviously have $\hat{s} = \phi$. Substituting back on the right hand side, (r.h.s.), we find

$$\hat{s}^2 \left[F/\phi^2 \right] = F - d\phi\tilde{a}F + o(d^2) . \tag{3.6}$$

If $\hat{s}$ and $\tilde{a}$ were simply numbers, the solution of Eq. (3.6) would be $\hat{s} = \phi - d\,\tilde{a}\phi^2/2$. We guess, and verify, that the correct solution is

$$\hat{s} = \phi - \frac{d}{2}\phi\tilde{a}\phi . \tag{3.7}$$

(A systematic expansion of $\hat{s}$ is obtained in the next section.) Explicitly then we have

$$\hat{s}\left[F/\phi^2 \right] = \frac{1}{\phi} \left\{ F - d \left[\frac{1}{2} \left(\phi\nabla^2\zeta - \nabla\zeta\cdot\nabla\phi \right) F + \phi\nabla\zeta\cdot\nabla F \right] \right\} + o(d^2) , \tag{3.8}$$

which can be used directly in Eq. (2.15) with the substitution $F \to \mathbf{B}$. To $\sim o(d)$, the large bracket under the integral sign in Eq. (2.15) becomes K independent and can be directly equated to zero. The expression that follows simplifies expanding the double vectorial product appearing in it as

$$d\phi\nabla\times \left(\frac{\hat{\mathbf{n}}}{\phi} \times \mathbf{B} \right) = d \Big[\hat{\mathbf{n}}\nabla \cdot \mathbf{B} - \phi(\mathbf{B}\cdot\nabla)\nabla\zeta + \phi\nabla^2\zeta\, \mathbf{B} + \phi(\nabla\zeta\cdot\nabla)\mathbf{B} \Big] . \tag{3.9}$$

We see in this way that the last term in square brackets above cancels the analogous last term in square brackets in (3.8), while the third term changes sign to the first in (3.8). The result is

$$\hat{\mathbf{n}} \times \mathbf{E} - \frac{1}{\sqrt{\epsilon}} \Big\{ -\mathbf{B}\left[1 + dK_m\right] - d\hat{\mathbf{n}}\nabla\cdot\mathbf{B} + d\phi(\mathbf{B}\cdot\nabla)\nabla\zeta + d\phi\nabla\left(\frac{\hat{\mathbf{n}}}{\phi} \cdot \mathbf{B} \right) \Big\} = o(d^2) , \tag{3.10}$$

where

$$K_m = \frac{1}{2}\left(\frac{1}{R_{\min}} + \frac{1}{R_{\max}} \right) = \frac{1}{2}\nabla\cdot(\phi\nabla\zeta) \tag{3.11}$$

is the mean curvature of the surface.[3] Recall that $\nabla \cdot \mathbf{B}$ stands for $\nabla_{\mathbf{R}} \cdot \mathbf{B}$ (thus, it does not vanish).

It is convenient to introduce the parallel projection operator $\mathbf{P}$ such that $\mathbf{P} \cdot \mathbf{E} = -\hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \mathbf{E}) = \mathbf{E}_{\parallel}$. The Cartesian components of the tensor $\mathbf{P}$ are

$$P_{ij} = \delta_{ij} - \hat{n}_i \hat{n}_j \ , \qquad i,j = 1,2,3 \ . \tag{3.12}$$

Projecting Eq. (3.10) over $\hat{\mathbf{n}}$ shows that $\hat{\mathbf{n}} \cdot \mathbf{B} \sim o(d)$. Thus, the last term in curly brackets is of $o(d^2)$ and can be omitted. The projection over $\hat{\mathbf{n}}$ gives then explicitly

$$-d\,\nabla \cdot \mathbf{B} = \hat{\mathbf{n}} \cdot \mathbf{B} - d\phi \mathbf{B} \cdot \nabla\nabla\zeta \cdot \hat{\mathbf{n}} + o(d^2) \ . \tag{3.13}$$

Substituting back in (3.10) and using the identity (2.16), we get

$$\hat{\mathbf{n}} \times \left(\mathbf{E} - \frac{1}{\sqrt{\epsilon}} \{ (\hat{\mathbf{n}} \times \mathbf{B})\,(1 + dK_m) - d\hat{\mathbf{n}} \times \phi\,(\mathbf{B} \cdot \nabla)\,\nabla\zeta \} \right) = o(d^2) \ . \tag{3.14}$$

Equation (3.13) is the *surface divergence constraint.* From the relation

$$-\phi \mathbf{B} \cdot \nabla\nabla\zeta \cdot \hat{\mathbf{n}} = -\frac{1}{\phi} \nabla\phi \cdot \mathbf{B} \ , \tag{3.15}$$

it can be rewritten as

$$\hat{\mathbf{n}} \cdot \mathbf{B} + d\,\nabla_{\parallel} \cdot \mathbf{B}_{\parallel} = o(d^2) \ , \tag{3.16}$$

where $\nabla_{\parallel} = \mathbf{P} \cdot \nabla$, as the notation implies, and

$$\nabla_{\parallel} \cdot \mathbf{B}_{\parallel} \equiv \phi \nabla \cdot \left(\frac{1}{\phi} \mathbf{B}_{\parallel} \right) \tag{3.17}$$

is the surface divergence.[2,3] We have used the fact that $\mathbf{B}_{\parallel}$ is the same as $\mathbf{B}$ to zero order. Equation (3.16) agrees with Eq. (3.37) of Ref. 3.

Equation (3.14) leads to the SI relation found by the coordinate transformation method.[2,3] To see this, we apply $\hat{\mathbf{n}} \times$ to both sides, and we also apply to the last term in curly brackets the identity (A9) of Appendix A. The result is

$$\mathbf{E}_{\parallel} = \frac{1}{\sqrt{\epsilon}} \{ (1 - dK_m) \hat{\mathbf{n}} \times \mathbf{B} + d\,\mathbf{P} \cdot \phi \nabla\nabla\zeta \mathbf{P} \cdot (\hat{\mathbf{n}} \times \mathbf{B}) \} + o(d^2) \ . \tag{3.18}$$

This local relation between the two fields at the surface can be expressed in terms of the geometrical quantities of the surface as

$$\mathbf{E}_{\parallel} = \frac{1}{\sqrt{\epsilon}} \mathbf{Z} \cdot (\hat{\mathbf{n}} \times \mathbf{B}) + o(d^2) \ , \tag{3.19}$$

where we introduce

$$Z_{ij} = P_{ij} + dS'_{ij} + o(d^2) \tag{3.20}$$

as the SI tensor, while

$$\mathbf{S}' = \mathbf{S} - \frac{1}{2} \operatorname{tr}(\mathbf{S}) \mathbf{P} \tag{3.21}$$

is the traceless part of the extrinsic curvature tensor

$$\mathbf{S} = \mathbf{P} \cdot \phi \nabla\nabla\zeta \cdot \mathbf{P} \tag{3.22}$$

and

$$\operatorname{tr}(\mathbf{S}) = 2K_m = \nabla \cdot (\phi \nabla\zeta) = -\nabla \cdot \hat{\mathbf{n}} \ , \tag{3.23}$$

showing the geometrical meaning of K_m in Eq. (3.11) as the mean curvature of the surface.

IV. SECOND-ORDER SOLUTION

The starting equation is again (3.4), which we now consider as an equation for the operator $\hat{s}$. We rewrite it as

$$\hat{s}^2 \left[F/\phi^2 \right] = F - d\,\hat{s} \left[\tilde{a} F \right] - d^2 \nabla^2 F \ . \tag{4.1}$$

We search for the solution of this equation by expanding $\hat{s}$ in power series of d and as suggested by (3.8) we try the form

$$\hat{s} \left[F/\phi^2 \right] = \frac{1}{\phi} \left\{ F - d\,\hat{U} F + d^2\,\hat{V} F - d^3\,\hat{W} F \right\} + o(d^4) \ , \tag{4.2}$$

where for $\hat{U}$ we take a linear operator

$$\hat{U} = U^{(0)} + \mathbf{U}^{(1)} \cdot \nabla \ , \tag{4.3}$$

and we try for $\hat{V}$, $\hat{W}$ a quadratic and cubic operator, respectively,

$$\hat{V} = V^{(0)} + \mathbf{V}^{(1)} \cdot \nabla + \mathbf{V}^{(2)} \cdot \nabla\nabla \ , \tag{4.4}$$

$$\hat{W} = W^{(0)} + \mathbf{W}^{(1)} \cdot \nabla + \mathbf{W}^{(2)} \cdot \nabla\nabla + \mathbf{W}^{(3)} \cdot \nabla\nabla\nabla \ . \tag{4.5}$$

Inserting (4.2) in Eq. (4.1) and equating coefficients of the same powers we get

$$\hat{U}\phi + \phi\hat{U} = \phi a \ , \tag{4.6}$$

$$\hat{V}\phi + \phi\hat{V} + \hat{U}\phi\hat{U} = \hat{U}\phi a - \phi\nabla^2 \ , \tag{4.7}$$

$$\hat{W}\phi + \phi\hat{W} + \hat{V}\phi\hat{U} + \hat{U}\phi\hat{V} = \hat{V}\phi a \ , \tag{4.8}$$

where for convenience we have put

$$a = \phi\tilde{a} \ . \tag{4.9}$$

We treat here the first two above equations, while Eq. (4.8) is postponed to the next section. From $\hat{U}\phi = \phi\hat{U} + \mathbf{U}^{(1)} \cdot \nabla\phi$, Eq. (4.6) is rewritten as

$$2\phi\hat{U} + \mathbf{U}^{(1)} \cdot \nabla\phi = \phi a \ . \tag{4.10}$$

In this equation, we first compare terms $\sim \nabla$ and get

$$\mathbf{U}^{(1)} = \phi \nabla \zeta \ . \tag{4.11}$$

Substituting back in Eq. (4.14), we find

$$U^{(0)} = \frac{1}{2}(\phi \nabla^2 \zeta - b) \ , \tag{4.12}$$

where

$$b = \nabla \zeta \cdot \nabla \phi \ . \tag{4.13}$$

Hence, in agreement with Eq. (3.8),

$$\hat{U} = \frac{1}{2}(a - b) \ . \tag{4.14}$$

Equation (4.7) can be treated similarly. Eliminating $\hat{U}$ and using the relation $(a-b)\phi = \phi(a+b)$, we have

$$\hat{V}\phi + \phi\hat{V} = \phi \left\{ \frac{1}{4}(a+b)^2 - \nabla^2 \right\} \ . \tag{4.15}$$

From Eq. (4.4), the left hand side (l.h.s.) is rewritten as

$$2\phi\hat{V} + \mathbf{V}^{(1)}\cdot\nabla\phi + \mathbf{V}^{(2)}\cdot\nabla\nabla\phi + 2\nabla\phi\cdot\mathbf{V}^{(2)}\cdot\nabla \ , \tag{4.16}$$

and from $\frac{1}{2}(a+b) = K_m + \nabla\zeta\cdot\nabla$ the r.h.s. becomes

$$-\phi\nabla_\parallel^2 + \phi K_m^2 + \phi^2 \nabla\zeta\cdot\nabla K_m + \phi^2 b \nabla\zeta\cdot\nabla - \nabla\phi\cdot\nabla \ , \tag{4.17}$$

where we have introduced the surface covariant Laplacian operator[2,3]

$$\begin{aligned} \nabla_\parallel^2 &= \nabla^2 - \hat{\mathbf{n}}\hat{\mathbf{n}}\cdot\nabla\nabla + 2K_m \hat{\mathbf{n}}\cdot\nabla \\ &= \nabla^2 - \phi^2 \nabla\zeta\nabla\zeta\cdot\nabla\nabla - \phi\nabla\cdot(\phi\nabla\zeta)\nabla\zeta\cdot\nabla \ , \end{aligned} \tag{4.18}$$

where as specified after Eq. (2.13), ∇ stands for $\nabla_{\mathbf{R}}$. Comparing terms of the type $\sim \nabla\nabla$ in Eqs. (4.16) and (4.17), one gets easily

$$\mathbf{V}^{(2)} = -\frac{1}{2}\mathbf{P} \ , \tag{4.19}$$

where $\mathbf{P}$ is the projection operator defined in Eq. (3.12). Eliminating $\mathbf{V}^{(2)}$, Eq. (4.16) becomes

$$\begin{aligned} &2\phi\hat{V} + \mathbf{V}^{(1)}\cdot\nabla\phi + \frac{1}{2}\phi^2\nabla\zeta\nabla\zeta\cdot\nabla\nabla\phi - \frac{1}{2}\nabla^2\phi \\ &\quad + \phi^2 b \nabla\zeta\cdot\nabla - \nabla\phi\cdot\nabla \end{aligned} \tag{4.20}$$

Equating the terms of $\sim \nabla$ in Eq. (4.17) and Eq. (4.20), we find

$$\mathbf{V}^{(1)} = \phi K_m \nabla\zeta \ , \tag{4.21}$$

which compares to (4.11). Using this in Eq. (4.20) and equating once more with (4.17), we find finally

$$\hat{V} = -\frac{1}{2}\nabla_\parallel^2 + \frac{1}{2}K_m^2 + \frac{1}{4}\left\{ \frac{1}{\phi}\nabla_\parallel^2\phi + (\hat{\mathbf{n}}\cdot\nabla\nabla\cdot\hat{\mathbf{n}}) \right\} \ . \tag{4.22}$$

The last term in curly brackets can be written in a covariant way. Using (4.18) and the identity

$$\begin{aligned} \nabla^2\phi &= \nabla\cdot\left(-\phi^3\nabla\zeta\cdot\nabla\nabla\zeta\right) \\ &= 3\left(\nabla\phi\right)^2/\phi - \phi^3\left(\nabla\nabla\zeta\right)^2 - \phi^3\nabla\zeta\cdot\nabla\left(\nabla^2\zeta\right) \ , \end{aligned} \tag{4.23}$$

a simple calculation shows it to be

$$-\left\{ \phi^2\left(\nabla\nabla\zeta\right)^2 - \frac{2}{\phi^2}\left(\nabla\phi\right)^2 + b^2 \right\} = -\mathrm{tr}\left(\mathbf{S}^2\right) \ . \tag{4.24}$$

One can also note that the traceless curvature tensor $\mathbf{S}'$ of Eq. (3.21), satisfies the relations

$$\mathrm{tr}\left(\mathbf{S}'^2\right) = \mathrm{tr}\left(\mathbf{S}^2\right) - \frac{1}{2}\left(\mathrm{tr}\mathbf{S}\right)^2 = 2\Delta^2 \ , \tag{4.25}$$

where 2Δ is the curvature difference introduced in Eq. (1.2). Then Eq. (4.22) has the simple expression

$$\hat{V} = -\frac{1}{2}\left(\nabla_\parallel^2 + \Delta^2\right) \ . \tag{4.26}$$

The operator $\hat{s}$ in Eq. (4.1) has now been found up to $o(d^2)$. From Eq. (2.15), and proceeding as in the previous section, we get

$$\begin{aligned} \hat{\mathbf{n}}\times\mathbf{E} = \frac{1}{\sqrt{\epsilon}}\Big\{ &-\mathbf{B}\left[1 + dK_m - \frac{d^2}{2}\Delta^2\right] - d\hat{\mathbf{n}}\nabla\cdot\mathbf{B} \\ &+ d\phi\left(\mathbf{B}\cdot\nabla\right)\nabla\zeta + d\phi\nabla\left(\frac{\hat{\mathbf{n}}}{\phi}\cdot\mathbf{B}\right) + \frac{d^2}{2}\nabla_\parallel^2\mathbf{B}\Big\} \\ &+ o(d^3) \end{aligned} \tag{4.27}$$

as a generalization of Eq. (3.10). Projecting over $\hat{\mathbf{n}}$ we get the analog of (3.13), which is the *surface divergence constraint.* As before, this constraint allows us to eliminate $\nabla\cdot\mathbf{B}$, so that Eq. (4.27) becomes

$$\begin{aligned} \hat{\mathbf{n}}\times\Bigg(\mathbf{E} - \frac{1}{\sqrt{\epsilon}}\Big\{&(\hat{\mathbf{n}}\times\mathbf{B})\left(1 + dK_m - \frac{d^2}{2}\Delta^2\right) \\ &- d\hat{\mathbf{n}}\times\phi\left(\mathbf{B}\cdot\nabla\right)\nabla\zeta - d\hat{\mathbf{n}}\times\phi\nabla\left(\frac{\hat{\mathbf{n}}}{\phi}\cdot\mathbf{B}\right) \\ &- \frac{d^2}{2}\hat{\mathbf{n}}\times\nabla_\parallel^2\mathbf{B}\Big\} + o(d^3)\Bigg) = 0 \ . \end{aligned} \tag{4.28}$$

Using Eqs. (3.15) and (3.23), it is easily shown that the surface divergence constraint used above becomes

$$\hat{\mathbf{n}}\cdot\mathbf{B}\left[1 - dK_m - \frac{d^2}{2}\Delta^2\right] + d\,\nabla_\parallel\cdot\mathbf{B}_\parallel - \frac{1}{2}d^2\,\hat{\mathbf{n}}\cdot\nabla_\parallel^2\mathbf{B} = o(d^3) \ , \tag{4.29}$$

which generalizes Eq. (3.16). Note that the $\mathbf{P}$ operator is now *effective* on the first-order field $\mathbf{B}$.

We now show that Eq. (4.28) leads to the result of Ref. 3 [their Eq. (3.47)] once the two terms appearing in the second row are transformed as follows. In the first, we separate the $\mathbf{B}$ field in a parallel and normal component to the surface and use Eq. (A9), thus getting

$$\phi\hat{\mathbf{n}}\times(\mathbf{B}\cdot\nabla)\nabla\zeta = 2K_m(\hat{\mathbf{n}}\times\mathbf{B}) - \mathbf{S}\cdot\hat{\mathbf{n}}\times\mathbf{B} + \phi(\hat{\mathbf{n}}\cdot\mathbf{B})\hat{\mathbf{n}}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta\,, \quad (4.30)$$

while for the second term we use the identity

$$\begin{aligned}\phi(\hat{\mathbf{n}}\cdot\mathbf{B})\,\hat{\mathbf{n}}\cdot\nabla\nabla\zeta + \phi\nabla\left(\frac{\hat{\mathbf{n}}}{\phi}\cdot\mathbf{B}\right) &= \left(\frac{\hat{\mathbf{n}}}{\phi}\cdot\mathbf{B}\right)\nabla\phi + \phi\nabla\left(\frac{\hat{\mathbf{n}}}{\phi}\cdot\mathbf{B}\right)\\ &= \nabla(\hat{\mathbf{n}}\cdot\mathbf{B}) = -d\nabla(\nabla_{\|}\cdot\mathbf{B}_{\|}) + o(d^2)\,, \quad (4.31)\end{aligned}$$

where in the last step we have used (3.16). With the above identities Eq. (4.28) becomes

$$\mathbf{E}_{\|} = \frac{1}{\sqrt{\epsilon}}\left\{\mathbf{Z}(\hat{\mathbf{n}}\times\mathbf{B}) + d^2\hat{\mathbf{n}}\times\left[\nabla_{\|}(\nabla_{\|}\cdot\mathbf{B}_{\|}) - \frac{1}{2}\nabla_{\|}^2\mathbf{B}_{\|}\right]\right\} + o(d^3)\,, \quad (4.32)$$

where

$$Z_{ij} = P_{ij}\left\{1 - \frac{d^2}{2}\Delta^2\right\} + dS'_{ij} \quad (4.33)$$

is the SI tensor up to order d^2.

V. THIRD-ORDER AND CONCLUSION

The starting equation is (4.8), which we rewrite as

$$\hat{W}\phi + \phi\hat{W} = \hat{V}\phi\left(a - \hat{U}\right) - \hat{U}\phi\hat{V}\,. \quad (5.1)$$

From Eq. (4.14), using also

$$(a-b)\phi = \phi(a+b) = 2\phi\left(K_m + \phi\nabla\zeta\cdot\nabla\right)\,, \quad (5.2)$$

which follows from the definitions in (4.9) and (4.13), we get

$$\hat{W}\phi + \phi\hat{W} = \left[\hat{V}\,,\,\phi K_m\right]_- + \left[\hat{V}\,,\,\phi^2\nabla\zeta\cdot\nabla\right]_-\,, \quad (5.3)$$

where $[\,,\,]_-$ denotes the commutator. On the r.h.s. of the last expression, the terms $\sim\nabla\nabla\nabla$ cancel out, hence

$$\mathbf{W}^{(3)} = 0\,. \quad (5.4)$$

The second commutator in Eq. (5.3) contains second derivative terms coming from

$$\left[\mathbf{V}^{(2)}\cdot\nabla\nabla\,,\,\phi^2\nabla\zeta\cdot\nabla\right]_- = -\phi\mathbf{S}\cdot\nabla\nabla\,, \quad (5.5)$$

where $\mathbf{S}$ is the extrinsic curvature tensor defined in Eq. (3.22). For clarity, we write out the expression for $\mathbf{S}\cdot\nabla\nabla$ in Cartesian components

$$\mathbf{S}\cdot\nabla\nabla = \left\{\phi\partial_\alpha\partial_\beta\zeta + (\partial_\alpha\zeta)\,\partial_\beta\phi + (\partial_\alpha\phi)\,\partial_\beta\zeta - b\phi^2\,(\partial_\alpha\zeta)\,\partial_\beta\zeta\right\}\partial_\alpha\partial_\beta\,, \quad (5.6)$$

and greek indices run over x, y. Here the sum over repeated indices is implied and we use for brevity, $\partial_\alpha \equiv \partial/\partial x^\alpha$. Taking into account Eq. (5.4), one gets from Eq. (5.3)

$$\mathbf{W}^{(2)} = -\frac{1}{2}\mathbf{S}\,, \quad (5.7)$$

which compares to (4.19). The calculation of the other terms contributing in $\hat{W}$ is more involved. We begin by expressing the l.h.s. of Eq. (5.3) as

$$\begin{aligned}&2\phi\hat{W} - \phi\nabla\phi\cdot\nabla\nabla\zeta\cdot\nabla - b\nabla\phi\cdot\nabla + \left[b^2\phi^2 - (\nabla\phi)^2\right]\nabla\zeta\cdot\nabla\\ &+ \mathbf{W}^{(1)}\cdot\nabla\phi - \frac{1}{2}\phi\nabla\nabla\zeta\cdot\nabla\nabla\phi\\ &-\frac{1}{2}\nabla\zeta\cdot\nabla\,(\nabla\phi)^2 + \frac{1}{2}b\phi^2\nabla\zeta\cdot\nabla\nabla\phi\cdot\nabla\zeta\,, \quad (5.8)\end{aligned}$$

while we proceed by brute force for the calculation of the commutators on the r.h.s. of the same equation. Comparison of the terms $\sim\nabla$ on the two sides then gives

$$\begin{aligned}\mathbf{W}^{(1)} = -\frac{1}{2}\{&\nabla\zeta\cdot\nabla\nabla\phi + \nabla\phi\cdot\nabla\nabla\zeta + (\nabla^2\zeta)\nabla\phi\\ &+\phi\nabla(\nabla^2\zeta) + [\nabla^2\phi - 2b\phi K_m\\ &-\phi^2(\nabla\zeta\cdot\nabla\nabla\phi\cdot\nabla\zeta)]\nabla\zeta\}\,, \quad (5.9)\end{aligned}$$

and the remaining terms give

$$\begin{aligned}W^{(0)} = -\frac{1}{4\phi}\Big\{&2\mathbf{W}^{(1)}\cdot\nabla\phi - \phi\nabla\nabla\zeta\cdot\nabla\nabla\phi\\ &+ b\phi^2\nabla\zeta\cdot\nabla\nabla\phi\cdot\nabla\zeta - \nabla\zeta\cdot\nabla\,(\nabla\phi)^2\\ &+ \nabla_{\|}^2\,(\phi K_m) - \phi^2\nabla\zeta\cdot\nabla\Delta^2\Big\}\,. \quad (5.10)\end{aligned}$$

Analogously to $\mathbf{W}^{(2)}$ in Eq. (5.7), $\mathbf{W}^{(1)}$ and $W^{(0)}$ can be expressed in terms of the geometrical quantities of the surface. Using Eqs. (4.23) and (4.24), an easy calculation shows that

$$\mathbf{W}^{(1)}\cdot\nabla = -\frac{1}{2}\left\{\nabla_{\|}\mathrm{tr}(\mathbf{S}) + \mathrm{tr}(\mathbf{S}^2)\,\hat{\mathbf{n}}\right\}\cdot\nabla\,. \quad (5.11)$$

Using this and

$$\nabla_{\|}^2\,(\phi K_m) = \phi\nabla_{\|}^2 K_m + K_m\nabla_{\|}^2\phi + 2\nabla_{\|}K_m\cdot\nabla_{\|}\phi\,, \quad (5.12)$$

and recalling the definition of Δ^2 given by Eqs. (4.24) and (4.25), we obtain

$$\begin{aligned}W^{(0)} = -\frac{1}{4}\Big\{&\nabla_{\|}^2 K_m + b\,\mathrm{tr}\,(\mathbf{S}^2) + K_m\left(\frac{1}{\phi}\nabla_{\|}^2\phi\right)\\ &-\left[\nabla\nabla\zeta\cdot\nabla\nabla\phi + \frac{1}{2}\phi\nabla\zeta\cdot\nabla\,\mathrm{tr}\,(\phi\nabla\nabla\zeta)^2\right]\\ &-b\frac{1}{\phi^2}\,(\nabla\phi)^2 + \phi K_m\nabla\zeta\cdot\nabla(2K_m)\Big\}\,. \quad (5.13)\end{aligned}$$

Now, by comparing Eq. (4.22) with (4.24), we have

$$K_m\left(\frac{1}{\phi}\nabla_{\|}^2\phi\right) = -K_m \mathrm{tr}\left(\mathbf{S}^2\right) - \phi K_m \nabla\zeta\cdot\nabla(2K_m)\ , \tag{5.14}$$

and the term in square brackets in Eq. (5.13) can be rewritten as

$$-\left[\nabla\nabla\zeta\cdot\nabla\nabla\phi + \frac{1}{2}\phi\nabla\zeta\cdot\nabla\mathrm{tr}\left(\phi\nabla\nabla\zeta\right)^2\right]$$
$$= \mathrm{tr}\left(\phi\nabla\nabla\zeta\right)^3 - 3\nabla\nabla\zeta\cdot\nabla\phi\cdot\nabla\phi/\phi - b\,\mathrm{tr}\left(\phi\nabla\nabla\zeta\right)^2$$
$$= \mathrm{tr}\left(\mathbf{S}^3\right) + b\frac{1}{\phi^2}\left(\nabla\phi\right)^2 - b\,\mathrm{tr}\left(\mathbf{S}^2\ ,\right) \tag{5.15}$$

where in the second identity we have used Eq. (4.24) and

$$\mathrm{tr}\left(\mathbf{S}^3\right) = \mathrm{tr}\left(\phi\nabla\nabla\zeta\right)^3 - 3\nabla\nabla\zeta\cdot\nabla\phi\cdot\nabla\phi/\phi - 3b\left(\nabla\phi\right)^2/\phi^2 + b^3\ . \tag{5.16}$$

With the help of these expressions we arrive at

$$W^{(0)} = -\frac{1}{4}\left\{\left[\mathrm{tr}\left(\mathbf{S}^3\right) - \frac{1}{2}\mathrm{tr}\mathbf{S}\,\mathrm{tr}\left(\mathbf{S}^2\right)\right] + \frac{1}{2}\nabla_{\|}^2(\mathrm{tr}\mathbf{S})\right\}\ , \tag{5.17}$$

which further simplifies by noting that

$$\mathrm{tr}\left(\mathbf{S}^3\right) - \frac{1}{2}\mathrm{tr}\left(\mathbf{S}\right)\mathrm{tr}\left(\mathbf{S}^2\right) = \mathrm{tr}\left(\mathbf{S}'^3\right) + \mathrm{tr}\left(\mathbf{S}\right)\mathrm{tr}\left(\mathbf{S}'^2\right)\ , \tag{5.18}$$

and that $\mathrm{tr}\left(\mathbf{S}'^3\right) = 0$, which is actually valid for any odd power. We have then

$$W^{(0)} = -\frac{1}{4}\left\{\mathrm{tr}\mathbf{S}\,\mathrm{tr}\left(\mathbf{S}'^2\right) + \frac{1}{2}\nabla_{\|}^2(\mathrm{tr}\mathbf{S})\right\}\ . \tag{5.19}$$

In conclusion, from Eqs. (4.5), (5.8), (5.12), and (5.20), the $\hat{W}$ operator can be rewritten as

$$\hat{W} = -\frac{1}{2}\mathbf{S}\cdot\nabla_{\|}\nabla_{\|} - \nabla_{\|}K_m\cdot\nabla_{\|} - \frac{1}{4}\nabla_{\|}^2K_m - K_m\Delta^2\ . \tag{5.20}$$

In writing the last equation above, we have made use of the relation

$$\mathbf{S}\cdot\nabla\nabla - \mathrm{tr}\left(\mathbf{S}^2\right)\phi\nabla\zeta\cdot\nabla = \mathbf{S}\cdot\nabla_{\|}\nabla_{\|}\ , \tag{5.21}$$

which follows from

$$\mathbf{S}\cdot\nabla\nabla = \mathbf{S}\cdot\nabla_{\|}\left\{\nabla_{\|} + \hat{\mathbf{n}}\left(\hat{\mathbf{n}}\cdot\nabla\right)\right\}$$
$$= \mathbf{S}\cdot\nabla_{\|}\nabla_{\|} + \mathbf{S}\cdot\left(\nabla_{\|}\hat{\mathbf{n}}\right)\left(\hat{\mathbf{n}}\cdot\nabla\right) \tag{5.22}$$

(recall that $\mathbf{S}\cdot\hat{\mathbf{n}} = 0$), and

$$\nabla_{\|}\hat{\mathbf{n}} = -\mathbf{S}\ . \tag{5.23}$$

Together with Eqs. (4.14) and (4.26), Eq. (5.20) defines the $\hat{s}$ operator in Eq. (4.2) up to $o(d^3)$.

We now insert $\hat{s}$ in the starting equation (2.15) and proceed as in Sec. IV. The main difference is, obviously, that we now consistently retain all terms of $o(d^3)$. Therefore, in the last identity in Eq. (4.31) we now use, from Eq. (4.29),

$$\hat{\mathbf{n}}\cdot\mathbf{B} = -d\left\{(1+dK_m)\nabla_{\|}\cdot\mathbf{B}_{\|} - \frac{d}{2}\hat{\mathbf{n}}\cdot\nabla_{\|}^2\mathbf{B}\right\} + o(d^3)\ . \tag{5.24}$$

Also, the term $-(d^2/2)\nabla_{\|}^2\mathbf{B}$ which appears in Eq. (4.28) can be conveniently transformed. To $o(d^2)$, one could make in Eq. (4.32) the simple replacement $\mathbf{B}\to\mathbf{B}_{\|}$, while including $o(d^3)$ one has, from Eq. (3.16)

$$\mathbf{B} \equiv \mathbf{B}_{\|} + \hat{\mathbf{n}}(\hat{\mathbf{n}}\cdot\mathbf{B}) \simeq \mathbf{B}_{\|} - d\,\hat{\mathbf{n}}\nabla_{\|}\cdot\mathbf{B}_{\|}\ . \tag{5.25}$$

Using a relation of the type (5.12) and Eq. (5.23), one gets

$$\hat{\mathbf{n}}\times\left\{-\frac{d^2}{2}\nabla_{\|}^2\mathbf{B}\right\} = \hat{\mathbf{n}}\times\left\{-\frac{d^2}{2}\nabla_{\|}^2\mathbf{B}_{\|} - d^3\,\mathbf{S}\cdot\nabla_{\|}\left(\nabla_{\|}\cdot\mathbf{B}_{\|}\right) - d^3\left(\nabla_{\|}\cdot\mathbf{B}_{\|}\right)\nabla_{\|}K_m\right\} + o(d^4)\ . \tag{5.26}$$

The last term in (5.26) requires some care. To get it we have used

$$-\nabla_{\|}^2\hat{\mathbf{n}} = \nabla_{\|}\cdot\mathbf{S} = \nabla_{\|}\mathrm{tr}(\mathbf{S}) + \hat{\mathbf{n}}\,\mathrm{tr}\left(\mathbf{S}^2\right)\ , \tag{5.27}$$

which can be proved as follows. One notes first that $\nabla_{\| j}\hat{n}_i = \nabla_{\| i}\hat{n}_j = S_{ij}$. Therefore, one has

$$-\nabla_{\|}^2\hat{n}_i = -\nabla_{\| j}\nabla_{\| i}\hat{n}_j$$
$$= \nabla_{\| i}\mathrm{tr}\mathbf{S} + \left(\nabla_{\| i}\nabla_{\| j} - \nabla_{\| j}\nabla_{\| i}\right)\hat{n}_j\ . \tag{5.28}$$

The last commutator is then computed using $\nabla_{\| i}P_{jk} = S_{ij}\hat{n}_k + S_{ik}\hat{n}_j$.

After some algebra and using the above relations, one gets

$$\mathbf{E}_{\|} = \frac{1}{\sqrt{\epsilon}}\left\{\mathbf{Z}\cdot(\hat{\mathbf{n}}\times\mathbf{B}) + d^2\hat{\mathbf{n}}\times\left(\nabla_{\|}\nabla_{\|}\cdot\mathbf{B}_{\|} - \frac{1}{2}\nabla_{\|}^2\mathbf{B}_{\|} - d\mathbf{S}'\cdot\nabla_{\|}\left(\nabla_{\|}\cdot\mathbf{B}_{\|}\right) - \frac{d}{2}\nabla_{\|}\left(\hat{\mathbf{n}}\cdot\nabla_{\|}^2\mathbf{B}_{\|}\right) + \frac{d}{2}\mathbf{S}\cdot\nabla_{\|}\nabla_{\|}\mathbf{B}_{\|} + d\left(\nabla_{\|}K_m\cdot\nabla_{\|}\right)\mathbf{B}_{\|}\right)\right\} + o(d^4)\ , \tag{5.29}$$

where

$$Z_{ij} = P_{ij}\left\{1 - d^2\Delta^2\left(\frac{1}{2} - dK_m\right) + \frac{d^3}{4}\nabla_{\|}^2(K_m)\right\} + dS'_{ij} \tag{5.30}$$

is the SI tensor to $o(d^3)$.

In the 1D case of a surface grating

$$z = \zeta(x) , \tag{5.31}$$

and, for instance, taking the magnetic field parallel to the grating grooves (p polarization), the SI Eq. (5.30) becomes a scalar quantity Z_p. From

$$\mathrm{tr}\,(\mathbf{S}^n) = (\mathrm{tr}\mathbf{S})^n = \left(\phi^3\zeta''\right)^n , \tag{5.32}$$

$\Delta = K_m$, and

$$\nabla_{\|}^2 \mathrm{tr}\mathbf{S} = \phi^2\left(\phi^3\zeta''\right)'' - \frac{1}{2}\phi\zeta'\left(\phi^6\zeta''^2\right)' , \tag{5.33}$$

one has

$$Z_p = \Big\{1 + \frac{d}{2}\phi^3\zeta'' - \frac{d^2}{8}\phi^6\zeta''^2 + \frac{d^3}{4}\Big[-\phi^9\zeta''^3 + \frac{15}{2}\phi^9\zeta'^2\zeta''^3 - 5\phi^7\zeta'\zeta''\zeta''' + \frac{1}{2}\phi^5\zeta^{iv}\Big]\Big\} , \tag{5.34}$$

which is the result given by Maradudin[4] [his Eq. (45)].

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APPENDIX

Start from the triple vector product

$$-\hat{\mathbf{n}}\times[\nabla\times(\mathbf{v}\times\nabla\zeta)] , \tag{A1}$$

where ∇ acts, by definition, on $\nabla\zeta$ variable only. Using the vector identity

$$\{\mathbf{a}\times(\mathbf{b}\times\mathbf{c})\}_i = \mathbf{a}b_i\cdot\mathbf{c} - (\mathbf{a}\cdot\mathbf{b})c_i , \tag{A2}$$

for terms in square brackets in (A1), we get the equivalent expressions

$$\hat{\mathbf{n}}\times(\mathbf{v}\cdot\nabla)\nabla\zeta - \nabla^2\zeta(\hat{\mathbf{n}}\times\mathbf{v}) , \tag{A3}$$

and

$$(\hat{\mathbf{n}}\cdot\nabla)(\mathbf{v}\times\nabla\zeta) - \nabla(\hat{\mathbf{n}}\cdot\mathbf{v}\times\nabla\zeta) . \tag{A4}$$

Equating (A3) and (A4), we have the relation

$$\hat{\mathbf{n}}\times(\mathbf{v}\cdot\nabla)\nabla\zeta = \nabla^2\zeta(\hat{\mathbf{n}}\times\mathbf{v}) - (\nabla\nabla\zeta\cdot\hat{\mathbf{n}}\times\mathbf{v}) + \mathbf{v}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta . \tag{A5}$$

If $\mathbf{v}$ is parallel to $\hat{\mathbf{n}}$, (A5) becomes a trivial identity. This suggests using, Eq. (2.16), in the last term above, to separate normal and parallel components to the surface. We have

$$\mathbf{v}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta = -[\hat{\mathbf{n}}\times(\hat{\mathbf{n}}\times\mathbf{v})]\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta + (\hat{\mathbf{n}}\cdot\mathbf{v})\,\hat{\mathbf{n}}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta \tag{A6}$$

$$= -\hat{\mathbf{n}}\cdot\nabla\nabla\zeta\cdot\hat{\mathbf{n}}(\hat{\mathbf{n}}\times\mathbf{v}) + \hat{\mathbf{n}}\hat{\mathbf{n}}\cdot(\nabla\nabla\zeta\cdot\hat{\mathbf{n}}\times\mathbf{v}) + (\hat{\mathbf{n}}\cdot\mathbf{v})\,\hat{\mathbf{n}}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta \tag{A7}$$

and in the second identity above, Eq. (A2) has been used. Substituting in (A5) get

$$\hat{\mathbf{n}}\times(\mathbf{v}\cdot\nabla)\nabla\zeta = \left(\nabla^2\zeta - \hat{\mathbf{n}}\cdot\nabla\nabla\zeta\cdot\hat{\mathbf{n}}\right)(\hat{\mathbf{n}}\times\mathbf{v}) - \mathbf{P}(\nabla\nabla\zeta\cdot\hat{\mathbf{n}}\times\mathbf{v}) + (\hat{\mathbf{n}}\cdot\mathbf{v})\,\hat{\mathbf{n}}\times(\hat{\mathbf{n}}\cdot\nabla)\nabla\zeta . \tag{A8}$$

If $\mathbf{v}$ lies on the tangent plane, the last term vanishes. One gets in this way the equivalent expression

$$\phi\hat{\mathbf{n}}\times(\mathbf{P}\mathbf{v}\cdot\nabla)\nabla\zeta = 2K_m(\hat{\mathbf{n}}\times\mathbf{v}) - \mathbf{P}\phi\nabla\nabla\zeta\mathbf{P}(\hat{\mathbf{n}}\times\mathbf{v}) . \tag{A9}$$

In writing the last, we have used the identity $\hat{\mathbf{n}}\times\mathbf{v} = \mathbf{P}(\hat{\mathbf{n}}\times\mathbf{v})$ which is valid for any vector $\mathbf{v}$ and

$$-\hat{\mathbf{n}}\cdot\nabla\nabla\zeta\cdot\hat{\mathbf{n}} = -\phi^2\nabla\zeta\cdot\nabla\nabla\zeta\cdot\nabla\zeta = \frac{1}{\phi}\nabla\zeta\nabla\phi , \tag{A10}$$

which follows from definitions (2.5) and (2.6).

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