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Systematic Splitting of Wavefields into Unidirectional Modes: Long-Range Asymptotic Methods for Weakly Uniform Media

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13. ABSTRACT (Maximum 200 words) A series of pseudo-unitary transforms is devised and applied to the Helmholtz equation for a weakly nonuniform one-dimensional medium, decoupling the wave field in a consistent order-by-order way into counter-propagating modes. The result is a generalized form of d'Alembert decomposition, providing an asymptotic solution without backscatter at arbitrary order. Low-order contributions correspond to the standard WKB approximation. Higher orders provide additional terms of potential importance in applications involving propagation over long ranges, e.g., long time-of-flight measurement and very-long-baseline interferometry. Evidence is presented that this decoupling scheme is equivalent to high-order Born approximations.			
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SYSTEMATIC SPLITTING OF WAVEFIELDS INTO UNIDIRECTIONAL MODES: LONG-RANGE ASYMPTOTIC METHODS FOR WEAKLY NONUNIFORM MEDIA

1. INTRODUCTION

This work aims to produce a unified understanding of the three analytic approximations — WKB, parabolic, and Born — that are most widely cited to justify approximating wave propagation through media with only “weak” nonuniformities as a purely one-way phenomenon. The particular focus is on backscatter — how to neglect it in a consistent way, and what impact this neglect has on the remaining forward-propagating component. To limit the complexity of the problem and yet retain most of the essential features, attention is restricted to waves in a single spatial dimension. The subject is introduced in section 2 in the context of the prototypical example — vibrations of a nonuniform string. This section explores the difficulties inherent in any attempt to generalize forward/backward mode splitting beyond uniform media, where it is a trivial matter, to nonuniform media, where it can generally be done only approximately. In section 3, the initial-value problem for the Helmholtz equation is first recast in first-order form and then transformed by a rotation into the “d’Alembert” representation where questions of mode coupling are more naturally addressed. Section 4 discusses the effect of such state-space transforms on the equation of motion — especially the class of “pseudo-unitary” rotations that strictly conserve the wave energy. A pseudo-unitary rotation is used in section 5 to go to the “Bremmer” representation, where it is evident what will be required to decouple the counter-propagating wave modes to first order. Section 6 introduces a scheme of successive pseudo-unitary Pauli-space rotations that reveals the conditions for decoupling the modes to any desired order, giving operational meaning to the phrase “weakly nonuniform medium”. In section 7, this weak nonuniformity is invoked, and the resulting asymptotic approximations are obtained for the long-range wave field through order $m = 6$. The phase in this expression is seen to agree with the WKB result through order $m = 3$, with differences appearing at $m = 4$. Endpoint amplitude effects are also discussed, and it is shown that these begin to differ from the WKB approximation at third order. Finally, section 8 presents an illustrative example involving a specific environment. Beginning with section 3, Pauli matrices are used to facilitate the analysis. Appendix A reviews their properties — particularly the fact that, when used as the infinitesimal generators of state-space transforms, the Pauli matrices just induce rotations. The relation of this work to the Born series approach is discussed in Appendix B.

2. BACKGROUND

This section sets the scene. The Helmholtz equation for continuous wave (cw) motion and its ancillary relations for energy density and power flux are obtained for one-dimensional nonuniform media, and the basic requirement for approximate mode splitting is identified.

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Consider the transverse motion of a string stretched along the x coordinate under tension τ . Suppose the string has a density $\rho(x)$ and consider its displacement $w(x, t)$ in the transverse y direction. Within the linear-response regime, w will obey the familiar linear wave equation. If the x dependence of ρ is only a gradual one relative to the wavelengths involved, the solution to be expected on physical grounds should consist of a pair of waveforms that travel in opposite directions along the string, changing only gradually with x and only weakly coupled to one another.

Uniform Medium

If τ and ρ are just constants, the displacement obeys a simple form of the wave equation

$$\rho \partial_t^2 w - \tau \partial_x^2 w = 0, \quad (1)$$

where the phase speed $c = \sqrt{\tau/\rho}$ is constant. (See various elementary books, e.g. Ref. 1.) The shorthand notation $\partial_{qr} = \partial r / \partial q$, $d_{qr} = dr / dq$ is used for derivatives throughout this work.

The kinetic energy is an inherently local quantity (because the mass is) with a density $K_w = (\rho/2)(\partial_t w)^2$. The potential energy can also be regarded as localized, with a density $V_w = (\tau/2)(\partial_x w)^2$. The total energy density for the wave motion is just their sum,

$$E_w = \frac{\rho}{2}(\partial_t w)^2 + \frac{\tau}{2}(\partial_x w)^2. \quad (2a)$$

The power flux, also known as energy current density, is

$$P_w = -\tau(\partial_x w)(\partial_t w). \quad (2b)$$

Since the medium is passive and lossless, wave energy is conserved,

$$\partial_x P_w + \partial_t E_w = (\partial_t w)(\rho \partial_t^2 w - \tau \partial_x^2 w) = 0. \quad (3)$$

Consider the distribution of energy in a wave field that is a superposition of two others: $w = \alpha + \beta$. Since the total wave energy is conserved, one might naively expect that $P_{\alpha+\beta}$ and $E_{\alpha+\beta}$ would simply reduce to $P_\alpha + P_\beta$ and $E_\alpha + E_\beta$, but this cannot be true in general; linear superposition does not apply to energy quantities because they are quadratic in the wave field. Thus, the differences

$$E_{\alpha,\beta} \stackrel{def}{=} E_{\alpha+\beta} - (E_\alpha + E_\beta) = \rho(\partial_t \alpha)(\partial_t \beta) + \tau(\partial_x \alpha)(\partial_x \beta) \quad (4a)$$

$$P_{\alpha,\beta} \stackrel{def}{=} P_{\alpha+\beta} - (P_\alpha + P_\beta) = -\tau(\partial_x \alpha)(\partial_t \beta) - \tau(\partial_x \beta)(\partial_t \alpha) \quad (4b)$$

do not vanish identically. However, there is one important case where this energy superposition *does* hold. When d'Alembert's decomposition into left/right-going waveforms is used, i.e.,

$$w(x, t) = \alpha(\xi) + \beta(\eta), \quad (5)$$

where $\xi = x - ct$ and $\eta = x + ct$, then

$$\begin{aligned} E_\alpha &= \tau(\partial_\xi \alpha)^2 \geq 0 & P_\alpha &= +cE_\alpha \geq 0 \\ E_\beta &= \tau(\partial_\eta \beta)^2 \geq 0 & P_\beta &= -cE_\beta \leq 0 \\ E_{\alpha+\beta} &= E_\alpha + E_\beta \geq 0 & P_{\alpha+\beta} &= P_\alpha + P_\beta \end{aligned} \quad (6)$$

so that both $E_{\alpha,\beta}$ and $P_{\alpha,\beta}$ vanish.

It is also well known [1] that w satisfies Eq. (1) if and only if d'Alembert's decomposition holds, i.e., that this decomposition provides the general solution for the wave equation in a uniform medium. Any wave field in such a medium is simply a pair of counter-propagating waveforms, the d'Alembert modes, and these partition the total energy. Energy superposition applies, and each mode separately transports its share of the total. These modes move at constant speed, propagate without distortion, and partition the energy exactly. Because there is no environmental inhomogeneity to couple the modes, there can be no backscatter. If the field is initialized with only one of these modes excited, the other one can never arise anywhere. The aim of this work is to extend this result in a controlled, approximate way to media with weak inhomogeneities, providing a generalized form of d'Alembert decomposition.

Nonuniform Media

The energy expressions in Eq. (2) remain valid even when τ and ρ are not simply constants. The Lagrangian density $L(w, \partial_x w, \partial_t w) = K_w - V_w$ is still governed by the appropriate Lagrange equation

$$\frac{\partial}{\partial t} \left[\frac{\partial L}{\partial(\partial_t w)} \right] + \frac{\partial}{\partial x} \left[\frac{\partial L}{\partial(\partial_x w)} \right] - \frac{\partial L}{\partial w} = 0, \quad (7)$$

i.e.,

$$\partial_t (\rho \partial_t w) + \partial_x (-\tau \partial_x w) = 0. \quad (8)$$

With $\rho = \rho(x)$ and even $\tau = \tau(t)$, this would reduce to Eq. (1) again. A time-dependent tension, however, would introduce a source term on the right-hand side of Eq. (3), so we will confine ourselves to cases with constant τ . In these static nonuniform environments, wave energy is still conserved — Eq. (3) remains valid — but d'Alembert's decomposition no longer holds in the original form. It must be generalized.

Complex Representation

This generalization will be easier to produce using a complex representation. Physically, the wave field is certainly a real-valued quantity. But since the wave equation is linear and has real coefficients, there is no harm in adding on some imaginary part to extend the physical field w_{re} to complex values: $w = w_{re} + iw_{im}$. Naturally, both w_{re} and w_{im} must satisfy Eq. (1), and the same is true of w and w^* . Also, the $\partial_x w$, $\partial_t w$ factors in the energy expressions now refer to $\partial_x w_{re}$, $\partial_t w_{re}$ so that

$$E_w = \left[\frac{\rho}{2} (\partial_t w + \partial_t w^*)^2 + \frac{\tau}{2} (\partial_x w + \partial_x w^*)^2 \right] / 4, \quad (9a)$$

$$P_w = -\tau (\partial_x w + \partial_x w^*) (\partial_t w + \partial_t w^*) / 4. \quad (9b)$$

As a result,

$$\partial_x P_w + \partial_t E_w = (\partial_t w + \partial_t w^*) \left[(\rho \partial_t^2 w - \tau \partial_x^2 w) + (\rho \partial_t^2 w^* - \tau \partial_x^2 w^*) \right] / 4 = 0, \quad (10)$$

as expected.

For the superposition field $w = \alpha + \beta$,

$$E_{\alpha,\beta} = [\rho(\partial_t\alpha + \partial_t\alpha^*)(\partial_t\beta + \partial_t\beta^*) + \tau(\partial_x\alpha + \partial_x\alpha^*)(\partial_x\beta + \partial_x\beta^*)] / 4 , \quad (11a)$$

$$P_{\alpha,\beta} = [-\tau(\partial_x\alpha + \partial_x\alpha^*)(\partial_t\beta + \partial_t\beta^*) - \tau(\partial_x\beta + \partial_x\beta^*)(\partial_t\alpha + \partial_t\alpha^*)] / 4 , \quad (11b)$$

but the right-hand sides fail to vanish because there is no d'Alembert decomposition to separate the field exactly into counter-propagating modes. However, there is a workable approximate approach.

CW Fields

It might be possible to deal successfully with fields whose time dependence is quite general. Narrowband fields, for example, could be handled using analytic-signal methods. Since this would be too great a diversion from the present purpose, however, the scope of this work is confined to continuous wave (cw) fields.

Since the medium itself is not time-dependent, each frequency component can be treated separately. With only a single frequency ω in its spectrum, the wave field can only be sinusoidal in time: $w_{re}(x, t) = F(x) \cos(\omega t - \varphi(x))$. If the imaginary part is chosen to be $w_{im}(x, t) = -F(x) \sin(\omega t - \varphi(x))$, then the complex representation of the wave field is

$$w(x, t) = u(x)e^{-i\omega t} , \quad (12)$$

where $u(x) = F(x)e^{i\varphi(x)}$. Thus the wave equation for $w_{re} = (w + w^*)/2$ reduces to

$$e^{-i\omega t}(u'' + k^2u) + e^{+i\omega t}(u^{*''} + k^2u^*) = 0 , \quad (13)$$

where the primes denote x -derivatives and $k(x) = \omega/c(x)$, so both u and u^* must satisfy the one-dimensional Helmholtz equation

$$u'' + k^2u = 0 . \quad (14)$$

The field's power flux is then

$$P_w = P_w^+ + P_w^0 + P_w^- , \quad (15)$$

where

$$P_w^+ = -e^{+i2\omega t}(u^{*'}u^*)i\omega\tau/4 \quad (16a)$$

$$P_w^- = +e^{-i2\omega t}(u'u)i\omega\tau/4 \quad (16b)$$

$$P_w^0 = (uu^{*'} - u^*u')i\omega\tau/4 , \quad (16c)$$

and its energy density is

$$E_w = E_w^+ + E_w^0 + E_w^- , \quad (17)$$

where

$$E_w^+ = e^{+i2\omega t}(u^{*'}u^* - k^2u^{*2})\tau/8 \quad (18a)$$

$$E_w^- = e^{-i2\omega t}(u'u - k^2u^2)\tau/8 \quad (18b)$$

$$E_w^0 = (k^2u^*u + u^{*'}u')\tau/4 . \quad (18c)$$

Here we apply time averaging (denoted by a bar). This effectively kills off the time-dependent '+' and '-' terms, leaving only the constant '0' terms. Thus

$$\bar{P}_w = W(u, u^*) i\omega\tau/4 \quad (19a)$$

$$\bar{E}_w = (k^2 u^* u + u'^* u')\tau/4, \quad (19b)$$

where W is a Wronskian.¹ It is clear from Eq. (19) that, although \bar{E}_w can depend on x , \bar{P}_w cannot. That is a statement of conservation of wave energy for the cw case.

Each component of a superposition field $w = \alpha + \beta$ can be represented in complex form, $\alpha(x, t) = a(x) \exp(-i\omega t)$ and $\beta(x, t) = b(x) \exp(-i\omega t)$. Then,

$$P_{\alpha,\beta} = P_{\alpha,\beta}^+ + P_{\alpha,\beta}^0 + P_{\alpha,\beta}^-, \quad (20)$$

where

$$P_{\alpha,\beta}^+ = -e^{+i2\omega t} (a'^* b^* + a^* b'^*) i\omega\tau/4 \quad (21a)$$

$$P_{\alpha,\beta}^- = +e^{-i2\omega t} (a' b + a b') i\omega\tau/4 \quad (21b)$$

$$P_{\alpha,\beta}^0 = [(a'^* b + a b'^*) - (a' b^* + a^* b')] i\omega\tau/4, \quad (21c)$$

and thus

$$\bar{P}_{\alpha,\beta} = [W(b, a^*) + W(a, b^*)] i\omega\tau/4. \quad (22)$$

This clearly shows what would be needed to partition the power between two modes α and β . Since a and a^* must be solutions to Eq. (14), \bar{P}_α cannot depend on x . The same is true of b and b^* , so \bar{P}_β cannot depend on x either. Finally, in order for $\bar{P}_{\alpha,\beta}$ to vanish identically, there must be a linear dependence between a and b^* (and thus between a^* and b):

$$a \propto b^*. \quad (23)$$

Similarly,

$$E_{\alpha,\beta} = E_{\alpha,\beta}^+ + E_{\alpha,\beta}^0 + E_{\alpha,\beta}^-, \quad (24)$$

where

$$E_{\alpha,\beta}^+ = e^{+i2\omega t} (a'^* b'^* - k^2 a^* b^*) \tau/4 \quad (25a)$$

$$E_{\alpha,\beta}^- = e^{-i2\omega t} (a' b' - k^2 a b) \tau/4 \quad (25b)$$

$$E_{\alpha,\beta}^0 = [(a' b'^* + a'^* b') + k^2 (a^* b + a b^*)] \tau/4. \quad (25c)$$

Again, under time averaging, the '+' and '-' terms vanish, leaving only

$$\bar{E}_{\alpha,\beta} = \Re \{ a' b'^* + k^2 a b^* \} \tau/2. \quad (26)$$

¹Recall that $W(u, v) = uv' - vu'$ is independent of x when u and v are solutions to Eq. (14), and vanishes whenever these solutions are linearly dependent, i.e., when $v \propto u$.

From Eq. (23) it is clear that $b^* = \zeta a$ where ζ is some complex x -independent quantity. Thus,

$$\bar{E}_{\alpha,\beta} = \Re \left[\zeta (a'^2 + k^2 a^2) \right] \tau/2 . \quad (27)$$

At the same time,

$$\bar{E}'_{\alpha} = \left[a' (a^{*''} + k^2 a^*) + a^{*'} (a'' + k^2 a) \right] \tau/4 \quad (28a)$$

$$\bar{E}'_{\beta} = \left[b' (b^{*''} + k^2 b^*) + b^{*'} (b'' + k^2 b) \right] \tau/4 . \quad (28b)$$

This is where difficulties appear in this attempt to separate the field *exactly* into counter-propagating modes that simultaneously obey the Helmholtz equation and partition the energy. Because a , b , a^* , and b^* are all solutions to the Helmholtz equation, both \bar{E}'_{α} and \bar{E}'_{β} vanish identically, leaving \bar{E}_{α} and \bar{E}_{β} independent of x . This cannot be right; \bar{E}_w itself did not have to be independent of x . Furthermore, $\bar{E}_{\alpha,\beta}$ can vanish only when $a' = \pm ika$. That implies a functional form for a ,

$$a(x) = a(x_0) \exp \left[\pm i \int_{x_0}^x d\chi k(\chi) \right] . \quad (29)$$

Unfortunately, it also implies that

$$a'' - k^2 a = \pm i k' a . \quad (30)$$

Since the right-hand side must vanish, it is essential that $k' = 0$. Clearly, the exact mode separation of the field can be done only in a uniform medium, where it is nothing more than the familiar d'Alembert representation. It cannot be done in nonuniform media — at least not in an *exact* way. Equation (30), however, suggests that mode separation might be achieved in some *approximate* sense based on the condition

$$|k'|/k^2 \ll 1 . \quad (31)$$

The remainder of this report is directed toward realizing that possibility.

3. INITIAL REFORMULATION

This section transmutes the whole wave motion problem into a form where the effects of environmental inhomogeneity on mode splitting are clearer and easier to begin dealing with. Initially, the Helmholtz equation and its power flux and energy density relations are recast in first-order form involving Pauli matrices. Then the Helmholtz equation's Picard series solution is presented and the reason for its generally slow convergence is underscored. Finally, the problem is transformed to the "d'Alembert" representation — an optimal starting point for subsequent perturbation analysis.

The one-dimensional Helmholtz equation has the form

$$d_x^2 u + k^2 u = 0 ,$$

where the wavenumber $k = \omega/c$ may be x -dependent. The complex field is $w(x, t) = u(x) \exp(-i\omega t)$ and the relevant energy quantities are

$$\begin{aligned} \bar{P}_w &= (-i\omega\tau/4) (u^* d_x u - u d_x u^*) \\ \bar{E}_w &= (\tau/4) \left[k^2 u^* u + (d_x u^*)(d_x u) \right] . \end{aligned}$$

First-Order Form

It is convenient to adopt some constant density value ρ_0 as a standard and then use the corresponding phase speed $c_0 = \sqrt{\tau/\rho_0}$ to define a reference wavenumber $k_0 = \omega/c_0$. The spatial coordinate will be rescaled to k_0x (so that distances are measured out in reference wavelengths), but this nondimensional coordinate will continue to be written as x . Thus the Helmholtz equation becomes

$$d_x^2 u + n^2 u = 0, \tag{32a}$$

where $n = c_0/c = k/k_0 = \sqrt{\rho/\rho_0}$ is the refractive index and, with constants lumped into $\gamma = \omega^2 \rho_0/4$, the energy terms are

$$\bar{P}_w = -ic_0\gamma (u^* d_x u - u d_x u^*) \tag{32b}$$

$$\bar{E}_w = \gamma [n^2 u^* u + (d_x u^*)(d_x u)]. \tag{32c}$$

Since Eq. (32a) is linear, the familiar trick of swapping order for dimensionality [3] can be used to convert it from a second-order one-dimensional form to a first-order two-dimensional one. To facilitate dealing with the complex 2-by-2 matrices that the latter form entails, we invoke the Pauli spin matrices whose properties are reviewed in Appendix A.

Initial Representation

The simplest way to produce a first-order form is to let the dependent variables be u and $\dot{u} = d_x u$ (the displacement of the string and the slope of its tangent) so that the state of the system is specified by the vector

$$\underline{\mathbf{u}} = \begin{bmatrix} u \\ \dot{u} \end{bmatrix}.$$

Then the Helmholtz equation takes the form

$$d_x \underline{\mathbf{u}} = \underline{\mathbf{G}} \underline{\mathbf{u}}, \tag{33}$$

where

$$\underline{\mathbf{G}} = \begin{bmatrix} 0 & 1 \\ -n^2 & 0 \end{bmatrix} = i \left(\frac{1+n^2}{2} \right) \sigma_2 + \left(\frac{1-n^2}{2} \right) \sigma_1 \tag{34a}$$

is the generator of the system's evolution along the x coordinate.

This is equivalent to the Schrödinger equation, $i d_x \underline{\mathbf{u}} = \underline{\mathbf{H}} \underline{\mathbf{u}}$, for a two-state quantum system with a Hamiltonian $\underline{\mathbf{H}} = i \underline{\mathbf{G}}$ where x plays the role of time (in a system of units where $\hbar = 1$). The Hamiltonian's eigenvalues, $\pm n$, correspond to time-dependent energy levels. The power flux and energy density are "matrix elements" (in the quantum mechanical sense)

$$\begin{aligned} \bar{P}(\underline{\mathbf{u}}) &= c_0 \gamma \underline{\mathbf{u}}^\dagger \underline{\mathbf{P}} \underline{\mathbf{u}} \\ \bar{E}(\underline{\mathbf{u}}) &= \gamma \underline{\mathbf{u}}^\dagger \underline{\mathbf{E}} \underline{\mathbf{u}} \end{aligned}$$

of a pair of Hermitian operators,

$$\underline{\mathbf{P}} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \sigma_2 \quad (34b)$$

$$\underline{\mathbf{E}} = \begin{bmatrix} n^2 & 0 \\ 0 & 1 \end{bmatrix} = \left(\frac{1+n^2}{2} \right) \mathbf{1} - \left(\frac{1-n^2}{2} \right) \sigma_3 . \quad (34c)$$

The only peculiar aspect of this as a quantum mechanics problem is that, except for the degenerate $n = 1$ case, $\underline{\mathbf{H}}$ is non-Hermitian. The work below is generally done in terms of $\underline{\mathbf{G}}$, with $\underline{\mathbf{H}}$ appearing only when analogies to quantum mechanics are pursued.

In a certain sense, the solution is already in hand. When Eq. (33) is combined with any initial condition $\underline{\mathbf{u}}(x_0)$ (forming an “initial-value” or “one-point boundary value” problem), the state vector at any x is simply

$$\underline{\mathbf{u}}(x) = \underline{\mathbf{K}}(x, x_0) \underline{\mathbf{u}}(x_0)$$

in terms of the propagator matrix $\underline{\mathbf{K}}(x, x_0)$. This matrix operator is defined by a Dyson-ordered integral [2] (also known as a “product integral” [4]) and is variously called a “matricant” [5] or “matrizant” [6]. It is the solution to the same ordinary differential equation with unit-matrix initial values:

$$d_x \underline{\mathbf{K}}(x, x_0) = \underline{\mathbf{G}}(x) \underline{\mathbf{K}}(x, x_0) \quad \dots \quad \underline{\mathbf{K}}(x_0, x_0) = \mathbf{1} , \quad (35)$$

or, equivalently, the integral equation

$$\underline{\mathbf{K}}(x, x_0) = \mathbf{1} + \int_{x_0}^x d\xi \underline{\mathbf{G}}(\xi) \underline{\mathbf{K}}(\xi, x_0) . \quad (36)$$

Under fairly general conditions,² this has a unique solution in the form of an infinite series

$$\underline{\mathbf{K}}(x, x_0) = \sum_{j=0}^{\infty} \underline{\mathbf{K}}_j(x, x_0) \quad (37a)$$

that begins with

$$\underline{\mathbf{K}}_0(x, x_0) = \mathbf{1} \quad (37b)$$

and continues by Picard iteration

$$\underline{\mathbf{K}}_{j+1}(x, x_0) = \int_{x_0}^x d\xi \underline{\mathbf{G}}(\xi) \underline{\mathbf{K}}_j(\xi, x_0) , \quad (37c)$$

converging uniformly and absolutely [5,6]. This Picard series³ is satisfying but less useful than it may appear, especially in nonuniform media, because the convergence is typically quite slow.

²Sufficient conditions are that, in an interval containing x and x_0 , $n^2(x)$ be single-valued, bounded, and integrable and that $d_x n^2(x)$ be piecewise continuous and bounded [6].

³It is also associated with the names Liouville and Neumann.

To see why that is, let

$$\epsilon = (n^2 - 1)/2 \quad (38)$$

measure the deviation of the refractive index from its reference value, 1, so that the three operators of Eq. (34) are

$$\underline{\mathbf{G}} = -\epsilon\sigma_1 + i(1 + \epsilon)\sigma_2 \quad (39a)$$

$$\underline{\mathbf{P}} = \sigma_2 \quad (39b)$$

$$\underline{\mathbf{E}} = (i + \epsilon)\mathbf{1} + \epsilon\sigma_3 . \quad (39c)$$

The generator $\underline{\mathbf{G}}$ has a constant term as well as ϵ -dependent ones. Thus $\underline{\mathbf{K}}_j$, a multiple integral of a product of the form

$$\underline{\mathbf{G}}(x_j) \underline{\mathbf{G}}(x_{j-1}) \cdots \underline{\mathbf{G}}(x_2) \underline{\mathbf{G}}(x_1) ,$$

contains contributions of multiple orders in $\epsilon(x)$. The integrand for $\underline{\mathbf{K}}_3$, for example, is

$$\underline{\mathbf{G}}(x_3) \underline{\mathbf{G}}(x_2) \underline{\mathbf{G}}(x_1) = \begin{bmatrix} 0 & -(1 + 2\epsilon(x_2)) \\ (1 + 2\epsilon(x_3))(1 + 2\epsilon(x_1)) & 0 \end{bmatrix} , \quad (40)$$

which has contributions of orders 0, 1, and 2 in ϵ . The convergence of Eq. (37) is slow because $\underline{\mathbf{K}}_j$ generally contains terms in $\epsilon^0, \epsilon^1, \epsilon^2, \dots, \epsilon^{j-1}, \epsilon^j$. Although it is mathematically allowable to expand all the terms and re-order the series so that the j th term contains only ϵ^j , no method is known for doing that with any generality. There is, however, a way to finesse a solution by applying Pauli-space rotations.

d'Alembert Representation

Before pursuing that option, it will be convenient to change the representation to one in which the generator $\underline{\mathbf{G}}$ is diagonal wherever the inhomogeneity ϵ vanishes. This is done by applying the unitary operator

$$\underline{\mathbf{U}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} \quad (41)$$

to transform state vectors and operators according to $\underline{\mathbf{u}} = \underline{\mathbf{U}}\mathbf{u}$ and $\underline{\mathbf{V}} = \underline{\mathbf{U}}\mathbf{V}\underline{\mathbf{U}}^{-1}$, respectively. The form of the problem remains the same,

$$d_x \underline{\mathbf{u}} = \underline{\mathbf{G}}\underline{\mathbf{u}} \quad (42a)$$

$$\underline{\bar{P}}(\underline{\mathbf{u}}) = c_0 \gamma \underline{\mathbf{u}}^\dagger \underline{\mathbf{P}}\underline{\mathbf{u}} \quad (42b)$$

$$\underline{\bar{E}}(\underline{\mathbf{u}}) = \gamma \underline{\mathbf{u}}^\dagger \underline{\mathbf{E}}\underline{\mathbf{u}} \quad (42c)$$

in terms of the transformed state vector

$$\underline{\mathbf{u}} = \frac{1}{\sqrt{2}} \begin{bmatrix} u + i\dot{u} \\ u - i\dot{u} \end{bmatrix}$$

and transformed operators $\underline{\mathbf{G}}, \underline{\mathbf{P}}, \underline{\mathbf{E}}$ in this new "d'Alembert" representation.

Equation (41) can be written as $\mathbf{U} = \exp\{-i\mathbf{S}\}$ in terms of an operator $\mathbf{S} = S_0\mathbf{1} + \vec{S}\cdot\vec{\sigma}$ that has a scalar part $S_0 = -\pi/4$ and a Pauli-vector part $\vec{S} = S\hat{s}$ with magnitude $S = \pi/3$ and direction $\hat{s} = (\hat{e}_1 - \hat{e}_2 + \hat{e}_3)/\sqrt{3}$. Thus, \mathbf{U} transforms operators into the d'Alembert representation by simply rotating their Pauli-vector parts about the $(1, -1, 1)$ direction through the angle $-2S = -2\pi/3$. That rotation amounts to a cyclic permutation of $(\hat{e}_2, -\hat{e}_3, -\hat{e}_1)$, i.e., to the replacement $(\hat{e}_1, \hat{e}_2, \hat{e}_3) \rightarrow (-\hat{e}_2, -\hat{e}_3, \hat{e}_1)$, which means that the effect of \mathbf{U} can be found by inspection. In particular, the three operators of Eq. (39) become

$$\mathbf{G} = -i(1 + \epsilon)\sigma_3 + \epsilon\sigma_2 \quad (43a)$$

$$\mathbf{P} = -\sigma_3 \quad (43b)$$

$$\mathbf{E} = (1 + \epsilon)\mathbf{1} + \epsilon\sigma_1 . \quad (43c)$$

Their scalar and Pauli-vector parts are

$$\begin{aligned} G_0 &= 0 & \vec{G} &= -i(1 + \epsilon)\hat{e}_3 + \epsilon\hat{e}_2 \\ P_0 &= 0 & \vec{P} &= -\hat{e}_3 \\ E_0 &= 1 + \epsilon & \vec{E} &= \epsilon\hat{e}_1 , \end{aligned}$$

and, with the positive sign chosen for square roots, the magnitudes and directions of the vector parts $\vec{G} = G\hat{g}$, $\vec{P} = P\hat{p}$, and $\vec{E} = E\hat{e}$ are

$$\begin{aligned} G &= in & \hat{g} &= -[(1 + \epsilon)\hat{e}_3 + i\epsilon\hat{e}_2]/n \\ P &= 1 & \hat{p} &= -\hat{e}_3 \\ E &= \epsilon & \hat{e} &= \hat{e}_1 . \end{aligned}$$

On first inspection, the initial-value problem seems no better behaved than before, since the generator in Eq. (43a) will also produce ϵ -ordering problems in the Picard series for its propagator. The advantage of this representation is that, within any x -interval where $k = k_0$, the generator reduces to a diagonal form: $\mathbf{G} \rightarrow -i\sigma_3$. Since the forthcoming solution will emerge from a perturbation process for $|\epsilon| \ll 1$, it is naturally simpler to begin in the d'Alembert representation where the unperturbed $\epsilon = 0$ problem is diagonal.

Mode Separation

At this point, it is worth noting that wherever $k = k_0$, the d'Alembert generator's eigenvectors are $|\zeta\rangle$ with corresponding eigenvalues $-\zeta i$, where $\zeta = \pm$. This means that the state vector separates exactly into a sum of counter-propagating modes

$$\mathbf{u}(x) = \mathbf{a}(x) + \mathbf{b}(x) ,$$

where

$$\mathbf{a}(x) = u_-(x_0) \exp[+i(x - x_0)] |-\rangle \quad (44a)$$

$$\mathbf{b}(x) = u_+(x_0) \exp[-i(x - x_0)] |+\rangle . \quad (44b)$$

It is easy to confirm that these modes partition both the power flux and the energy density,

$$\begin{aligned} \bar{P}(\mathbf{a} + \mathbf{b}) &= \bar{P}(\mathbf{a}) + \bar{P}(\mathbf{b}) \\ \bar{E}(\mathbf{a} + \mathbf{b}) &= \bar{E}(\mathbf{a}) + \bar{E}(\mathbf{b}) , \end{aligned}$$

that their individual energies are separately conserved,

$$\begin{aligned}\bar{P}(\mathbf{a}(x)) &= \bar{P}(\mathbf{a}(x_0)) = +c_0\gamma|u_-(x_0)|^2 \\ \bar{P}(\mathbf{b}(x)) &= \bar{P}(\mathbf{b}(x_0)) = -c_0\gamma|u_+(x_0)|^2\end{aligned}$$

and that their energy densities are spatially uniform,

$$\begin{aligned}\bar{E}(\mathbf{a}(x)) &= \bar{E}(\mathbf{a}(x_0)) = \gamma|u_-(x_0)|^2 \\ \bar{E}(\mathbf{b}(x)) &= \bar{E}(\mathbf{b}(x_0)) = \gamma|u_+(x_0)|^2.\end{aligned}$$

This is d'Alembert's decomposition again — an exact result for uniform media, but only approximate otherwise.

4. STATE-SPACE TRANSFORMS

Later on, the convergence of Picard-series solutions will be improved by the application of well chosen transforms. This section previews the properties of such transforms — particularly those of the wave-energy conserving “pseudo-unitary” class.

The challenge is to find some expression for the solution to the d'Alembert initial-value problem,

$$d_x \mathbf{K}(x, x_0) = \mathbf{G}(x) \mathbf{K}(x, x_0) \dots \mathbf{K}(x_0, x_0) = \mathbf{1}, \quad (45)$$

that is better behaved than Eq. (37). The general idea is to do this by transforming to still other representations where the generator assumes more tractable forms. A perfectly diagonal form would seem ideal, but it is not generally attainable. Instead, we apply a series of transforms that improve the diagonality incrementally with each step.

The first step is along the general lines of the work by Keller and Keller [6]. The essence of it is to find a change of representation that converts the generator \mathbf{G} into the form

$$\tilde{\mathbf{G}} = \tilde{\mathbf{A}} + \tilde{\mathbf{R}}, \quad (46)$$

where

- $\tilde{\mathbf{A}}$ is diagonal and proportional to a suitably defined quantity $\tilde{\nu} \approx n$, and
- $\tilde{\mathbf{R}}$ is off-diagonal and proportional to a suitably defined small quantity $\tilde{\rho}$.

Once that is achieved, one can transform to the $\tilde{\mathbf{A}}$ -interaction representation, where the j th term in the propagator's Picard series will contain only $\tilde{\rho}^j$. For small $|\tilde{\rho}|$, this approach leads to a perturbative formulation for the field in terms of multiply reflected left- and right-going modes. This series constitutes an algorithm for computing the field at limited ranges, and its leading term provides an asymptotic expression for the field at long range. The transform that splits the generator according to Eq. (46) is a simple rotation in Pauli space.

In fact, the second, third and all subsequent steps are achieved through a regular succession of such rotations. Given certain assumptions about the range dependence of the medium, each one improves both the perturbative formulation and the long-range asymptotic approximation. The operators that produce these rotations, however, differ in two respects from the transform \mathbf{U} in Eq. (41), namely, they are

- x -dependent, and
- “pseudo-unitary” (a generalization of the unitary class).

Ultimately this means that all the $\tilde{\nu}$ and $\tilde{\varrho}$ quantities are functions of x , and that all the rotation angles are imaginary. These points are explored in the remainder of this section, and then the rotations themselves are obtained explicitly in the following sections.

Pseudo-Unitarity

This section makes some analogies to quantum mechanics, and thus uses the Hamiltonian $\mathbf{H} = i\mathbf{G}$. For any operator \mathbf{V} , it is clear from Eq. (42a) that

$$d_x (\mathbf{u}^\dagger \mathbf{V} \mathbf{u}) = \mathbf{u}^\dagger [i(\mathbf{H}^\dagger \mathbf{V} - \mathbf{V} \mathbf{H}) + d_x \mathbf{V}] \mathbf{u} \quad (47)$$

represents the total x -derivative of the matrix element of \mathbf{V} with the state vector \mathbf{u} — the rate of change due to both the dynamic evolution of \mathbf{u} and any explicit x dependence in \mathbf{V} . Since the Hamiltonian is “pseudo-Hermitian”, i.e.

$$\mathbf{H}^\dagger \mathbf{P} = \mathbf{P} \mathbf{H} \quad \dots \quad \text{pseudo-Hermitian} , \quad (48)$$

and \mathbf{P} itself is independent of x , any matrix element of \mathbf{P} must also be x -independent. That fact itself is nothing new (it was implicit in Eq. (19a)); the novel element is its relation to the pseudo-Hermiticity of \mathbf{H} . Note that there is *no* comparable result for \mathbf{E} . Since

$$\mathbf{E} = -\mathbf{P} \mathbf{H} , \quad (49)$$

that operator, although pseudo-Hermitian, is x -dependent wherever \mathbf{H} is. As a result, \mathbf{P} is a constant of the motion, but \mathbf{E} is *not*.

The dynamic evolution of the state vector can be summarized in terms of the propagator as $\mathbf{u}(\xi) = \mathbf{K}(\xi, \zeta) \mathbf{u}(\zeta)$. From the identity

$$\mathbf{u}^\dagger(\xi) \mathbf{P} \mathbf{u}(\xi) = \mathbf{u}^\dagger(\zeta) [\mathbf{K}^\dagger(\xi, \zeta) \mathbf{P} \mathbf{K}(\xi, \zeta)] \mathbf{u}(\zeta) ,$$

together with the initial value $\mathbf{K}(\zeta, \zeta) = \mathbf{1}$, it follows that, since \mathbf{P} is an invariant of the motion, the propagator is “pseudo-unitary”, i.e.

$$\mathbf{P} = \mathbf{K}^\dagger(\xi, \zeta) \mathbf{P} \mathbf{K}(\xi, \zeta) \quad \dots \quad \text{pseudo-unitary} \quad (50)$$

for any ξ, ζ . This property is responsible for the invariance of \mathbf{P} during the evolution. By definition, \mathbf{P} will be invariant under *any* pseudo-unitary transform \mathbf{M} , whether, like \mathbf{K} , it is related to the dynamic evolution of the system or not.⁴

Using the fact that \mathbf{P} is Hermitian, the pseudo-Hermiticity of \mathbf{H} and the pseudo-unitarity of a transform \mathbf{M} can be rewritten in various equivalent ways, such as

$$\begin{aligned} (\mathbf{P} \mathbf{H})^\dagger &= \mathbf{P} \mathbf{H} \\ (\mathbf{P} \mathbf{M})^\dagger &= \mathbf{P} \mathbf{M}^{-1} . \end{aligned}$$

⁴Strictly speaking, the way things have been defined, it is \mathbf{M}^{-1} , not \mathbf{M} itself, that is directly analogous to \mathbf{K} . However, pseudo-unitarity for one implies pseudo-unitarity for the other.

These results have better-known analogs in quantum mechanics, where the operator $\mathbf{P}^2 = \mathbf{1}$ is a constant of the motion rather than \mathbf{P} itself. Although the vibrating string problem and the two-state quantum problem are very similar in a mathematical sense, it would be a mistake to press the analogy too far, since the two state vectors have entirely different physical meanings — one being a classical displacement and the other a probability amplitude.

In a quantum mechanical setting, the physical observables are represented by Hermitian operators. Any such operator \mathbf{V} has real Pauli coefficients V_0, \dots, V_3 . In the present context, \mathbf{V} may be pseudo-Hermitian, in which case V_0 and V_3 are real while V_1 and V_2 are imaginary.

State-Space Transforms

A linear transform $\mathbf{M}\tilde{\mathbf{u}} = \mathbf{u}$ will preserve the appearance of the problem

$$d_x \tilde{\mathbf{u}} = \tilde{\mathbf{G}} \tilde{\mathbf{u}} \tag{51a}$$

$$\tilde{\mathbf{P}}(\tilde{\mathbf{u}}) = c_0 \gamma \tilde{\mathbf{u}}^\dagger \tilde{\mathbf{P}} \tilde{\mathbf{u}} \tag{51b}$$

$$\tilde{\mathbf{E}}(\tilde{\mathbf{u}}) = \gamma \tilde{\mathbf{u}}^\dagger \tilde{\mathbf{E}} \tilde{\mathbf{u}} \tag{51c}$$

in terms of the transformed operators

$$\tilde{\mathbf{G}} = \tilde{\mathbf{A}} + \tilde{\mathbf{R}} \tag{52a}$$

$$\tilde{\mathbf{P}} = \mathbf{M}^\dagger \mathbf{P} \mathbf{M} \tag{52b}$$

$$\tilde{\mathbf{E}} = \mathbf{M}^\dagger \mathbf{E} \mathbf{M} \tag{52c}$$

The first part of the generator,

$$\tilde{\mathbf{A}} = \mathbf{M}^{-1} \mathbf{G} \mathbf{M} \tag{53a}$$

is a similarity transform; the second part,

$$\tilde{\mathbf{R}} = -\mathbf{M}^{-1} d_x \mathbf{M} \tag{53b}$$

involves the explicit x dependence of \mathbf{M} (which is assumed to be nonsingular and differentiable so that $\tilde{\mathbf{R}}$ is well-defined).

To conserve energy, \mathbf{M} will be restricted to pseudo-unitary transforms. When that is done, Eq. (49) is enough to determine the forms of the transformed energy operators:

$$\tilde{\mathbf{E}} = -i\mathbf{P}\tilde{\mathbf{A}} \tag{54}$$

and $\tilde{\mathbf{P}} = \mathbf{P}$. In quantum mechanical terminology, such an \mathbf{M} is an innocuous “change of picture,” and all that is needed to characterize its effect is usable expressions for $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{R}}$. To obtain them, it will be sufficiently general to use

$$\mathbf{M} = \exp(-i\mathbf{S}) \tag{55}$$

with a pseudo-Hermitian \mathbf{S} to guarantee that \mathbf{M} is pseudo-unitary. Thus,

$$\tilde{\mathbf{A}} = \exp(+i\mathbf{S})\mathbf{G}\exp(-i\mathbf{S}) \tag{56a}$$

$$\tilde{\mathbf{R}} = -\exp(+i\mathbf{S})d_x\exp(-i\mathbf{S}) \tag{56b}$$

Since Eq. (56a) is a similarity transform, $\tilde{\Lambda} = \tilde{\Lambda}_0 \mathbf{1} + \tilde{\Lambda} \cdot \vec{\sigma}$ is the result of a simple Pauli-space rotation of \mathbf{G} , as discussed in Appendix A. Specifically,

$$\tilde{\Lambda}_0 = G_0 = 0 \quad (57a)$$

and $\tilde{\Lambda} = \tilde{\Lambda} \hat{\lambda}$ where

$$\tilde{\Lambda} = G = in, \quad (57b)$$

with $\hat{\lambda}$ obtained by rotating \hat{g} about the \hat{s} direction through the angle $\phi = -2S$. But, since \mathbf{S} is pseudo-Hermitian rather than Hermitian, this angle need not be real. If \hat{s} points mainly in the \hat{e}_3 direction (i.e., if $|\hat{s} \cdot \hat{e}_3|^2 > |\hat{s} \cdot \hat{e}_1|^2 + |\hat{s} \cdot \hat{e}_2|^2$), then ϕ is a real angle — otherwise it is imaginary.

The second term of the transformed generator has the form

$$\tilde{\mathbf{R}} = - \left\{ e^{+iS_0} [\cos(S) + i \sin(S) \hat{s} \cdot \vec{\sigma}] \right\} d_x \left\{ e^{-iS_0} [\cos(S) - i \sin(S) \hat{s} \cdot \vec{\sigma}] \right\}. \quad (58)$$

With the help of $\hat{s} \cdot \dot{\hat{s}} = 0$ and Eq. (A6), this reduces to

$$\tilde{\mathbf{R}} = i \dot{S}_0 \mathbf{1} + i \left[\dot{S} \hat{s} + \cos(S) \sin(S) \dot{\hat{s}} - \sin^2(S) (\hat{s} \times \dot{\hat{s}}) \right] \cdot \vec{\sigma}. \quad (59)$$

(As always, the dot indicates differentiation by the scaled coordinate x .) The scalar part of \mathbf{S} affects only the scalar term $\tilde{R}_0 = i \dot{S}_0$. Since S_0 has no impact on the vector part of $\tilde{\mathbf{R}}$ and had none at all on $\tilde{\Lambda}$, it is entirely irrelevant to the problem of diagonalizing $\tilde{\Lambda} + \tilde{\mathbf{R}}$. For convenience, let $S_0 = 0$ so that only the vector part

$$\vec{\tilde{R}} = -\frac{i}{2} \left[\dot{\phi} \hat{s} + \sin \phi \dot{\hat{s}} + (1 - \cos \phi) \hat{s} \times \dot{\hat{s}} \right] \quad (60)$$

remains. This involves rates of change for both the length and direction of \vec{S} (i.e., both $\dot{\phi}$ and $\dot{\hat{s}}$), and that appears to be about all that can be said about it in general. However, if the direction is fixed, the expression simplifies to

$$\vec{\tilde{R}} = -\frac{i}{2} \dot{\phi} \hat{s}. \quad (61)$$

One case is useful enough to deserve special attention, namely an \vec{S} that is parallel to one of the Pauli axes: $\hat{s} \cdot \hat{e}_j = \pm 1$ for $j = 1, 2$, or 3 . To maintain pseudo-unitarity, $\dot{\phi}$ must be real when $j = 3$ and imaginary when $j = 1, 2$.

5. BREMMER REPRESENTATION

This section implements a pseudo-unitary transform to the ‘‘Bremmer’’ representation, where the generator of the wave evolution is diagonal to order ϵ . This fact improves the convergence of the Picard series for the solution and provides the impetus for additional transforms that are developed in the next section to improve it still further.

Change of Notation

The previous section dealt with state-space transforms in a fairly general sense: $\mathbf{u} = \mathbf{M}\tilde{\mathbf{u}}$, where \mathbf{u} was a d'Alembert state vector and $\tilde{\mathbf{u}}$ was the state vector in some transformed representation. Here we devise a particular form for that. Since it will ultimately be the first in a series, we switch to an indexed notation at this point. Quantities in the d'Alembert representation together with the transform that produces them are indicated by a ⁽⁰⁾ superscript, e.g., \mathbf{G} , \mathbf{A} , \mathbf{R} , \mathbf{u} and \mathbf{M} , \mathbf{S} are written hereafter as $\mathbf{G}^{(0)}$, $\mathbf{A}^{(0)}$, $\mathbf{R}^{(0)}$, $\mathbf{u}^{(0)}$ and $\mathbf{M}^{(0)}$, $\mathbf{S}^{(0)}$. The transformed or "Bremmer" representation is labeled with a ⁽¹⁾ superscript, so $\tilde{\mathbf{G}}$, $\tilde{\mathbf{A}}$, $\tilde{\mathbf{R}}$, $\tilde{\mathbf{u}}$ are denoted $\mathbf{G}^{(1)}$, $\mathbf{A}^{(1)}$, $\mathbf{R}^{(1)}$, $\mathbf{u}^{(1)}$. The transform, then, is written $\mathbf{u}^{(0)} = \mathbf{M}^{(0)}\mathbf{u}^{(1)}$.

Rotation

Making $\mathbf{A}^{(1)}$ diagonal is tantamount to aligning $\tilde{\mathbf{A}}^{(1)}$ with \hat{e}_3 . Since $\tilde{\mathbf{A}}^{(1)}$ results from a rotation of $\tilde{\mathbf{G}}^{(0)} = \epsilon\hat{e}_2 - i(1+\epsilon)\hat{e}_3$, the diagonalization can be accomplished by using \hat{e}_1 as the axis and rotating through the angle $\tan^{-1}(i\epsilon/(1+\epsilon))$, i.e., by using a vector $\tilde{\mathbf{S}}^{(0)}$ with components $S_2^{(0)} = S_3^{(0)} = 0$ and

$$S_1^{(0)} = -i\psi^{(0)}/2, \quad (62)$$

where

$$\tanh \psi^{(0)} = \frac{\epsilon}{1+\epsilon}. \quad (63)$$

Thus

$$\mathbf{S}^{(0)} = -\frac{i}{2}\psi^{(0)}\sigma_1, \quad (64)$$

and the transform $\mathbf{M}^{(0)} = \exp\{-i\mathbf{S}^{(0)}\}$ is

$$\begin{aligned} \mathbf{M}^{(0)} &= \cosh(\psi^{(0)}/2) \mathbf{1} - \sinh(\psi^{(0)}/2) \sigma_1 \\ &= \frac{1+n}{2\sqrt{n}} \mathbf{1} + \frac{1-n}{2\sqrt{n}} \sigma_1. \end{aligned} \quad (65)$$

The transformed operators are

$$\mathbf{A}^{(1)} = -i\nu^{(1)}\sigma_3 \quad (66a)$$

$$\mathbf{R}^{(1)} = \varrho^{(1)}\sigma_1 \quad (66b)$$

$$\mathbf{P}^{(1)} = -\sigma_3 \quad (66c)$$

$$\mathbf{E}^{(1)} = \nu^{(1)}\mathbf{1}, \quad (66d)$$

where

$$\nu^{(1)} = n \quad (67)$$

$$\varrho^{(1)} = \frac{\dot{n}}{2n} = d_x(\log \sqrt{n}). \quad (68)$$

Note that $|\varrho^{(1)}| \ll \nu^{(1)}$ is precisely the condition anticipated by Eq. (31) at the end of section 2.

Using a pseudo-unitary transform automatically produces an off-diagonal $\mathbf{R}^{(1)}$. The converse is also true. Keller and Keller [6] began by requiring $\mathbf{R}^{(1)}$ to be off-diagonal and arrived at a pseudo-unitary transformation (the same one, to within an arbitrary constant). Pseudo-unitarity distinguishes an essentially unique “splitting” among all the possible transforms [7]. It is appropriate to acknowledge here that, despite a somewhat altered appearance in the present context, the transform developed in this section is a type of Foldy-Wouthuysen transform [8]. This sort of transform was introduced in the early 1950s [9] to produce asymptotic mode decoupling in a very different physical context — relativistic quantum mechanics.

Mode Separation

This is a convenient point to pause and consider the case of an environmental region where the wavenumber k is a constant — possibly different from the reference value k_0 . Since ϵ is constant in such a region, $\mathbf{G}^{(0)}$ is independent of x and can thus be diagonalized by an x -independent $\mathbf{S}^{(0)}$. This means that $\mathbf{R}^{(1)}$ vanishes so that Eq. (64) diagonalizes the whole generator $\mathbf{G}^{(1)} = -i\nu^{(1)}\sigma_3$, and that $\nu^{(1)} = n$ is independent of x . As in section 3, the generator’s eigenvectors are $|\zeta\rangle$; here, however the corresponding eigenvalues are $-\zeta i\nu^{(1)}$. Again the state vector separates exactly into a sum of counter-propagating modes

$$\mathbf{u}^{(1)}(x) = \mathbf{a}^{(1)}(x) + \mathbf{b}^{(1)}(x), \quad (69)$$

where

$$\mathbf{a}^{(1)}(x) = u_{-}^{(1)}(x_0) \exp \left[+i\nu^{(1)} \times (x - x_0) \right] |-\rangle \quad (70a)$$

$$\mathbf{b}^{(1)}(x) = u_{+}^{(1)}(x_0) \exp \left[-i\nu^{(1)} \times (x - x_0) \right] |+\rangle. \quad (70b)$$

It is easy to confirm that these modes also partition both the power flux and the energy density,

$$\begin{aligned} \bar{P}(\mathbf{a}^{(1)} + \mathbf{b}^{(1)}) &= \bar{P}(\mathbf{a}^{(1)}) + \bar{P}(\mathbf{b}^{(1)}) \\ \bar{E}(\mathbf{a}^{(1)} + \mathbf{b}^{(1)}) &= \bar{E}(\mathbf{a}^{(1)}) + \bar{E}(\mathbf{b}^{(1)}), \end{aligned}$$

that their individual energies are separately conserved,

$$\begin{aligned} \bar{P}(\mathbf{a}^{(1)}(x)) &= \bar{P}(\mathbf{a}^{(1)}(x_0)) = +c_0\gamma|u_{-}^{(1)}(x_0)|^2 \\ \bar{P}(\mathbf{b}^{(1)}(x)) &= \bar{P}(\mathbf{b}^{(1)}(x_0)) = -c_0\gamma|u_{+}^{(1)}(x_0)|^2, \end{aligned}$$

and their energy densities are spatially uniform,

$$\begin{aligned} \bar{E}(\mathbf{a}^{(1)}(x)) &= \bar{E}(\mathbf{a}^{(1)}(x_0)) = \gamma\nu^{(1)}|u_{-}^{(1)}(x_0)|^2 \\ \bar{E}(\mathbf{b}^{(1)}(x)) &= \bar{E}(\mathbf{b}^{(1)}(x_0)) = \gamma\nu^{(1)}|u_{+}^{(1)}(x_0)|^2. \end{aligned}$$

This is the d’Alembert decomposition of section 3 again, this time for $n \neq 1$.

Bremmer Series

In the Bremmer representation, the initial-value problem is

$$d_x \mathbf{u}^{(1)}(x) = [\mathbf{A}^{(1)}(x) + \mathbf{R}^{(1)}(x)] \mathbf{u}^{(1)}(x) \quad \dots \quad \mathbf{u}^{(1)}(x_0) = [\mathbf{M}^{(0)}(x_0)]^{-1} \mathbf{u}^{(0)}(x_0). \quad (71)$$

Since $\mathbf{A}^{(1)}(x)$, the "large" part of the generator, is diagonal, it can be used to construct an "interaction" transform [10],

$$\mathbf{L}(x, x_0) = \exp \left(\int_{x_0}^x d\xi \mathbf{A}^{(1)}(\xi) \right) = \begin{bmatrix} \exp(-i\varphi^{(1)}(x, x_0)) & 0 \\ 0 & \exp(+i\varphi^{(1)}(x, x_0)) \end{bmatrix} \quad (72)$$

in which

$$\varphi^{(1)}(x, x_0) = \int_{x_0}^x d\xi \nu^{(1)}(\xi). \quad (73)$$

This \mathbf{L} converts the state vector to the interaction representation via

$$\mathbf{u}^{(1)}(x) = \mathbf{L}(x, x_0) \mathbf{q}(x), \quad (74)$$

and is itself the propagator for an artificial problem,

$$d_x \mathbf{L}(x, x_0) = \mathbf{A}^{(1)}(x) \mathbf{L}(x, x_0) \quad \dots \quad \mathbf{L}(x_0, x_0) = \mathbf{1} \quad (75)$$

in which the perturbation $\varrho^{(1)}$ is "turned off" [2] so that $|+\rangle$ and $|-\rangle$ are decoupled.

In this interaction representation, the initial-value problem for state vectors is

$$d_x \mathbf{q}(x) = \mathbf{V}(x, x_0) \mathbf{q}(x) \quad \dots \quad \mathbf{q}(x_0) = \mathbf{u}^{(1)}(x_0) \quad (76)$$

in terms of the generator,⁵

$$\mathbf{V}(x, x_0) = \mathbf{L}^{-1}(x, x_0) \mathbf{R}^{(1)}(x) \mathbf{L}(x, x_0). \quad (77)$$

The propagator, $\mathbf{Z}(x, x_0)$, evolves the state vector from its initial value in the usual way,

$$\mathbf{q}(x) = \mathbf{Z}(x, x_0) \mathbf{q}(x_0), \quad (78)$$

and thus satisfies the initial-value differential problem,

$$d_x \mathbf{Z}(x, x_0) = \mathbf{V}(x, x_0) \mathbf{Z}(x, x_0) \quad \dots \quad \mathbf{Z}(x_0, x_0) = \mathbf{1}. \quad (79)$$

As before, the equivalent integral equation is

$$\mathbf{Z}(x, x_0) = \mathbf{1} + \int_{x_0}^x d\xi \mathbf{V}(\xi, x_0) \mathbf{Z}(\xi, x_0), \quad (80)$$

and its Picard series solution (often called a Born series in this context [10]) is

⁵In quantum-mechanical terms, the interaction Hamiltonian would be $i\mathbf{V}$.

$$\mathbf{Z}(x, x_0) = \sum_{j=0}^{\infty} \mathbf{Z}_j(x, x_0), \quad (81a)$$

where

$$\mathbf{Z}_0(x, x_0) = \mathbf{1} \quad (81b)$$

and

$$\mathbf{Z}_{j+1}(x, x_0) = \int_{x_0}^x d\xi \mathbf{V}(\xi, x_0) \mathbf{Z}_j(\xi, x_0). \quad (81c)$$

Equations (79)–(81) are identical in form to Eqs. (35)–(37). Here, however, $\mathbf{V} \propto \rho^{(1)}$:

$$\mathbf{V}(\xi, x_0) = \rho^{(1)}(\xi) \begin{bmatrix} 0 & \exp[+2i\varphi^{(1)}(\xi, x_0)] \\ \exp[-2i\varphi^{(1)}(\xi, x_0)] & 0 \end{bmatrix}. \quad (82a)$$

Thus \mathbf{Z}_j involves *only* the j th power of $\rho^{(1)}$, so the convergence problem that was caused by the presence of terms containing both ϵ^0 and ϵ^1 in $\underline{\mathbf{G}}$ (the generator in Eq. (39a)) is avoided. For $|\rho^{(1)}| \ll 1$, the series should converge rapidly.

Furthermore, \mathbf{V} is off-diagonal. Consequently the \mathbf{Z}_j terms are alternately diagonal and off-diagonal. \mathbf{Z}_2 , for instance, is just the double integral of

$$\mathbf{V}(\xi, x_0)\mathbf{V}(\zeta, x_0) = \rho^{(1)}(\xi)\rho^{(1)}(\zeta) \begin{bmatrix} \exp[+2i\varphi^{(1)}(\xi, \zeta)] & 0 \\ 0 & \exp[-2i\varphi^{(1)}(\xi, \zeta)] \end{bmatrix}. \quad (82b)$$

As a result, when Eq. (81a) is used with Eq. (78) with the state vector expanded in the unperturbed eigenstates, $\mathbf{q}(x) = \sum_{\varsigma=\pm} q_{\varsigma}(x)|\varsigma\rangle$, one finds

$$\begin{aligned} q_{\varsigma}(x) &= q_{\varsigma}(x_0) + \int_{x_0}^x dx_1 \rho^{(1)}(x_1) \exp[+2\varsigma i\varphi^{(1)}(x_1, x_0)] q_{-\varsigma}(x_0) \\ &+ \int_{x_0}^x dx_2 \int_{x_0}^{x_2} dx_1 \rho^{(1)}(x_2)\rho^{(1)}(x_1) \exp[+2\varsigma i\varphi^{(1)}(x_2, x_1)] q_{\varsigma}(x_0) + \dots \end{aligned} \quad (83)$$

for $\varsigma = \pm$. This is essentially the Bremmer series [11] — an expression whose j th term represents a wave that been reflected j times on its way from x_0 to x , with $\rho^{(1)}(x)$ acting as a distributed reflection coefficient for the medium. Clearly, if $q_{-\varsigma}$ vanishes at x_0 , the odd-numbered terms all vanish. Then the state vector reduces to $q_{\varsigma}(x)|\varsigma\rangle$, a mode that propagates purely in one direction, but has an amplitude $q_{\varsigma}(x)$ composed of contributions that have undergone an even number (0, 2, 4, ...) of distributed reflections. The $j > 2$ terms were left implicit in Eq. (83). More of them could have been included without much trouble, but there would be little reason for it in this context because our interest is in long-range propagation. For computational purposes, the infinite series must be truncated at some order, and this implies a maximum x beyond which the truncated series no longer faithfully represents $q_{\varsigma}(x)$. For long-range use, a large- x asymptotic expansion is needed instead. The first term in the asymptotic expansion of the Bremmer series for small $\rho^{(1)}$ is just the leading term in the series [6],

$$u_{\zeta}^{(1)}(x) \sim \exp \left[-i\zeta\varphi^{(1)}(x, x_0) \right] q_{\zeta}(x_0) . \quad (84)$$

This expression is an asymptotic approximation for one-way propagation that excludes backscatter in all forms (all the $j > 0$ terms).

Note that this would all have been equally simple had $\mathbf{R}^{(0)}$ involved σ_2 instead of σ_1 , i.e., if $\vec{G}^{(0)}$ had turned out to be orthogonal to \hat{e}_2 rather than to \hat{e}_1 . In that case, a diagonal $\Lambda^{(1)}$ could have been produced by simply rotating around that axis instead.

6. HIGHER-ORDER REPRESENTATIONS

Building on the results of the preceding section, this section introduces a hierarchy of trans-Bremmer rotations. In these the wave-evolution generator is diagonal, and thus the forward/backward modes are decoupled, to progressively higher orders.

Chain of Rotations

Pseudo-unitary rotations similar to the one in the preceding section will be used to generate further representations, which will be denoted by superscripts $^{(m)}$, with $m > 1$. Let \hat{e}_j, \hat{e}_ℓ be the first two Pauli unit vectors \hat{e}_1, \hat{e}_2 in either order and suppose that $\vec{G}^{(m)}$ is orthogonal to \hat{e}_j (i.e., $G_j^{(m)} = 0$). Then choosing $\hat{s}^{(m)}$ to lie along the j axis ($|\hat{s}^{(m)} \cdot \hat{e}_j| = 1$) allows the first term on the right-hand side of

$$\vec{G}^{(m+1)} = \left(\cosh \psi^{(m)} \vec{G}^{(m)} + i \sinh \psi^{(m)} \vec{G}^{(m)} \times \hat{s}^{(m)} \right) + \frac{1}{2} \hat{s}^{(m)} d_x \psi^{(m)} \quad (85)$$

(see Eq. (A11)) to be aligned with \hat{e}_3 by the proper choice of $\psi^{(m)}$. This is still only a partial diagonalization because the second term remains orthogonal to \hat{e}_3 ; however, if $|G_j^{(m+1)}|/|G_3^{(m+1)}| < |G_\ell^{(m)}|/|G_3^{(m)}|$, it is a step in the right direction. Furthermore, since $G_\ell^{(m+1)} = 0$, the process can easily be repeated, this time by a rotation about the ℓ axis. In fact, it can be iterated indefinitely in an alternating series of rotations about the first and second Pauli-space axes.

The process begins with the Pauli vector part of the d'Alembert generator rewritten as

$$\vec{G}^{(0)} = -i\nu^{(0)}\hat{e}_3 + \varrho^{(0)}\hat{e}_3 \times \hat{s}^{(0)} \quad (86a)$$

in terms of

$$\hat{s}^{(0)} = \hat{e}_1 \quad (86b)$$

$$\nu^{(0)} = 1 + \epsilon \quad (86c)$$

$$\varrho^{(0)} = \epsilon . \quad (86d)$$

The axis $\hat{s}^{(0)}$ and the rotation angle

$$\psi^{(0)} = \tanh^{-1} \left(\varrho^{(0)} / \nu^{(0)} \right) \quad (86e)$$

determine the transform $\mathbf{M}^{(0)}$ that produces $\vec{G}^{(1)}$.

The j th iterate has the same form,

$$\vec{G}^{(j)} = -i\nu^{(j)}\hat{e}_3 + \rho^{(j)}\hat{e}_3 \times \hat{s}^{(j)}, \quad (87a)$$

with

$$\hat{s}^{(j)} = \hat{s}^{(j-1)} \times \hat{e}_3 \quad (87b)$$

$$\nu^{(j)} = \nu^{(j-1)} / \cosh \psi^{(j-1)} \quad (87c)$$

$$\rho^{(j)} = \frac{1}{2} d_x \psi^{(j-1)}. \quad (87d)$$

The axis $\hat{s}^{(j)}$ and rotation angle

$$\psi^{(j)} = \tanh^{-1} (\rho^{(j)} / \nu^{(j)}) \quad (87e)$$

determine the transform $\mathbf{M}^{(j)}$ that produces $\vec{G}^{(j+1)}$.

This procedure produces a chain of generators

$$\mathbf{G}^{(0)} \rightarrow \mathbf{G}^{(1)} \rightarrow \mathbf{G}^{(2)} \rightarrow \mathbf{G}^{(3)} \rightarrow \dots \rightarrow \mathbf{G}^{(m)} \quad (88)$$

linked by a series of pseudo-unitary transforms, $\mathbf{u}^{(j)} = \mathbf{M}^{(j)}\mathbf{u}^{(j+1)}$, where

$$\mathbf{M}^{(j)} = \cosh(\psi^{(j)}/2) \mathbf{1} - \sinh(\psi^{(j)}/2) \hat{s}^{(j)} \cdot \vec{\sigma}. \quad (89)$$

Only one assumption is implicit in the construction of link m at the end: that $d_x^m \epsilon$ exists for the environment in question. As m is increased, lengthening the chain, $\mathbf{P}^{(m)}$ always remains identical to the original $\mathbf{P}^{(0)}$, and the system evolves by the transformed equation

$$d_x \mathbf{u}^{(m)} = \mathbf{G}^{(m)} \mathbf{u}^{(m)}. \quad (90)$$

As m is increased by 1, $\hat{s}^{(m)}$ simply rotates by $-\pi/2$ about \hat{e}_3 . (It is periodic: $\hat{s}^{(m+4)} = \hat{s}^{(m)}$.) In addition, *provided* the ratio $|\nu^{(m)}/\rho^{(m)}|$ diminishes with increasing m , the generator becomes more and more diagonal. Together these mean that successive $\vec{G}^{(m)}$ vectors spiral in toward alignment with $-\hat{e}_3$ as sketched in Fig. (1).

As in the $m = 1$ case of section 5, the transformed generator for $m > 1$ is split into $\mathbf{G}^{(m)} = \mathbf{A}^{(m)} + \mathbf{R}^{(m)}$, where

$$\mathbf{A}^{(m)} = -i\nu^{(m)}\sigma_3 \quad (91a)$$

$$\mathbf{R}^{(m)} = \rho^{(m)}(\hat{e}_3 \times \hat{s}^{(m)}) \cdot \vec{\sigma}. \quad (91b)$$

And, as always,

$$\mathbf{P}^{(m)} = -\sigma_3. \quad (91c)$$

Thanks to the nature of the transform that produced them, all three operators have conveniently simple forms: $\mathbf{P}^{(m)}$ is invariant, $\mathbf{A}^{(m)} \propto \nu^{(m)}$ is diagonal, and $\mathbf{R}^{(m)} \propto \rho^{(m)}$ involves only one of the two off-diagonal Pauli operators σ_1, σ_2 . It would be too much to hope that the simplicity of Eq. (66d) would persist in a form like $\mathbf{E}^{(m)} = \nu^{(m)}\mathbf{1}$, and indeed it does not. But there is no physical reason why it should.

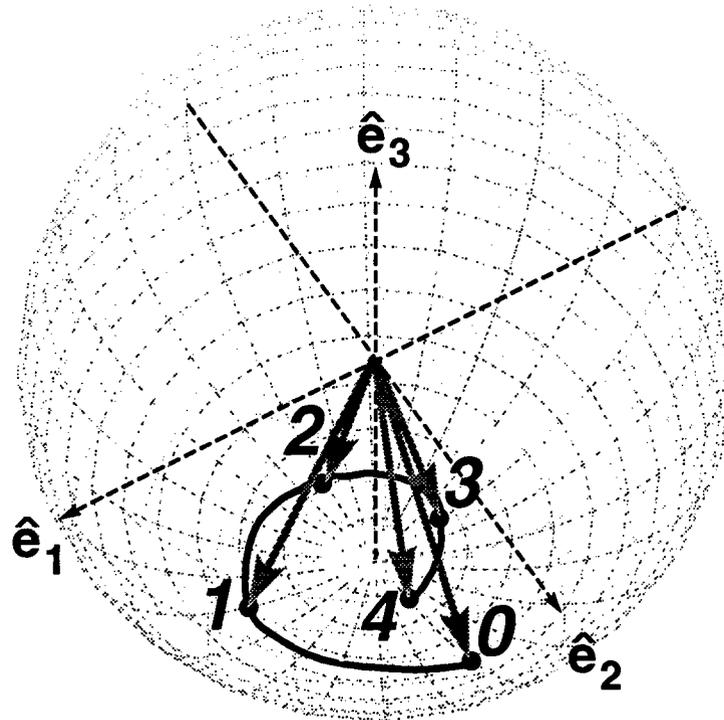


Fig. 1 – Pauli-space illustration of $\vec{G}^{(m)}$ for $m = 0 \dots 4$. Since $G_3^{(m)}$ is imaginary, the figure is only qualitative. The m th gray arrow has components $(G_1^{(m)}, G_2^{(m)}, \Im G_3^{(m)})$.

Mode Separation

Suppose, for the moment, that the environment has an interval I where $\rho^{(m)}(x) = 0$. Then the generator is diagonal in that interval

$$\mathbf{G}^{(m)}(x) = -i\nu^{(m)}(x)\sigma_3 \quad \dots \quad x \in I$$

and so is the propagator

$$\mathbf{K}^{(m)}(x, x_0) = \exp \left\{ -i\sigma_3 \int_{x_0}^x d\zeta \nu^{(m)}(\zeta) \right\} \quad \dots \quad x, x_0 \in I,$$

so that the state vector separates exactly into a sum of counter-propagating modes

$$\mathbf{u}^{(m)}(x) = \mathbf{a}^{(m)}(x) + \mathbf{b}^{(m)}(x), \quad (92)$$

where

$$\mathbf{a}^{(m)}(x) = u_-^{(m)}(x_0) \exp \left[+i \int_{x_0}^x d\zeta \nu^{(m)}(\zeta) \right] |-\rangle \quad (93a)$$

$$\mathbf{b}^{(m)}(x) = u_+^{(m)}(x_0) \exp \left[-i \int_{x_0}^x d\zeta \nu^{(m)}(\zeta) \right] |+\rangle. \quad (93b)$$

It is easy to confirm that the power flux is partitioned between these modes

$$\bar{P}(\mathbf{a}^{(m)} + \mathbf{b}^{(m)}) = \bar{P}(\mathbf{a}^{(m)}) + \bar{P}(\mathbf{b}^{(m)})$$

and separately conserved

$$\begin{aligned}\bar{P}(\mathbf{a}^{(m)}(x)) &= \bar{P}(\mathbf{a}^{(m)}(x_0)) = +c_0\gamma|u_-^{(m)}(x_0)|^2 \\ \bar{P}(\mathbf{b}^{(m)}(x)) &= \bar{P}(\mathbf{b}^{(m)}(x_0)) = -c_0\gamma|u_+^{(m)}(x_0)|^2.\end{aligned}$$

This result is exact but, of course, it is not general because the condition $\rho^{(m)}(x) = 0$ limits its validity to a particular type of environment. The $m = 1$ case was encountered in section 5, where $\rho^{(1)}(x) = 0$ was seen to imply a uniform medium having $n(x) = n(x_0)$, with standard d'Alembert mode separation prevailing everywhere. The limitation is even greater for $m > 1$. For example, $\rho^{(2)}(x) = 0$ presupposes a medium where $n^{-1}(x) - n(x_0)^{-1} = (x - x_0)g$ for some constant g . This, in turn, means that $0 < n(x) < \infty$ is possible only on the semi-infinite interval $I = \{x | (x - x_0)gn(x_0) > 0\}$. This is just another reminder that, except for tailor-made special cases, mode separation is an approximate result, not an exact one.

Higher-Order Bremmer Series

In parallel to section 5, the initial-value problem for $\mathbf{u}^{(m)}$ can be solved via the $\mathbf{A}^{(m)}$ interaction representation. The eigenvectors of $\mathbf{A}^{(m)}$ are still $|\zeta\rangle$, and the counterpart of Eq. (83) for the components of the interaction-representation state vector is again a Bremmer series,

$$\begin{aligned}q_\zeta(x) &= q_\zeta(x_0) + \int_{x_0}^x dx_1 \rho^{(m)}(x_1) \exp\left[+2\zeta i\varphi^{(m)}(x_1, x_0)\right] q_{-\zeta}(x_0) \\ &\quad + \int_{x_0}^x dx_2 \int_{x_0}^{x_2} dx_1 \rho^{(m)}(x_2) \rho^{(m)}(x_1) \exp\left[+2\zeta i\varphi^{(m)}(x_2, x_1)\right] q_\zeta(x_0) + \dots\end{aligned}\quad (94)$$

The first term in the asymptotic expansion of this m th-order Bremmer series for small $\rho^{(m)}$ is again just the leading term in the series,

$$u_\zeta^{(m)}(x) \sim \exp\left[-\zeta i\varphi^{(m)}(x, x_0)\right] q_\zeta(x_0) \quad \dots \quad \zeta = \pm. \quad (95)$$

This is a higher-order asymptotic approximation for one-way propagation.

7. EXPANSION IN ϵ DERIVATIVES

This section introduces a smallness criterion for spatial derivatives of ϵ that renders the m th-order Bremmer representation's generator diagonal to order ϵ^m , thus eliminating backscatter to that order. Further, it obtains the resulting x -dependent amplitude and phase of the field and interprets each of these as having a contribution that accumulates along the propagation path and another contribution from the path's endpoints.

If the environmental variations are adiabatic in the sense that $x \sim \epsilon^{-1}$, then one should expect that

$$d_x^m \epsilon \sim \epsilon^{m+1}. \quad (96)$$

Since $\tanh \psi^{(0)} = \epsilon/(1 + \epsilon)$ and $\tanh \psi^{(1)} = d_x \epsilon / 2n$, one would have

$$\begin{aligned}\tanh \psi^{(0)} &\sim \epsilon \\ \tanh \psi^{(1)} &\sim \epsilon^2\end{aligned}$$

and, indeed, for any order m ,

$$\tanh \psi^{(m)} \sim \epsilon^{m+1} . \quad (97)$$

The symbolic mathematics system Maple® has been used to confirm through $m = 5$ that, assuming Eq. (96),

$$\tanh \psi^{(m)} = 2^{-m} d_x^m \epsilon + O(\epsilon^{m+2}) ,$$

which provides a direct verification of Eq. (97). This means that, as m increases, $\rho^{(m)}$ grows steadily smaller in relation to $\nu^{(m)}$ in the sense that $\rho^{(m)}/\nu^{(m)} \sim \epsilon^{m+1}$. Thus, under these assumptions, $\mathbf{G}^{(m)}$ is diagonal to order ϵ^m .

The notation $\zeta^{(m)}$ has been used generally for any quantity ζ in the m th representation. When the ϵ series for $\zeta^{(m)}$ is truncated at the m th order, the result will be denoted $\zeta^{[m]}$. For the generator $\mathbf{G}^{(m)}$, this is

$$\mathbf{G}^{[m]} = -i\nu^{[m]}\sigma_3 , \quad (98)$$

where $\nu^{[m]}$ consists of all the terms of $\nu^{(m)}$ up through order ϵ^m , i.e., $\nu^{(m)} = \nu^{[m]} + O(\epsilon^{m+1})$. Since Eq. (98) is diagonal, the evolution that it generates can be found by a trivial integration, *provided* that the function $\nu^{[m]}(x)$ is known. As m grows larger, the calculation of $\nu^{[m]}$ becomes an increasingly intricate task, but one that reduces to a fixed pattern of routine operations — an ideal job for symbolic computation software. Maple has been used to generate the result out to $m = 6$. (Farther, actually, but this has to be stopped somewhere.) The result can be expressed as

$$\begin{aligned}\nu &= 1 + \epsilon - \frac{1}{2}\epsilon^2 + \frac{1}{2}\epsilon^3 \\ &\quad - \left(\frac{5}{8}\epsilon^4 + \frac{1}{8}\epsilon^2\right) + \left(\frac{7}{8}\epsilon^5 + \frac{5}{8}\epsilon\epsilon^2\right) - \left(\frac{21}{16}\epsilon^6 + \frac{35}{16}\epsilon^2\epsilon^2 + \frac{1}{32}\epsilon^2\right) + O(\epsilon^7) ,\end{aligned} \quad (99)$$

with $\nu^{[m]}$ found by simply truncating ν at the m th order. Maple has also been used to verify that $\rho^{[m]} = 0 = \psi^{[m]}$.

Cumulative Contribution

With $\nu^{[m]}(x)$ in hand, it is a trivial matter to solve the problem approximated at order m ,

$$d_x \mathbf{u}^{(m)} = \mathbf{G}^{[m]} \mathbf{u}^{(m)} . \quad (100)$$

The state vector has the separated form

$$\mathbf{u}^{(m)} = \mathbf{a}^{(m)} + \mathbf{b}^{(m)} ,$$

where the modes are

$$\mathbf{a}^{(m)}(x) = u_+^{(m)}(x_0) \exp\left(+i\varphi^{[m]}(x, x_0)\right) |-\rangle \quad (101a)$$

$$\mathbf{b}^{(m)}(x) = u_-^{(m)}(x_0) \exp\left(-i\varphi^{[m]}(x, x_0)\right) |+\rangle \quad (101b)$$

in terms of the phase function

$$\varphi(x, x_0) = \int_{x_0}^x d\xi \nu(\xi) . \quad (102)$$

($\varphi^{[m]}$ is formed in the usual way, by using $\nu^{[m]}$ as the integrand.) A few points should be noted here:

1. The important quantity here is this phase, specifically the deviation from $\varphi^{[0]}(x, x_0) = x - x_0$ (its value in a uniform medium with $n = 1$).
2. The even-order contributions to $\nu^{[m]} - \nu^{[0]}$ are all negative. For $x - x_0 > 0$ (< 0), this means that all the even-order contributions to $\varphi^{[m]}$ serve to retard (advance) the phase in a strictly *cumulative* way.
3. The odd-order contributions to $\nu^{[m]}$ do not have definite signs (thanks to their odd powers of ϵ) so they are likely to do quite a lot of zero-crossing when $|x - x_0|$ is large enough. In that event, their contributions to $\varphi^{[m]}$ should oscillate about zero rather than accumulating.
4. Comparison of Eq. (99) to the Taylor series for the refractive index,

$$n = 1 + \epsilon - \frac{1}{2}\epsilon^2 + \frac{1}{2}\epsilon^3 - \frac{5}{8}\epsilon^4 + \frac{7}{8}\epsilon^5 - \frac{21}{16}\epsilon^6 + O(\epsilon^7)$$

shows that ν begins to deviate from n at order ϵ^4 . Thus the WKB phase approximation — the consequence of invoking the estimate $\nu \approx n$ in the phase integrand — begins to depart from the above results at fourth order.

Endpoint Contribution

The procedure detailed above yields $\mathbf{u}^{(m)}$, the state vector in the m th transformed representation. That still has to be transformed back to the d'Alembert (0-th) representation via

$$\mathbf{u}^{(0)} = \mathbf{W}^{(m)} \mathbf{u}^{(m)} , \quad (103)$$

where

$$\mathbf{W}^{(m)} = \mathbf{M}^{(0)} \mathbf{M}^{(1)} \dots \mathbf{M}^{(m-1)} . \quad (104)$$

So $\mathbf{W}^{(m)}$ needs to be calculated. Of course, since it is going to be applied to $\mathbf{u}^{(m)}$, the m th order estimated state vector that results from approximating $\mathbf{G}^{(m)}$ by $\mathbf{G}^{[m]}$, a suitable approximation for $\mathbf{W}^{(m)}$ will do. But what is “suitable”? A knee-jerk option might be $\mathbf{W}^{[m]}$, the transform truncated at the same order as the generator. On consideration, however, that appears to be overdoing it. The phase deviation $\varphi^{[m]} - \varphi^{[0]}$ embodies the effects of environmental nonuniformities accumulated throughout the propagation from $\xi = x_0$ to $\xi = x$. But the back-transform $\mathbf{W}^{(m)}$ is not cumulative; it depends only on environmental conditions at the final point $\xi = x$. It might be sufficient to approximate it by $\mathbf{W}^{[\ell]}$ for some $\ell < m$. We proceed for the moment with $\mathbf{W}^{[\ell]}$.

The unitary transform in Eq. (41) needs to be applied to return to the initial representation (where the first component of the state vector was simply the string displacement and the second was the slope of its tangent)

$$\underline{\mathbf{a}} = \mathbf{U}\mathbf{a}^{(0)} = \mathbf{U}\mathbf{W}^{[\ell]}\mathbf{a}^{(\ell)} \quad (105a)$$

and

$$\underline{\mathbf{b}} = \mathbf{U}\mathbf{b}^{(0)} = \mathbf{U}\mathbf{W}^{[\ell]}\mathbf{b}^{(\ell)}. \quad (105b)$$

In view of Eqs. (93) and (101), only the matrix elements $\langle +|\mathbf{U}\mathbf{W}^{[\ell]}|+\rangle$ and $\langle +|\mathbf{U}\mathbf{W}^{[\ell]}|-\rangle$ are needed to obtain the displacement fields for the left- and right-going d'Alembert modes, respectively. Another resort to Maple yields

$$\langle +|\mathbf{U}\mathbf{W}^{[\ell]}|+\rangle = \frac{Q^{[\ell]}}{\sqrt{2}} e^{+i\vartheta^{[\ell]}} \quad (106a)$$

$$\langle +|\mathbf{U}\mathbf{W}^{[\ell]}|-\rangle = \frac{Q^{[\ell]}}{\sqrt{2}} e^{-i\vartheta^{[\ell]}} , \quad (106b)$$

where the phase is

$$\vartheta = \frac{1}{4}\dot{\epsilon} - \frac{3}{4}\epsilon\dot{\epsilon} + \left(\frac{15}{8}\epsilon^2\dot{\epsilon} + \frac{1}{16}\ddot{\epsilon} \right) + O(\epsilon^5) , \quad (107)$$

and the amplitude term is

$$Q = 1 - \frac{1}{2}\epsilon + \frac{5}{8}\epsilon^2 - \left(\frac{15}{16}\epsilon^3 - \frac{1}{8}\ddot{\epsilon} \right) + \left(\frac{195}{128}\epsilon^4 - \frac{9}{16}\epsilon\ddot{\epsilon} - \frac{5}{16}\dot{\epsilon}^2 \right) + O(\epsilon^5) . \quad (108)$$

The endpoint phase vanishes to first order, $\vartheta^{[1]} = 0$. When the endpoint x lies in a uniform region (where n is constant, but not necessarily 1), the phase vanishes entirely, and if $n = 1$ the amplitude term also reduces to unity. Comparison of Eq. (108) to the power series

$$n^{-1/2} = 1 - \frac{1}{2}\epsilon + \frac{5}{8}\epsilon^2 - \frac{15}{16}\epsilon^3 + \frac{195}{128}\epsilon^4 + O(\epsilon^5) \quad (109)$$

shows that the standard WKB amplitude expression $Q \approx 1/\sqrt{n}$ is valid only through order ϵ^2 . It might be guessed that $Q \approx 1/\sqrt{\nu}$ would be an improvement on that, but the ϵ -series

$$\nu^{-1/2} = 1 - \frac{1}{2}\epsilon + \frac{5}{8}\epsilon^2 - \frac{15}{16}\epsilon^3 + \left(\frac{195}{128}\epsilon^4 + \frac{1}{16}\dot{\epsilon}^2 \right) + O(\epsilon^5)$$

shows that it, too, is valid only through order ϵ^2 .

Conclusion

The final result for the string displacement field is

$$u(x) = \frac{Q^{[\ell]}(x)}{\sqrt{2}} \left(u_+^{(m)}(x_0) \exp \left\{ +i[\varphi^{[m]}(x, x_0) - \vartheta^{[\ell]}(x)] \right\} + u_-^{(m)}(x_0) \exp \left\{ -i[\varphi^{[m]}(x, x_0) - \vartheta^{[\ell]}(x)] \right\} \right), \quad (110)$$

where m is the ‘‘cumulative’’ order and $\ell \leq m$ is the ‘‘endpoint’’ order.

8. EXAMPLE

This section introduces a specific weakly nonuniform medium and presents a numerical example of 4th-order, non-WKB phase accumulation.

Consider a class of environments characterized by a periodic inhomogeneity of the form

$$\epsilon(x) = Ag \sin(ax) + Bg \sin(bgx). \quad (111)$$

As an example, take the case where $(A, B, a, b, g) = (1.0, 0.4, 1.0, 0.8, 0.1)$. Figure 2 illustrates the first- through fourth-order contributions to Eq. (99), namely,

$$\begin{aligned} & \text{first-order index contribution} \cdots +\epsilon \\ & \text{second-order index contribution} \cdots -\frac{1}{2}\epsilon^2 \\ & \text{third-order index contribution} \cdots +\frac{1}{2}\epsilon^3 \\ & \text{fourth-order index contribution} \cdots \underbrace{-\frac{5}{8}\epsilon^4}_{\text{WKB}} \underbrace{-\frac{1}{8}\epsilon^2}_{\text{non-WKB}} \end{aligned}$$

plotted from top to bottom in the figure. As should be expected, this $\epsilon(x)$ exhibits spatial interference in the form of a pattern of beats in the top plot with a spacing

$$L \approx 2\pi/[(a - b)g] = 100\pi,$$

and the second through fourth orders follow suit. The amplitude of the beats in the m th order is $g^m = 10^{-m}$, with the odd orders being about equally positive and negative, and the even orders purely negative. In the bottom plot, the small non-WKB part of the fourth-order contribution is shown along with the total.

Figure 3 shows the phase contributions according to Eq. (102). Each plot results from integrating the corresponding plot in Fig. 2 from $x_0 = 0$ to x . Their behavior is as anticipated: the odd orders oscillate around small ‘dc’ values; the even orders decrease monotonically, contributing steadily accumulating phase retardations. In the even case, the phase retardation rate drops sharply with increasing order. In the bottom plot, the WKB and non-WKB parts of the fourth-order contribution are shown in addition to the total. In that plot, the rate of non-WKB phase retardation is about 15% of the WKB rate, which is itself only about 1.5% of the second-order rate. Clearly, fourth-order effects could be prominent only at long ranges. In fact, it is only when ranges

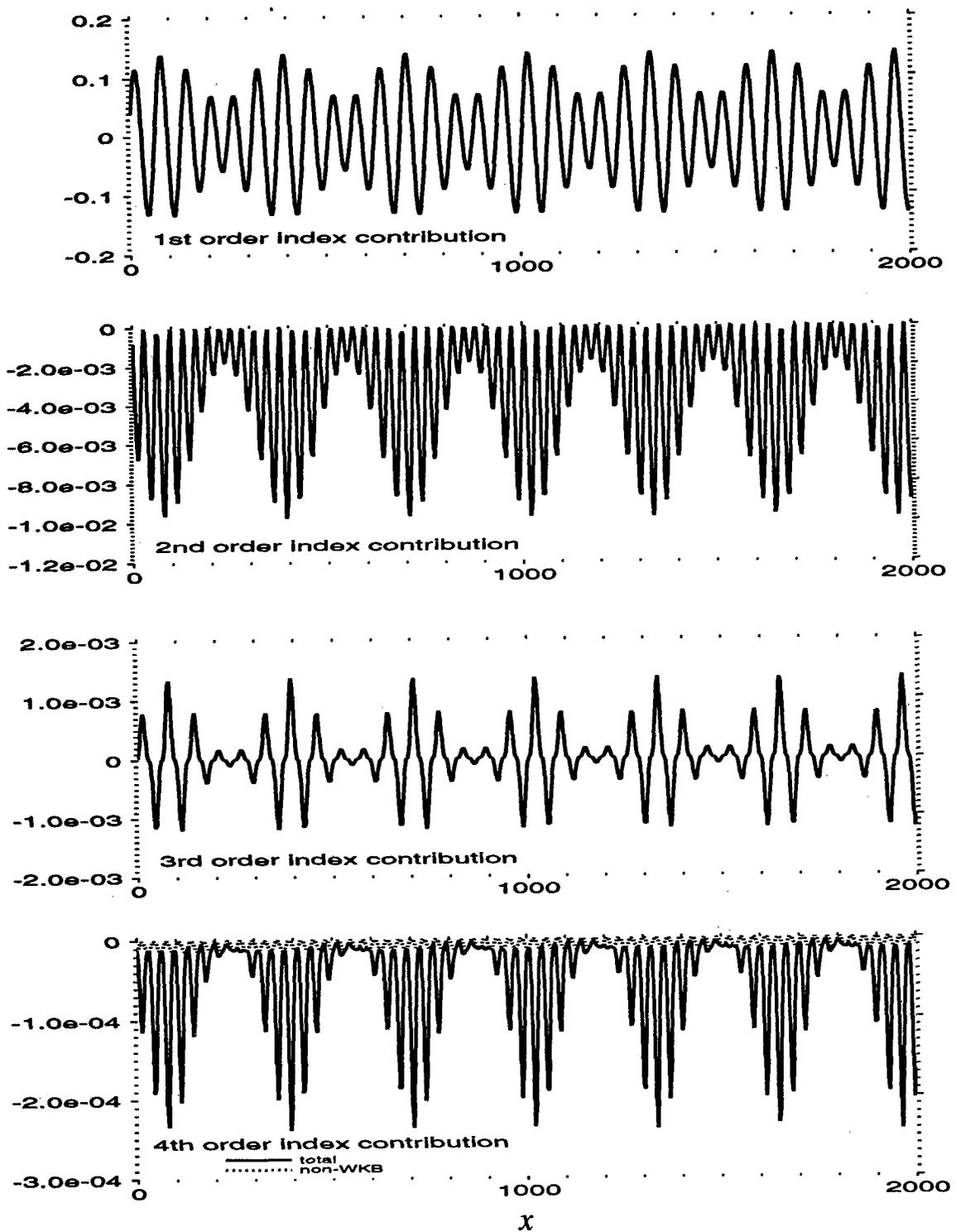


Fig. 2 - Index contributions to Eq. (99) for the example described in the text. Plots contain 500 points each and are computed at 20-digit precision.

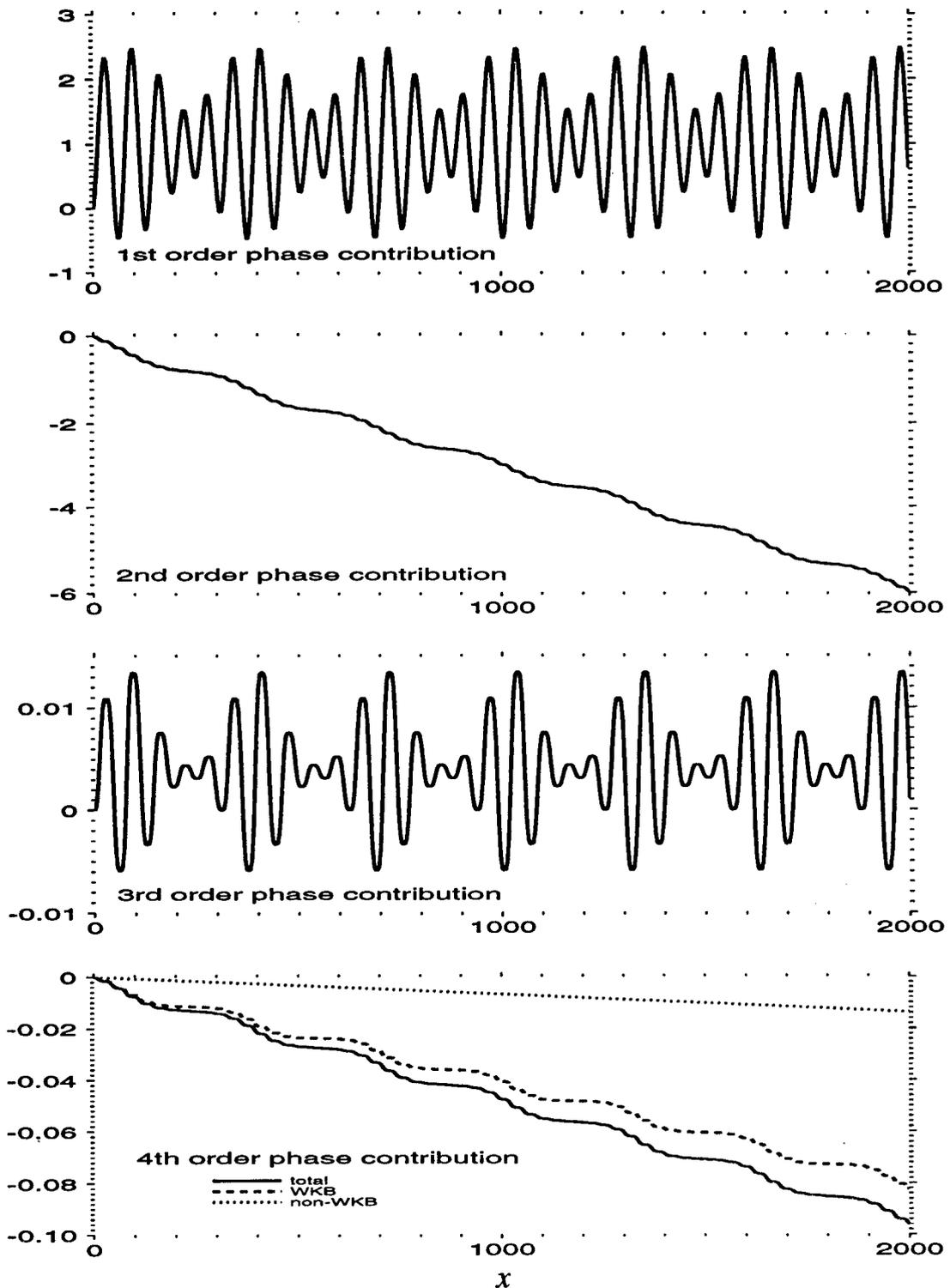


Fig. 3 – Phase contributions to Eq. (102) for the example described in the text. Plots contain 500 points each and are computed using 20-digit precision. (The tiny ripples in the even orders do not seem to be artificial. They look the same when computed with 10-digit precision.)

of $x \approx 224,000 \approx 714L$ are reached that the fourth-order non-WKB phase contribution reaches $-\pi/2$. At that range, the WKB contribution to the fourth-order phase is -3π , while the second-order contribution is approximately $-214\pi = 107 * (-2\pi)$. The example serves to underscore the following points:

- For situations that demand the relative phase of the signal at points only a few dozen wavelengths apart ($\Delta x \approx 10$ to 100), fourth-order phase corrections are quite small. In practice, a first-order estimate will usually be accurate enough.
- When the demand is for accurate phase values at very long ranges (e.g., in some long-range interferometry and long time-of-flight applications), fourth-order phase estimation, including the non-WKB contribution, may be indicated.

9. DISCUSSION

For the one-dimensional case of interest here, it has been shown that a properly chosen series of pseudo-unitary transforms converts the equation for the dynamic evolution of the wave field — the Helmholtz equation in this case — to a far more tractable (in fact, diagonal) approximate form. This can be done to any desired order m in the small environmental inhomogeneity $\epsilon(x)$. The resulting equation can be integrated immediately to provide m th-order expressions for the amplitude and phase of the wave field at long range. An inherent part of this construct is that backscatter is neglected at all orders so that the field consists of a pair of asymptotically decoupled counter-propagating modes.

The approach taken in sections 6 and 7 is not without historical precedent. Most notable is the 1950 application by Foldy and Wouthuysen [9] of such methods in quantum physics to obtain the Schrödinger equation from its relativistic precursor, the Klein-Gordon equation. More recently, Wurmser et al. [12] brought these techniques to bear on a case of classical wave motion in which the medium is also allowed to vary in directions *transverse* to the direction of propagation (e.g., along y as well as x). The resulting two-dimensional Helmholtz equation (Eq. (32a) with $d_x^2 \rightarrow d_x^2 + d_y^2$) leads to a d'Alembert representation of the dynamics that is similar to Eq. (42a) except that ϵ is a differential operator in y . The upshot is a pair of asymptotically decoupled parabolic equations for propagation in the $\pm x$ directions. These involve fourth-order non-WKB “corrections” to the refractive index like those seen here. They also contain novel features related to the additional transverse degree of freedom, notably a classical analog of the quantum mechanical phenomenon of *Zitterbewegung* [8].

Bremmer originally developed the representation of section 5, Eq. (83) in particular, by different means [11]. He first “stratified” the medium, approximating the refractive index by a piecewise constant staircase function; then he accounted for all the multiple reflections at each discontinuity; and finally, he took the limit of infinitely many steps of vanishing height. This “infinitesimal” approach is perfectly valid and can lead to physical insights [13]. It has been avoided here only because it is difficult to generalize.

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Appendix A

PAULI OPERATORS

Pauli matrices are used to facilitate the analysis throughout the body of this work. This section reviews their properties — especially their role as infinitesimal generators of rotation transforms in state space.

The Pauli spin matrices⁶

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = i \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (\text{A1})$$

have seen long service as a labor-saving device in quantum mechanics and will prove useful here also. Although certainly not essential, they do have some attributes that reduce the work involved in doing linear algebra on complex two-dimensional state spaces, e.g.,

$$\begin{aligned} \text{trace } \sigma_j &= 0 & \sigma_j^2 &= 1 \\ \det \sigma_j &= -1 & \sigma_j^\dagger &= \sigma_j \end{aligned}$$

In addition, the eigen-basis of σ_3 :

$$\sigma_3 |\varsigma\rangle = \varsigma |\varsigma\rangle \quad \dots \quad \varsigma = \pm$$

where

$$|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

is convenient for representing complex vectors

$$\mathbf{q} = \sum_{\varsigma=\pm} q_\varsigma |\varsigma\rangle.$$

The main advantage of Pauli operators, however, relates to the representation of linear transforms.

Pauli Space

The three Pauli operators are complete in the sense that, together with the unit matrix, they form a basis for complex 2-by-2 matrix operators. Any such operator can be represented as

$$\mathbf{V} = V_0 \mathbf{1} + V_1 \sigma_1 + V_2 \sigma_2 + V_3 \sigma_3 \quad (\text{A2a})$$

⁶No distinction is observed between the operators themselves and their matrix representation.

in terms of the four coefficients

$$V_0 = \text{trace}(\mathbf{V})/2 \quad (\text{A2b})$$

$$V_j = \text{trace}(\mathbf{V}\sigma_j + \sigma_j\mathbf{V})/4 \quad \dots \quad j = 1, 2, 3, \quad (\text{A2c})$$

all of which have real values if \mathbf{V} is Hermitian. In brief,

$$\mathbf{V} = V_0\mathbf{1} + \vec{V} \cdot \vec{\sigma}, \quad (\text{A3})$$

where

$$\vec{\sigma} = \sigma_1\hat{e}_1 + \sigma_2\hat{e}_2 + \sigma_3\hat{e}_3 \quad (\text{A4a})$$

$$\vec{V} = V_1\hat{e}_1 + V_2\hat{e}_2 + V_3\hat{e}_3 \quad (\text{A4b})$$

are vectors in an abstract three-dimensional 'Pauli space'. The original operator is equivalent to a scalar part V_0 and a Pauli-vector part \vec{V} . A magnitude and direction can be defined for this vector part through $V = (\vec{V} \cdot \vec{V})^{1/2}$ and $\hat{v} = \vec{V}/V$, although these need not generally be real valued.

Products and Exponentials

Products and exponentials of Pauli operators can be evaluated by using the fundamental combination rule

$$\sigma_j\sigma_k = i\epsilon_{jkl}\sigma_l + \delta_{jk}\mathbf{1} \quad (\text{A5})$$

and its various spinoffs [A1] such as

$$(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = (\vec{a} \cdot \vec{b})\mathbf{1} + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma} \quad (\text{A6})$$

and

$$\exp(\pm iS\hat{s} \cdot \vec{\sigma}) = \cos(S)\mathbf{1} \pm i\sin(S)\hat{s} \cdot \vec{\sigma}. \quad (\text{A7})$$

Similarity Transforms as Pauli-Space Rotations

For any Hermitian operator \mathbf{S} , the result of using the unitary operator $\exp(-i\mathbf{S})$ to perform a similarity transformation

$$\mathbf{V}' = \exp(+i\mathbf{S})\mathbf{V}\exp(-i\mathbf{S}) \quad (\text{A8})$$

on the \mathbf{V} of Eq. (A3) is necessarily an operator of the same form,

$$\mathbf{V}' = V'_0\mathbf{1} + \vec{V}' \cdot \vec{\sigma}. \quad (\text{A9})$$

Clearly, the scalar parts of \mathbf{S} and \mathbf{V} play only a trivial role in this (S_0 is irrelevant and V_0 is invariant), and the vector parts are related through

$$\vec{V}' \cdot \vec{\sigma} = \exp(+i\vec{S} \cdot \vec{\sigma})\vec{V} \cdot \vec{\sigma} \exp(-i\vec{S} \cdot \vec{\sigma}). \quad (\text{A10})$$

Expansion of the exponentials using Eq. (A7), followed by two applications of Eq. (A6) results in

$$\vec{V}' = \cos(2S) [\vec{V} - (\vec{V} \cdot \hat{s})\hat{s}] + \sin(2S)\vec{V} \times \hat{s} + (\vec{V} \cdot \hat{s})\hat{s} . \quad (\text{A11})$$

To clarify the form of this, let $S = -\phi/2$ and write $\vec{V} = V\hat{v}$ so that

$$\vec{V}' = V \{ \cos \phi [\hat{v} - (\hat{v} \cdot \hat{s})\hat{s}] - \sin \phi \hat{v} \times \hat{s} + (\hat{v} \cdot \hat{s})\hat{s} \} . \quad (\text{A12})$$

For a given \hat{v} , any choice of \hat{s} — provided it is not collinear with \hat{v} — determines a right-handed orthogonal Pauli-space basis $\hat{q}, \hat{r}, \hat{s}$ in the following way. Take \hat{r} to be the direction of $\hat{s} \times \hat{v}$, i.e., $\hat{s} \times \hat{v} = \sin \theta \hat{r}$ with $\theta = \angle(\hat{s}, \hat{v})$. Then, since \hat{v} is orthogonal to \hat{r} , it can be written as

$$\hat{v} = \sin \theta \hat{q} + \cos \theta \hat{s} ,$$

where $\hat{q} = \hat{r} \times \hat{s}$. Thus Eq. (A12) becomes

$$V' = V \quad (\text{A13a})$$

$$\hat{v}' = \sin \theta (\cos \phi \hat{q} + \sin \phi \hat{r}) + \cos \theta \hat{s} , \quad (\text{A13b})$$

which means that \vec{V}' is just a rotated version of \vec{V} . In standard spherical coordinates relative to the $\hat{q}, \hat{r}, \hat{s}$ axes, \hat{v}' is a unit vector with spherical angles (θ, ϕ) , whereas \hat{v} was a unit vector with spherical angles $(\theta, 0)$. Clearly, since $V_0' = V_0$ and $V' = V$, the entire $\mathbf{V} \rightarrow \mathbf{V}'$ transformation amounts to nothing more than a Pauli-space rotation of the vector part of \mathbf{V} about the direction \hat{s} through an angle $\phi = -2S$. Since \mathbf{S} is Hermitian, S_1, S_2, S_3 are all real, making the rotation angle real also.

If \mathbf{S} is not Hermitian, then the magnitude S , as defined above, can become imaginary, giving the unit vector \hat{s} both real and imaginary components. A more general class of "pseudo-Hermitian" \mathbf{S} operators (with real S_3 but imaginary S_1, S_2) is encountered below. The above result still applies, provided the rotation angle is allowed to be imaginary.

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Appendix B

RELATION TO THE BORN SERIES

This appendix relates the “Foldy-Wouthuysen” (FW) solution obtained in the body of the report to the solution achieved in a scattering context by the Born method. The two are shown to agree through second order.

Scattering Problem in Integral Form

The Helmholtz equation of interest is

$$d_x^2 u(x) + u(x) = -2\epsilon(x)u(x), \quad (\text{B1})$$

in the scaled x coordinate. A scattering problem is being considered, so there are no sources at finite x . The retarded Green’s function for a uniform medium (one with $\epsilon = 0$) is

$$g(x, y) = \frac{i}{2} e^{i|x-y|}. \quad (\text{B2})$$

It satisfies

$$d_x^2 g(x, y) + g(x, y) = -\delta(x - y) \quad (\text{B3})$$

and allows Eq. (B1) to be re-expressed, within any interval $a < x < b$, as

$$u(x) = [g(x, y)d_y u(y) - u(y)d_y g(x, y)]_{y=a}^{y=b} + \int_a^b dy 2g(x, y)\epsilon(y)u(y). \quad (\text{B4})$$

Bounded Scattering Region

For simplicity, suppose that all environmental nonuniformity lies in a bounded “scattering region” — specifically that the support of $\epsilon(x)$ is the finite interval $\ell < x < r$. Outside that interval the field must have the form

$$u(x) = \begin{cases} Ae^{+i(x-a)} + Be^{-i(x-a)} & \dots x \leq \ell \\ Ce^{+i(x-a)} + De^{-i(x-a)} & \dots r \leq x \end{cases} \quad (\text{B5})$$

where the point $x = a$ has been used for the (arbitrary) phase reference and A, B, C, D are parameters. One can always arrange for $A = 1$ and $D = 0$ by normalizing appropriately and taking the incident signal to come from the left. Then if $a \leq \ell$ and $r \leq b$, the $[\dots]_a^b$ term in Eq. (B4) reduces to $e^{i(x-a)}$, leaving

$$u(x) = e^{i(x-a)} + i \int_a^b dy e^{i|x-y|}\epsilon(y)u(y) \quad \dots a < x < b. \quad (\text{B6})$$

Now we rename $a = x_0$ and let $b \rightarrow \infty$ so that the integral equation to be solved is

$$u(x) = u_0(x) + i \int_{x_0}^{\infty} dy e^{i|x-y|} \epsilon(y) u(y) \quad \dots \quad x_0 < x < \infty, \quad (\text{B7})$$

given the incident signal $u_0(x) = e^{i(x-x_0)}$.

Born Method

The smallness of $\epsilon(x)$ suggests that one attempt to obtain the solution u as a Born series

$$u^B(x) = w_0(x) + w_1(x) + w_2(x) + \dots \quad (\text{B8})$$

with $w_n = O(\epsilon^n)$, starting with the incident field $w_0 = u_0$. Born's method obtains the partial sums, $u_n = w_0 + \dots + w_n$, of this series by iteration,

$$u_n(x) = u_0(x) + i \int_{x_0}^{\infty} dy e^{i|x-y|} \epsilon(y) u_{n-1}(y) \quad \dots \quad n > 0. \quad (\text{B9})$$

In other words, successive terms in the Born series, Eq. (B8), are generated via

$$w_n(x) = i \int_{x_0}^{\infty} dy e^{i|x-y|} \epsilon(y) w_{n-1}(y) \quad \dots \quad n > 0, \quad (\text{B10})$$

and the n th Born approximation is $u^B = u_n + O(\epsilon^{n+1})$.

Preliminaries

Before proceeding in that direction, it will be convenient to introduce some shorthand notation and a preliminary result.

Differentiation will be denoted by superscripts in parentheses,

$$q^{(n)}(x) = \frac{d^n q(x)}{dx^n} \quad \dots \quad n \geq 0, \quad (\text{B11})$$

which is a departure from the usage in the body of the report. ($n = 0$ is the trivial case $q^{(0)} = q$.) This will be extended to $n < 0$ so that, for example, $q^{(-1)}$ denotes the anti-derivative,

$$q^{(-1)}(x) = \int_{x_0}^x dy q(y). \quad (\text{B12})$$

In this notation, a typical Taylor series takes the form

$$q(x+y) = \sum_{n=0}^{\infty} \frac{y^n}{n!} q^{(n)}(x). \quad (\text{B13})$$

We will also need the following result:

$$\int_0^{\infty} dy e^{i2y} \frac{y^n}{n!} = \left(\frac{i}{2}\right)^{n+1}. \quad (\text{B14})$$

This may be obtained by first changing the integration variable to $t = 2y$, thereby converting the left-hand side to

$$\frac{1}{n! 2^{n+1}} \int_0^{\infty} dt e^{it} t^n.$$

For physical reasons⁷, that singular integral is to be understood as the $|\gamma| \rightarrow 0$ limit of

$$\int_0^{\infty} dt e^{-|\gamma|t} e^{it} t^n ,$$

which can be found in tables [B1]:

$$\int_0^{\infty} dt t^{\mu-1} e^{-|\gamma|t} e^{i\delta t} = \frac{\Gamma(\mu)}{(\delta^2 + \gamma^2)^{\mu/2}} e^{i\mu \arctan(\delta/|\gamma|)} \dots \Re(\mu) > -1, \quad |\gamma| > |\Im(\delta)| .$$

With $\mu = n + 1$ and $\delta = 1$, the $|\gamma| \rightarrow 0$ limit is $\Gamma(n + 1)e^{i(n+1)\pi/2} = n! i^{n+1}$, confirming Eq. (B14).

First Born Approximation

The first Born term is

$$w_1(x) = i \int_{x_0}^{\infty} dy e^{i(y-x_0+|x-y|)} \epsilon(y) ,$$

or, with the integration range partitioned at $y = x$,

$$w_1(x) = \underbrace{\left[i \int_{x_0}^x dy \epsilon(y) \right]}_{f(x)} e^{+i(x-x_0)} + \underbrace{\left[i \int_x^{\infty} dy e^{i2(y-x_0)} \epsilon(y) \right]}_{b(x)} e^{-i(x-x_0)} . \quad (\text{B15})$$

Outside the scattering region, where the functions f and b are constant, the significance of the two terms in Eq. (B15) is unambiguous. To the right (for $r < x$), b vanishes and the first term reduces to $f(+\infty)e^{+i(x-x_0)}$ where

$$f(+\infty) = i \int_{-\infty}^{\infty} dy \epsilon(y) ,$$

while to the left (for $x < \ell$), f vanishes and the second term reduces to $b(-\infty)e^{-i(x-x_0)}$ where

$$b(-\infty) = i \int_{-\infty}^{\infty} dy e^{i2(y-x_0)} \epsilon(y) .$$

On the right side of the scattering region, w_1 is a constant-amplitude wave that moves to the right; on the left, it has a different constant amplitude and moves to the left. Note also that for $x < \ell$,

$$u_1(x) = e^{i(x-x_0)} + e^{-i(x-x_0)} i \int_{-\infty}^{\infty} dy e^{i2y} \epsilon(y) .$$

In terms of the unscaled lengths $X = x/k_0$, $Y = y/k_0$, this is

$$u_1(X) = e^{-ik_0 X_0} \{ e^{ik_0 X} + [ik_0 \tilde{\epsilon}(2k_0)] e^{-ik_0 X} \} ,$$

in which the $[\dots]$ factor is recognizable as the first-order Born reflection coefficient expressed in the standard way [B2] as a Fourier transform $\tilde{\epsilon}(\kappa) = \int_{-\infty}^{+\infty} dY e^{i\kappa Y} \epsilon(Y)$.

⁷ $|\gamma|$ embodies the effect of attenuation in the medium.

But we are interested mainly in the field *within* the scattering region, where w_1 does not yield to any such simple, unambiguous reduction into forward and backward components. In the scattering region, however, Eq. (B15) can be written

$$w_1(x) = w_0(x) \left[i \int_{x_0}^x dy \epsilon(y) + i \int_0^\infty dy e^{i2y} \epsilon(x+y) \right]. \quad (\text{B16})$$

Then, with $\epsilon(x+y) = [\epsilon(x+y) - \epsilon(x)] + \epsilon(x)$ in the second integrand and with $\int_0^\infty dy e^{i2y} = i/2$ (Eq. (B14) with $n = 0$), one has

$$w_1(x) = w_0(x) \left\{ \underbrace{i \int_{x_0}^x dy \epsilon(y) - \frac{1}{2} \epsilon(x)}_{\mu} + \underbrace{i \int_0^\infty dy e^{i2y} [\epsilon(x+y) - \epsilon(x)]}_{\nu} \right\}. \quad (\text{B17})$$

This form emphasizes the fact that w_1 can always be regarded, without any approximation at all, as a forward-propagating carrier $w_0(x) = \exp\{i(x - x_0)\}$ with an x -dependent modulation $\mu + \nu$. It also suggests that, although $\mu \sim \epsilon$, it may be possible, when ϵ is a slowly varying function, to relegate ν to the $O(\epsilon^2)$ terms so that it contributes nothing to the Born approximation at this order. The remainder of this appendix is basically a systematic pursuit of this possibility through first and second order.

When $\epsilon(x+y)$ in the second integrand in Eq. (B16) is expanded in a Taylor series about $y = 0$, and Eq. (B14) is used to evaluate the resulting $\int_0^\infty dy e^{i2y} y^n/n!$ terms, the outcome is

$$w_1/w_0 = i \sum_{n=-1}^{\infty} \left(\frac{i}{2}\right)^{n+1} \epsilon^{(n)}. \quad (\text{B18})$$

(Note that μ comes from $n = -1, 0$ and ν from $n \geq 1$.) Thus the first Born partial sum is given by

$$u_1/w_0 = 1 + i \sum_{n=-1}^{\infty} \left(\frac{i}{2}\right)^{n+1} \epsilon^{(n)}, \quad (\text{B19})$$

i.e.,

$$u_1(x) = e^{i(x-x_0)} \left[1 + i \int_{x_0}^x dy \epsilon(y) - \frac{1}{2} \epsilon(x) + i \sum_{n=1}^{\infty} \left(\frac{i}{2}\right)^{n+1} \epsilon^{(n)}(x) \right]. \quad (\text{B20})$$

With

$$\epsilon^{(-1)} \sim \epsilon, \quad (\text{B21})$$

the first Born approximation $u^B = u_1 + O(\epsilon^2)$ can then be written

$$u^B(x) = e^{i(x-x_0)} \left[\left(1 - \frac{1}{2} \epsilon(x)\right) e^{i \int_{x_0}^x dy \epsilon(y)} + i \sum_{n=1}^{\infty} \left(\frac{i}{2}\right)^{n+1} \epsilon^{(n)}(x) \right] + O(\epsilon^2), \quad (\text{B22})$$

but that is as far as one can go without some knowledge of the behavior of the derivative terms in the remaining sum. If, as in section 7, one assumes that

$$\epsilon^{(n)} \sim \epsilon^{n+1} \quad \dots \quad n > 0, \quad (\text{B23})$$

then all of them belong with the $O(\epsilon^2)$ terms and one has

$$u^B(x) = \left(1 - \frac{1}{2}\epsilon(x)\right) e^{i \int_{x_0}^x dy [1+\epsilon(y)]} + O(\epsilon^2). \quad (\text{B24})$$

Term-by-term comparison with the first-order form of Eq. (110), namely,

$$u^{FW}(x) = Q^{[1]}(x) e^{-i\vartheta^{[1]}(x)} e^{i\varphi^{[1]}(x, x_0)} + O(\epsilon^2), \quad (\text{B25})$$

confirms that they agree through first order,

$$u^B - u^{FW} = O(\epsilon^2). \quad (\text{B26})$$

Second Born Approximation

The second Born series term is given by the double integral

$$w_2(x)/w_0(x) = - \int_{x_0}^{\infty} dy \int_{x_0}^{\infty} dz E(y, z) \quad (\text{B27})$$

with the integrand⁸

$$E(y, z) = e^{i\{|y-x|+|z-y|+(z-x)\}} \epsilon(y)\epsilon(z). \quad (\text{B28})$$

When the integration ranges are partitioned at $y = x$ and $z = y$, this becomes

$$w_2/w_0 = -(a + b + c + d) \quad (\text{B29})$$

in terms of the four quantities

$$a(x) = \int_{x_0}^x dy \int_y^{\infty} dz e^{i2(z-y)} \epsilon(y)\epsilon(z) \quad (\text{B30a})$$

$$b(x) = \int_{x_0}^x dy \int_{x_0}^y dz \epsilon(y)\epsilon(z) \quad (\text{B30b})$$

$$c(x) = \int_x^{\infty} dy \int_{x_0}^y dz e^{i2(y-x)} \epsilon(y)\epsilon(z) \quad (\text{B30c})$$

$$d(x) = \int_x^{\infty} dy \int_y^{\infty} dz e^{i2(z-x)} \epsilon(y)\epsilon(z) \quad (\text{B30d})$$

which will now be evaluated in turn.

The a term is

$$a(x) = \int_{x_0}^x dy \epsilon(y) \int_0^{\infty} dz e^{i2z} \epsilon(y+z) \quad (\text{B31a})$$

$$= \int_{x_0}^x dy \epsilon(y) \sum_{n=0}^{\infty} \epsilon^{(n)}(y) \left[\int_0^{\infty} dz e^{i2z} \frac{z^n}{n!} \right] \quad (\text{B31b})$$

$$= \sum_{n=0}^{\infty} \left(\frac{i}{2}\right)^{n+1} \alpha_n(x) \quad (\text{B31c})$$

⁸ E 's x dependence is left implicit.

where expanding $\epsilon(y + z)$ in a Taylor series about $z = 0$ produces Eq. (B31b), and Eq. (B31c) comes from evaluating $[\dots]$ via Eq. (B14) and using the definition

$$\alpha_n(x) = \int_{x_0}^x dy \epsilon(y) \epsilon^{(n)}(y) . \quad (\text{B32})$$

The b term is, with no approximation,

$$b(x) = \frac{1}{2} \left[\int_{x_0}^x dy \epsilon(y) \right]^2 . \quad (\text{B33})$$

The c term is

$$c(x) = \int_x^\infty dy e^{i2(y-x)} \gamma(y) \quad (\text{B34a})$$

$$= \int_0^\infty dy e^{i2y} \gamma(x + y) \quad (\text{B34b})$$

$$= \sum_{n=0}^\infty \gamma^{(n)}(x) \left[\int_0^\infty dy e^{i2y} \frac{y^n}{n!} \right] \quad (\text{B34c})$$

$$= \sum_{n=0}^\infty \left(\frac{i}{2} \right)^{n+1} \gamma^{(n)}(x) \quad (\text{B34d})$$

where the definition

$$\gamma(x) = \epsilon(x) \int_{x_0}^x dy \epsilon(y) \quad (\text{B35})$$

is used in Eq. (B34a), then expanding $\gamma(x + y)$ about $y = 0$ produces Eq. (B34c), and evaluation of $[\dots]$ through Eq. (B14) produces Eq. (B34d).

The d term is

$$d(x) = \int_x^\infty dy e^{i2(y-x)} a^{(1)}(y) \quad (\text{B36a})$$

$$= \int_0^\infty dy e^{i2y} a^{(1)}(x + y) \quad (\text{B36b})$$

$$= \sum_{\ell=0}^\infty \sum_{n=0}^\infty \left(\frac{i}{2} \right)^{n+1} \alpha_n^{(\ell+1)}(x) \left[\int_0^\infty dy e^{i2y} \frac{y^\ell}{\ell!} \right] \quad (\text{B36c})$$

$$= \sum_{n=0}^\infty \sum_{\ell=0}^\infty \left(\frac{i}{2} \right)^{n+\ell+2} \alpha_n^{(\ell+1)}(x) \quad (\text{B36d})$$

$$= \sum_{n=0}^\infty \left(\frac{i}{2} \right)^{n+2} \sum_{\ell=0}^n \alpha_{n-\ell}^{(\ell+1)}(x) \quad (\text{B36e})$$

where expanding $a^{(1)}(x + y)$ about $y = 0$ and using the definition Eq. (B32) produce Eq. (B36c), then evaluating $[\dots]$ using Eq. (B14) produces Eq. (B36d), and summation in an alternate order yields Eq. (B36e).

The second Born partial sum is given by

$$u_2/w_0 = 1 + w_1/w_0 + w_2/w_0 \quad (\text{B37})$$

with w_1/w_0 and w_2/w_0 obtained from Eq. (B18) and Eq. (B29), respectively. For the second Born approximation, we will need to identify and retain contributions through order ϵ^2 . For w_1/w_0 that is easy; to second order it is simply

$$-\frac{i}{4}\epsilon^{(1)}.$$

For w_2/w_0 , we need all the second-order terms from a , b , c , and d . Since b is purely second-order, its contribution is simply $\epsilon^{(-1)2}/2$.

For a , we need to assess the $\alpha_n = [\epsilon^{(0)}\epsilon^{(n)}]^{(-1)}$ terms, the first two of which are

$$\begin{aligned} \alpha_0(x) &= \int_{x_0}^x dy \epsilon^2(y) \\ \alpha_1(x) &= \int_{x_0}^x dy \epsilon(y) \epsilon^{(1)}(y) = \frac{1}{2} \epsilon^2(y) \Big|_{x_0}^x. \end{aligned}$$

Since $\epsilon^{(n)}(x_0) = 0$ for all $n \geq 0$, we have

$$\alpha_0 = \epsilon^{2(-1)} \sim \epsilon^2 \quad (\text{B38})$$

$$\alpha_1 = \frac{1}{2} \epsilon^2 \sim \epsilon^2, \quad (\text{B39})$$

both of which contribute at order ϵ^2 . The α_n for $n = 2, 3, \dots$ can be evaluated by repeated integration by parts. For even and odd n , respectively, they are

$$\begin{aligned} \alpha_{2\ell}(x) &= \underbrace{\sum_{k=0}^{\ell-1} (-)^k \epsilon^{(k)}(x) \epsilon^{(2\ell-k-1)}(x)}_{\sim \epsilon^{2\ell+1}} + \underbrace{(-)^{\ell} \int_{x_0}^x dy \epsilon^{(\ell)2}(y)}_{\sim \epsilon^{2\ell+2}} \\ \alpha_{2\ell+1}(x) &= \underbrace{\sum_{k=0}^{\ell-1} (-)^k \epsilon^{(k)}(x) \epsilon^{(2\ell-k)}(x)}_{\sim \epsilon^{2\ell+2}} + \underbrace{(-)^{\ell} \frac{1}{2} \epsilon^{(\ell)2}(x)}_{\sim \epsilon^{2\ell+2}} \end{aligned}$$

for $\ell \geq 1$. Since $2\ell + 1 \geq 3$, all of these belong in $O(\epsilon^3)$ and we are left with

$$\begin{aligned} a &= \frac{i}{2} \alpha_0 - \frac{1}{4} \alpha_1 + O(\epsilon^3) \\ &= \frac{i}{2} \epsilon^{2(-1)} - \frac{1}{8} \epsilon^2 + O(\epsilon^3). \end{aligned} \quad (\text{B40})$$

For c , we need the $\gamma^{(n)} = [\epsilon^{(0)}\epsilon^{(-1)}]^{(n)}$ terms. Since

$$\gamma^{(0)} = \underbrace{\epsilon^{(0)}\epsilon^{(-1)}}_{\sim \epsilon^2}, \quad (\text{B41})$$

these can easily be obtained from the standard expression for the n th derivative of a product,

$$\gamma^{(n)} = \sum_{k=0}^n \binom{n}{k} \epsilon^{(k)} \epsilon^{(n-k-1)} \quad \dots \quad n > 0.$$

With the $k = n$ term written separately, this is

$$\gamma^{(n)} = \underbrace{\epsilon^{(n)} \epsilon^{(-1)}}_{\sim \epsilon^{n+2}} + \underbrace{\sum_{k=0}^{n-1} \binom{n}{k} \epsilon^{(k)} \epsilon^{(n-k-1)}}_{\sim \epsilon^{n+1}} \quad \dots \quad n > 0. \quad (\text{B42})$$

Clearly, the only contribution below the third order is the $k = 0$ one for $n = 1$. Thus

$$\begin{aligned} c &= \frac{i}{2} \gamma_0 - \frac{1}{4} \gamma_1 + O(\epsilon^3) \\ &= \underbrace{\frac{i}{2} \epsilon^{(0)} \epsilon^{(-1)} - \frac{1}{4} \epsilon^{(0)2}}_{\sim \epsilon^2} + O(\epsilon^3). \end{aligned} \quad (\text{B43})$$

The fact that $\alpha_m^{(\ell+1)} = [\alpha_m^{(1)}]^{(\ell)} = [\epsilon^{(0)} \epsilon^{(m)}]^{(\ell)}$ is the ℓ th derivative of a product allows it to be written as

$$\alpha_m^{(\ell+1)} = \sum_{k=0}^{\ell} \binom{\ell}{k} \epsilon^{(k)} \epsilon^{(m+\ell-k)}.$$

Contributions to d come from $m = n - \ell$. Since these are

$$\alpha_{n-\ell}^{(\ell+1)} = \sum_{k=0}^{\ell} \binom{\ell}{k} \underbrace{\epsilon^{(k)} \epsilon^{(n-k)}}_{\sim \epsilon^{n+2}} \quad \dots \quad n \geq 0, \quad (\text{B44})$$

only $n = 0$ contributes below the third order. Thus

$$\begin{aligned} d &= \left(\frac{i}{2}\right)^2 \alpha_0^{(1)} + O(\epsilon^3) \\ &= \underbrace{-\frac{1}{4} \epsilon^{(0)2}}_{\sim \epsilon^2} + O(\epsilon^3). \end{aligned} \quad (\text{B45})$$

In light of the above results, the second Born approximation is given by

$$u^B/w_0 = 1 + \underbrace{\left(i\epsilon^{(-1)} - \frac{1}{2}\epsilon - \frac{i}{4}\epsilon^{(1)}\right)}_{\sim \epsilon} + \underbrace{\left(-\frac{1}{2}\epsilon^{(-1)2} - \frac{i}{2}\epsilon^{2(-1)} + \frac{5}{8}\epsilon^2 - \frac{i}{2}\epsilon\epsilon^{(-1)}\right)}_{\sim \epsilon^2} + O(\epsilon^3), \quad (\text{B46})$$

or, in the conventional notation,

$$\begin{aligned} u^B(x) &= e^{i(x-x_0)} \left[1 + i \int_{x_0}^x dy \epsilon(y) - \frac{1}{2} \left(\int_{x_0}^x dy \epsilon(y) \right)^2 - \frac{1}{2} \epsilon(x) \right. \\ &\quad \left. + \frac{5}{8} \epsilon^2(x) - \frac{i}{2} \dot{\epsilon}(x) - \frac{i}{2} \epsilon(x) \int_{x_0}^x dy \epsilon(y) - \frac{i}{2} \int_{x_0}^x dy \epsilon^2(y) \right] + O(\epsilon^3). \end{aligned} \quad (\text{B47})$$

Term-by-term comparison with the second-order form of Eq. (110), i.e.,

$$\begin{aligned} u^{FW}(x) &= Q^{[2]}(x) e^{-i\vartheta^{[2]}(x)} e^{i\varphi^{[2]}(x, x_0)} + O(\epsilon^3) \\ &= \left(1 - \frac{1}{2}\epsilon(x) + \frac{5}{8}\epsilon^2(x)\right) e^{-i\dot{\epsilon}(x)/4} e^{i \int_{x_0}^x dy (1 + \epsilon(y) - \epsilon^2(y)/2)} + O(\epsilon^3) \end{aligned} \quad (\text{B48})$$

confirms their agreement through second order,

$$u^B - u^{FW} = O(\epsilon^3). \quad (\text{B49})$$

To extend this investigation to the third Born approximation would mean analyzing w_3/w_0 — a triple integral analogous to Eq. (B27). The analog of Eq. (B30) would involve $2^3 = 8$ terms; furthermore, their third-order contributions, along with those of w_2/w_0 and w_1/w_0 , would need to be identified and retained. The effort appears prohibitive, but it seems compelling to conjecture that $u^B - u^{FW}$ vanishes to *all* orders.

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