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X-ray scattering from a randomly rough surface

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Abstract. On the basis of the method of reduced Rayleigh equations we present a simple and reciprocal theory of the coherent and incoherent scattering of x-rays from one- and two-dimensional randomly rough surfaces, that appears to be free from the limitations of earlier theories of such scattering based on the Born and distorted-wave Born approximations. In our approach, the reduced Rayleigh equation for the scattering amplitude(s) is solved perturbatively, with the small parameter of the theory $\eta(\omega) = 1 - \epsilon(\omega)$, where $\epsilon(\omega)$ is the dielectric function of the scattering medium. The magnitude of $\eta(\omega)$ for x-rays is in the range from 10^{-6} to 10^{-3}, depending on the wavelength of the x-rays. The contributions to the mean differential reflection coefficient from the coherent and incoherent components of the scattered x-rays are calculated through terms of second order in $\eta(\omega)$. The resulting expressions are valid to all orders in the surface profile function. The results for the incoherent scattering display a Yoneda peak when the scattering angle equals the critical angle for total internal reflection from the vacuum-scattering medium interface for a fixed angle of incidence, and when the angle of incidence equals the critical angle for total internal reflection for a fixed scattering angle. The approach used here may also be useful in theoretical studies of the scattering of electromagnetic waves from randomly rough dielectric–dielectric interfaces, when the difference between the dielectric constants on the two sides of the interface is small.

1. Introduction

The scattering of x-rays from rough surfaces and interfaces has been used extensively as a powerful experimental tool for investigating surface and interface properties (see, e.g., the recent review articles [1, 2] and references therein). A significant feature of x-ray scattering from condensed media is that the dielectric function of the scattering medium $\epsilon(\omega)$ in the x-ray frequency region is close to, and a little smaller than, unity, $\epsilon(\omega) = 1 - \eta(\omega)$. In this frequency range $\eta(\omega)$ can be assumed to be real and positive, and its magnitude lies in the range 10^{-6}–10^{-3}, depending on the wavelength of the x-rays. This can be seen most directly by starting from the simple, free-electron form of the dielectric function of a metal,

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \tag{1.1}$$

where ω_p is the plasma frequency of the conduction electrons, and γ is an inverse electronic relaxation time. It follows that $\eta(\omega)$ in this case is given by

$$\eta(\omega) = \frac{\omega_p^2}{\omega(\omega + i\gamma)} \cong \frac{\omega_p^2}{\omega^2}\left(1 - i\frac{\gamma}{\omega}\right) = \frac{\omega_p^2}{\omega^2}\left(1 - i\frac{\gamma}{\omega_p}\frac{\omega_p}{\omega}\right). \tag{1.2}$$

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A typical value of ω_p, in energy units, is 10 eV [3]. For 1 keV x-rays, the ratio ω_p/ω is therefore of the order of 10^{-2}. At the same time, the ratio γ/ω_p is of the order of 10^{-2} or smaller [3]. Consequently, the value of the imaginary part of $\eta(\omega)$ in the x-ray frequency range is four orders of magnitude smaller than the real part, which itself is of the order of 10^{-4} in this example. It follows, therefore, that to a very good approximation, the imaginary part of $\eta(\omega)$ can be neglected in comparison with the real part; we shall therefore neglect it in this paper.

Most of the attention in the existing experimental investigations of x-ray scattering from rough surfaces has been paid to x-ray specular reflectivity measurements. Since the x-rays are incident from an optically more dense medium onto an optically less dense medium, the phenomenon of total internal reflection of x-rays occurs when the angle of incidence θ_0 equals the critical angle $\theta_c = \arccos\sqrt{\eta(\omega)}$. As a result, the reflectivity for grazing angles of incidence tends to unity, and the intensity of the incoherent (diffuse) component of the scattered x-rays tends to zero. For angles of incidence smaller than the critical angle for total internal reflection, however, the coherent scattering rapidly tends to zero. As a result, the incoherent scattering becomes dominant. In addition, the angular dependence of this intensity displays a sharp asymmetric peak, called the Yoneda peak [4], at a scattering angle θ_s equal to the critical angle for total internal reflection for a fixed angle of incidence (see figure 1, taken from [5]), and at an angle of incidence θ_0 equal to the critical angle for total internal reflection for a fixed scattering angle. The Yoneda peak has been observed in x-ray scattering from rough solid and liquid surfaces, and from the interfaces in multilayer structures [4–9].

Theories of x-ray scattering from surfaces and multilayered structures have been constructed on the basis of the Born and distorted-wave Born approximations, which exploit

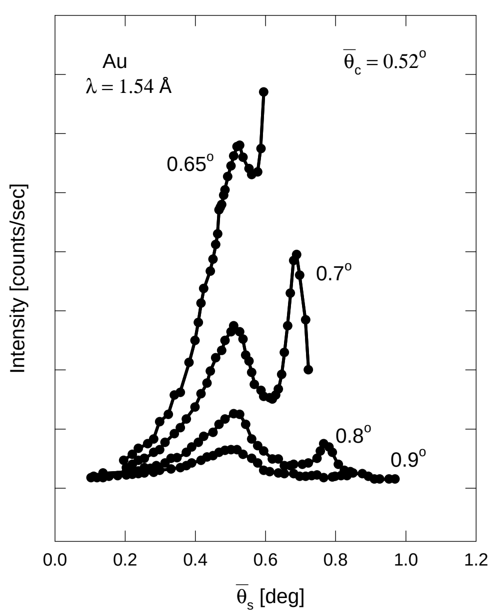

Figure 1. The angular distribution of the total power reflected from a gold surface as a function of the grazing scattering angle $\bar{\theta}_s = \pi/2 - \theta_s$ for several values of the grazing angle of incidence $\bar{\theta}_0 = \pi/2 - \theta_0$ greater than $\bar{\theta}_c = \pi/2 - \theta_c$. The wavelength of the incident x-rays is $\lambda = 1.54$ Å. $\bar{\theta}_c = 0.54^\circ$. (After [4]).

the weak interaction of x-rays and the scattering medium [1, 2, 7, 10–13]. The Born approximation is valid for small angles of incidence and scattering, but breaks down in the vicinity of the critical angle for total internal reflection, because in the initial and final states of the scattering process the reflection from the interface is neglected. In the distorted-wave Born approximation the basis for the perturbation approach is provided by the Fresnel eigenstates, i.e. the solutions of the Fresnel problem for a flat interface, which take into account the refraction of both the initial and final states. As a result, this approximation provides a good description of the scattering of x-rays for angles of incidence in the vicinity of the critical angle for total internal reflection. However, it fails at smaller angles. The distorted-wave Born approximation yields an expression for the specular reflectivity that is valid for grazing angles of incidence larger than the critical angle for total internal reflection and for not very rough surfaces, i.e. surfaces for which $\sqrt{\eta(\omega)}(\omega/c)\delta < 1$, where δ is the RMS height of the surface, in the form of the Fresnel reflectivity multiplied by a factor similar to the Debye–Waller factor which accounts for the surface roughness [7, 10, 13]. From such a result only the RMS height of the surface δ can be deduced from experimental data [7, 10, 13]. The second-order distorted-wave Born approximation yields a correction to the reflectivity proportional to the surface height autocorrelation function [13]. The angular dependence of the intensity of the incoherent component of the scattered x-rays obtained in the distorted-wave Born approximation displays the Yoneda peak as a result of the strong enhancement of the total field amplitude at the surface, which reaches a maximum value that is twice that of the incident field at the critical angle for total internal reflection [7].

The modified Born approximation [2] also takes refraction into account. It thus improves the Born approximation for grazing angles of incidence and yields the same results as the distorted-wave Born approximation.

When the grazing angle of incidence or scattering is smaller than the critical angle for total internal reflection, both the Born and distorted-wave Born approximations break down: the reflectivity obtained in the Born approximation diverges instead of saturating at the critical angle, while the reflectivity obtained in the distorted-wave Born approximation is greater than unity or, for a weakly rough surface, exactly equal to unity.

The interaction of electromagnetic waves with a randomly rough surface is weak when either the surface is weakly rough or the dielectric contrast between the medium of incidence and the scattering medium is small, even if the interface between them is not weakly rough. When this interaction is weak some form of perturbation theory can be used in the theoretical study of the scattering of electromagnetic waves from a randomly rough surface. If the roughness itself is weak, the perturbation theory is constructed on the basis of an expansion of some quantity in the theory in powers of the surface profile function. For example, in small-amplitude perturbation theory the scattering amplitude is expanded in powers of the surface profile function [14]. In self-energy perturbation theory [15] it is the proper self-energy entering the Green's function through which the scattering amplitude is expressed that is expanded in powers of the surface profile function. In phase perturbation theory [16] it is the phase of the scattering amplitude that is expanded in powers of the surface profile function.

If the dielectric contrast $\eta(\omega)$ between the medium of incidence and the scattering medium is small, even if the interface between them is not weakly rough, as is the case in the scattering of x-rays from rough surfaces and interfaces, it can be used as the small parameter in a perturbation theory of such scattering, with no restrictions on the surface roughness parameters except those inherent to the theoretical approach used.

In this paper we present a theory of x-ray scattering from one- and two-dimensional randomly rough surfaces, based on the method of reduced Rayleigh equations [15], that possesses the advantages of the Born and distorted-wave Born approximations and lacks their disadvantages. The method of reduced Rayleigh equations is based on the Rayleigh hypothesis [17, 18], which is the assumption that only that part of the scattered electromagnetic field that satisfies the (outgoing) boundary condition at infinity can be used in satisfying the electromagnetic boundary conditions on the rough surface. In the method of reduced Rayleigh equations the coupled integral equations for the amplitudes of the scattered and refracted fields are decoupled to yield integral equations for the amplitudes of the scattered field alone. In our approach, the scattering amplitude is calculated perturbatively as an expansion in powers of the small parameter $\eta(\omega)$. The validity of the resulting solution is restricted only by the condition for the validity of the Rayleigh hypothesis, i.e. $\mathrm{d}\zeta(x_1)/\mathrm{d}x_1 \ll 1$ in the case of a one-dimensional random surface, and $|\nabla\zeta(x_1, x_2)| \ll 1$ in the case of a two-dimensional random surface, where $\zeta(x_1)$ ($\zeta(x_1, x_2)$) is the surface profile function which defines the position of the surface through the equation $x_3 = \zeta(x_1)$ ($x_3 = \zeta(x_1, x_2)$) [19–21]. Moreover, in contrast with earlier theories of x-ray scattering from randomly rough surfaces in which either the incident x-rays were assumed to be s-polarized [7, 13] or the polarization of the incident and scattered x-rays was not taken into account at all through a scalar wave treatment [10–12], the approach adopted here, in which the x-rays are treated as electromagnetic waves, allows the polarizations of the incident and scattered x-rays to be included readily in calculations of the contributions to the mean differential reflection coefficients from both the coherent and incoherent components of the scattered x-rays; we have included these contributions.

For the specular reflectivity to the lowest order in $\eta(\omega)$, i.e. $\mathrm{O}(\eta^0(\omega))$, we obtain a result in the form of the Fresnel reflectivity multiplied by a 'Debye–Waller factor' that is consistent with the Debye–Waller factor obtained in [7, 10, 13]. We also obtain the lowest-order correction to this result by summing an infinite subset of terms in the perturbation series for the mean scattering amplitude, and find that it is of second order in the small parameter of our theory $\eta(\omega)$. The contribution to the mean differential reflection coefficient from the incoherent component of the scattered x-rays is calculated to the lowest non-zero order in $\eta(\omega)$, which is $\mathrm{O}(\eta^2(\omega))$. It displays the Yoneda peak when the scattering angle or the angle of incidence equals the critical angle for total internal reflection.

These results are obtained on the basis of the assumption that the scattering medium is homogeneous on the length scale being probed, i.e. the atomic structure of the scattering medium is ignored. This assumption is valid provided we deal with small angle scattering, where the condition $4\pi(a/\lambda)\sin\theta \ll 1$ is satisfied, where 2θ is the scattering angle, λ is the wavelength of the x-rays, and a is a typical length scale for any inhomogeneity within the scattering medium [7].

The outline of this paper is as follows. In section 2 we study the coherent and incoherent scattering of p-polarized x-rays incident from vacuum onto a one-dimensional, randomly rough metal surface, when the plane of incidence is perpendicular to the generators of this surface. This simpler version of the problem already displays all the features present in the theory of the scattering of x-rays from a two-dimensional randomly rough surface, without the complications caused by the possibility of out-of-plane and cross-polarized scattering present in the latter case. With the results of section 2 as a guide, in section 3 we present a theory of the scattering of x-rays from a two-dimensional randomly rough, metal surface. Numerical results calculated from the expressions derived in the preceding two sections are presented in section 4, and conclusions drawn from them are presented and discussed in section 5. Two appendices, in which results needed in the text are derived, conclude this paper.

2. A one-dimensional random surface

The physical system we consider here consists of vacuum in the region $x_3 > \zeta(x_1)$, and the scattering medium, which is characterized by an isotropic, complex, frequency-dependent dielectric function ϵ, in the region $x_3 < \zeta(x_1)$. The surface profile function $\zeta(x_1)$ is assumed to be a single-valued function of x_1 which is differentiable as many times as necessary. It is also assumed to constitute a stationary, zero-mean, Gaussian random process, which is defined by the properties

$$\langle \zeta(x_1) \rangle = 0 \tag{2.1}$$

$$\langle \zeta(x_1)\zeta(x_1') \rangle = \delta^2 W(|x_1 - x_1'|) \tag{2.2}$$

where the angular brackets denote an average over the ensemble of realizations of $\zeta(x_1)$, and $\delta = \sqrt{\langle \zeta^2(x_1) \rangle}$ is the RMS height of the surface. In the numerical work carried out in this paper we shall assume for the surface height autocorrelation function $W(|x_1|)$ the Gaussian form

$$W(|x_1|) = \exp(-x_1^2/a^2). \tag{2.3}$$

The characteristic length a appearing in this expression is the transverse correlation length of the surface roughness.

We assume that the random surface is illuminated from the vacuum side by a plane electromagnetic wave which, for definiteness, we assume is p-polarized. The plane of incidence is the x_1x_3-plane. In this scattering geometry there is no cross-polarized scattering, and it is convenient to work with the single non-zero component of the magnetic vector. In the vacuum region $x_3 > \zeta(x_1)_{\max}$ it is the sum of an incident plane wave and the scattered field,

$$H_2^{>}(x_1, x_3|\omega) = e^{ikx_1 - i\alpha_0(k)x_3} + \int_{-\infty}^{\infty} \frac{dq}{2\pi} R(q|k) e^{iqx_1 + i\alpha_0(q)x_3} \tag{2.4}$$

where

$$\alpha_0(q) = \left(\frac{\omega^2}{c^2} - q^2\right)^{1/2} \qquad |q| < \frac{\omega}{c} \tag{2.5a}$$

$$= i\left(q^2 - \frac{\omega^2}{c^2}\right)^{1/2} \qquad |q| > \frac{\omega}{c}. \tag{2.5b}$$

In writing equation (2.4) we have assumed a time dependence of the electromagnetic field of the form $\exp(-i\omega t)$, and have suppressed explicit mention of this factor.

The angles of incidence (θ_0) and scattering (θ_s), measured counterclockwise and clockwise from the x_3-axis, respectively, are related to the wavenumbers k and q by

$$k = \frac{\omega}{c} \sin\theta_0 \qquad q = \frac{\omega}{c} \sin\theta_s. \tag{2.6}$$

The differential reflection coefficient (DRC) $\partial R/\partial\theta_s$ is the fraction of the power in the incident wave that is scattered into an angular interval of width $d\theta_s$ about the scattering angle θ_s. Since the scattering surface is random, we are interested not in the differential reflection coefficient itself, but in its average over the ensemble of realizations of the surface profile function, $\langle \partial R/\partial\theta_s \rangle$. This is given in terms of the scattering amplitude $R(q|k)$ by [22]

$$\left\langle \frac{\partial R}{\partial \theta_s} \right\rangle = \frac{1}{L_1} \frac{\omega}{2\pi c} \frac{\cos^2\theta_s}{\cos\theta_0} \langle |R(q|k)|^2 \rangle \tag{2.7}$$

where L_1 is the length of the x_1-axis covered by the random surface. The wavenumbers q and k in equation (2.7) must be replaced by their equivalents given by (2.6).

As it stands, the expression given by equation (2.7) contains contributions from both the coherent (specular) and incoherent (diffuse) components of the scattered electromagnetic field. The former is given by

$$\left\langle \frac{\partial R}{\partial \theta_s} \right\rangle_{\text{coh}} = \frac{1}{L_1} \frac{\omega}{2\pi c} \frac{\cos^2\theta_s}{\cos\theta_0} |\langle R(q|k)\rangle|^2. \tag{2.8}$$

The latter is therefore given by

$$\left\langle \frac{\partial R}{\partial \theta_s} \right\rangle_{\text{incoh}} = \frac{1}{L_1} \frac{\omega}{2\pi c} \frac{\cos^2\theta_s}{\cos\theta_0} \left[\langle |R(q|k)|^2\rangle - |\langle R(q|k)\rangle|^2\right]. \tag{2.9}$$

We now turn to the determination of the scattering amplitude $R(q|k)$.

The method of reduced Rayleigh equations [23], which is based on the Rayleigh hypothesis [17, 18], Green's second integral identity [24], and the extinction theorem [25], yields the following integral equation satisfied by the scattering amplitude $R(q|k)$:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \frac{I(\alpha(q)-\alpha_0(p)|q-p)}{\alpha(q)-\alpha_0(p)} [\alpha(q)\alpha_0(p)+qp] R(p|k)$$
$$= \frac{I(\alpha(q)+\alpha_0(k)|q-k)}{\alpha(q)+\alpha_0(k)} [\alpha(q)\alpha_0(k)-qk] \tag{2.10}$$

where

$$\alpha(q) = \left[\epsilon\frac{\omega^2}{c^2} - q^2\right]^{1/2} \qquad \mathrm{Re}\,\alpha(q) > 0 \qquad \mathrm{Im}\,\alpha(q) > 0 \tag{2.11}$$

and

$$I(\gamma|Q) = \int_{-\infty}^{\infty} \mathrm{d}x_1 \mathrm{e}^{-\mathrm{i}Qx_1 - \mathrm{i}\gamma\zeta(x_1)}. \tag{2.12}$$

We begin the solution of equation (2.10) by rewriting the function $I(\gamma|Q)$ in the form

$$I(\gamma|Q) = 2\pi\delta(Q) + J(\gamma|Q) \tag{2.13}$$

where

$$J(\gamma|Q) = \int_{-\infty}^{\infty} \mathrm{d}x_1 \mathrm{e}^{-\mathrm{i}Qx_1}(\mathrm{e}^{-\mathrm{i}\gamma\zeta(x_1)} - 1). \tag{2.14}$$

Equation (2.10) is transformed by this step into

$$R(q|k) = 2\pi\delta(q-k)R_0(k) + \frac{\eta}{d(q)} N(q|k) + \frac{\eta}{d(q)} \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} M(q|p) R(p|k) \tag{2.15}$$

where

$$R_0(k) = \frac{\epsilon\alpha_0(k) - \alpha(k)}{\epsilon\alpha_0(k) + \alpha(k)} \tag{2.16a}$$

$$N(q|k) = \frac{qk - \alpha(q)\alpha_0(k)}{\alpha(q)+\alpha_0(k)} J(\alpha(q)+\alpha_0(k)|q-k) \tag{2.16b}$$

$$M(q|p) = \frac{qp + \alpha(q)\alpha_0(p)}{\alpha(q)-\alpha_0(k)} J(\alpha(q)-\alpha_0(p)|q-p) \tag{2.16c}$$

$$d(q) = \epsilon\alpha_0(q) + \alpha(q). \tag{2.16d}$$

In obtaining equation (2.15) we have accomplished two objectives. The first is that we have explicitly separated from the scattering amplitude $R(q|k)$ the contribution $2\pi\delta(q-k)R_0(k)$

that describes the scattering from a planar surface ($\zeta(x_1) \equiv 0$). The remaining terms on the right-hand side of equation (2.15) therefore arise from the surface roughness. The second is that the terms arising from the surface roughness are explicitly proportional to the small parameter of our theory, η.

We shall seek the solution of equation (2.15) in the form

$$R(q|k) = 2\pi\delta(q-k)R_0(k) + B(q|k) \tag{2.17}$$

where the function $B(q|k)$ satisfies the equation

$$B(q|k) = \eta A(q|k) + \eta \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} m(q|p)B(p|k) \tag{2.18}$$

with

$$A(q|k) = n(q|k) + m(q|k)R_0(k) \tag{2.19a}$$

$$m(q|k) = \hat{m}(q|k)J(\alpha(q) - \alpha_0(k)|q-k) \tag{2.19b}$$

$$n(q|k) = \hat{n}(q|k)J(\alpha(q) + \alpha_0(k)|q-k) \tag{2.19c}$$

$$\hat{m}(q|k) = \frac{qk + \alpha(q)\alpha_0(k)}{d(q)[\alpha(q) - \alpha_0(k)]} \tag{2.19d}$$

$$\hat{n}(q|k) = \frac{qk - \alpha(q)\alpha_0(k)}{d(q)[\alpha(q) + \alpha_0(k)]}. \tag{2.19e}$$

The iterative solution of equation (2.18) is formally an expansion of $B(q|k)$ in powers of η:

$$B(q|k) = \eta A(q|k) + \eta^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}p_1}{2\pi} m(q|p_1)A(p_1|k) + \eta^3 \int_{-\infty}^{\infty} \frac{\mathrm{d}p_1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_2}{2\pi} m(q|p_1)m(p_1|p_2)A(p_2|k) + \cdots. \tag{2.20}$$

2.1. Coherent scattering

From equation (2.8) we see that the contribution to the mean DRC from the coherent component of the scattered x-rays is expressed in terms of $\langle R(q|k)\rangle$, where

$$\langle R(q|k)\rangle = 2\pi\delta(q-k)R_0(k) + \langle B(q|k)\rangle. \tag{2.21}$$

To obtain $\langle B(q|k)\rangle$ we average equation (2.20) term by term:

$$\langle B(q|k)\rangle = \eta\langle A(q|k)\rangle + \eta^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}p_1}{2\pi} \langle m(q|p_1)A(p_1|k)\rangle + \eta^3 \int \frac{\mathrm{d}p_1}{2\pi} \int \frac{\mathrm{d}p_2}{2\pi} \langle m(q|p_1)m(p_1|p_2)A(p_2|k)\rangle + \cdots. \tag{2.22}$$

In view of equations (2.19*a*)–(2.19*c*) we see that the *n*th-order term in this expansion contains the average of the product of n $J(\gamma|Q)$ functions. This average is given by

$$\langle J(\gamma_1|Q_1)J(\gamma_2|Q_2)\cdots J(\gamma_n|Q_n)\rangle = \prod_{j=1}^{n} 2\pi\delta(Q_j)(\mathrm{e}^{-\frac{1}{2}\gamma_j^2\delta^2} - 1) + \theta(n-2) \sum_{\substack{i,j=1 \\ (i>j)}}^{n} 2\pi\delta(Q_i + Q_j)\mathrm{e}^{-\frac{1}{2}(\gamma_i^2+\gamma_j^2)\delta^2}$$

$$\times \int_{-\infty}^{\infty} du\, e^{-iQ_i u} (e^{-\gamma_i \gamma_j \delta^2 W(|u|)} - 1) \prod_{\substack{k=1 \\ (k \neq i,j)}}^{n} 2\pi \delta(Q_k)(e^{-\frac{1}{2}\gamma_k^2 \delta^2} - 1)$$

$$+ \text{ terms containing the product of } n-2 \text{ or fewer delta functions} \qquad (2.23a)$$

$$= \prod_{j=1}^{n} \langle J(\gamma_j|Q_j)\rangle + \theta(n-2) \sum_{\substack{i,j=1 \\ (i>j)}}^{n} \{J(\gamma_i|Q_i)J(\gamma_j|Q_j)\} \prod_{\substack{k=1 \\ (k \neq i,j)}}^{n} \langle J(\gamma_k|Q_k)\rangle$$

$$+ \text{ terms containing the product of } n-2 \text{ or fewer delta functions} \qquad (2.23b)$$

where $\theta(n) = 1$ for $n \geqslant 1$ and $\theta(n) = 0$ for $n < 0$, and we have introduced the notation that for any two random processes A and B

$$\{AB\} = \langle AB\rangle - \langle A\rangle\langle B\rangle \qquad (2.24)$$

is the correlated part of the average of their product.

The significance of grouping terms in the average $\langle J(\gamma_1|Q_1) \cdots J(\gamma_n|Q_n)\rangle$ according to the number of delta functions they contain stems from the fact that the diagonal elements of the functions $\hat{m}(q|k)$ and $\hat{n}(q|k)$ defined by equations (2.19*d*) and (2.19*e*) are proportional to η^{-1}:

$$\hat{m}(q|q) = -\frac{1}{\eta} \qquad \hat{n}(q|q) = \frac{R_0(q)}{\eta}. \qquad (2.25)$$

This result together with the result given by the first term on the right-hand side of equation (2.23) means that *each* term on the right-hand side of equation (2.22) has a contribution of order $O(\eta^0)$. Thus, in order to obtain the contribution to $\langle B(q|k)\rangle$ that is of zero order in η we have to sum the contribution of this order in each of the terms on the right-hand side of equation (2.22). To obtain this contribution it suffices to replace the average in each term on the right-hand side of equation (2.22) by the product of the averages of the individual factors, according to equation (2.23). In this way, we obtain

$$\langle B(q|k)\rangle_{(0)} = 2\pi\delta(q-k)[1 - X(k) + X(k)^2 - \cdots]a(k) \qquad (2.26)$$

where we have used the results that

$$\langle m(q|k)\rangle = 2\pi\delta(q-k)\left[-\frac{X(k)}{\eta}\right] \qquad (2.27a)$$

with

$$X(k) = e^{-\frac{1}{2}(\alpha(k)-\alpha_0(k))^2\delta^2} - 1 \qquad (2.27b)$$

and

$$\langle A(q|k)\rangle = 2\pi\delta(q-k)\left[\frac{a(k)}{\eta}\right] \qquad (2.28a)$$

with

$$a(k) = R_0(k)[e^{-\frac{1}{2}(\alpha(k)+\alpha_0(k))^2\delta^2} - e^{-\frac{1}{2}(\alpha(k)-\alpha_0(k))^2\delta^2}]. \qquad (2.28b)$$

It follows that

$$\langle B(q|k)\rangle_{(0)} = 2\pi\delta(q-k)R_0(k)[e^{-2\alpha_0(k)\alpha(k)\delta^2} - 1]. \qquad (2.29)$$

To obtain the leading contribution to $\langle B(q|k)\rangle$ that is of non-zero order in η we have to take into account the contribution to the average in each term on the right-hand side of equation (2.22) from the second term on the right-hand side of equation (2.23). Operationally, the latter tells us that in each term (starting with the second) we have to pair two factors and evaluate the correlated part of the average of their product, and then multiply the result by the product of the average of each of the remaining factors. In the nth-order term two types of contributions arise. The first consists of the $n-1$ terms in which one of the $m(p_i|p_j)$ is paired with $A(p_{n-1}|k)$, while the remaining $n-2$ factors of $m(p_i|p_j)$ are averaged individually; the second consists of the $(n-1)(n-2)/2$ terms in which two of the $m(p_i|p_j)$ are paired, while the remaining $n-2$ factors (including $A(p_{n-1}|k)$) are averaged individually. The correlated part of the average of two factors contains no explicit power of η in either case; the product of the $n-2$ averages of the remaining factors is proportional to $\eta^{-(n-2)}$. Consequently, the leading correction to the result given by equation (2.29) is of order $\mathrm{O}(\eta^2)$.

Let us consider first the sum of all the terms on the right-hand side of equation (2.22), starting with the second-order term, in which one of the $m(p_i|p_j)$ is paired with $A(p_{n-1}|k)$, and the product averaged, while the remaining factors are averaged individually. We find that this is given by

$$\begin{aligned}\langle B(q|k)\rangle_{(21)} &= \eta^2[1 - X(q) + X(q)^2 - \cdots] \\ &\quad\times \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \{m(q|p)[1 - X(p) + X(p)^2 - \cdots]A(p|k)\}. \qquad (2.30)\end{aligned}$$

The first series, in powers of $-X(q)$, is associated with the product of the averages of the individual $m(p_i|p_j)$ which stand to the left of the factor $m(p_i|p_j)$ that is paired with $A(p_{n-1}|k)$; the second series, in powers of $-X(p)$, is associated with the product of the averages of the individual $m(p_i|p_j)$ which stand between the factor $m(p_i|p_j)$ that is paired with $A(p_{n-1}|k)$ and $A(p_{n-1}|k)$ itself.

We next consider the sum of all terms on the right-hand side of equation (2.22), starting with the third-order term, in which two of the $m(p_i|p_j)$ are paired and the correlated average of their product evaluated, while the remaining factors are averaged individually. We find that this is given by

$$\begin{aligned}\langle B(q|k)\rangle_{(22)} &= \eta^2[1 - X(q) + X(q)^2 - \cdots] \\ &\quad\times \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \left\{m(q|p)[1 - X(p) + X(p)^2 - \cdots]m(p|k)\right\} \\ &\quad\times[1 - X(k) + X(k)^2 - \cdots]a(k). \qquad (2.31)\end{aligned}$$

Again, the first series, in powers of $-X(q)$, is associated with the product of the averages of the individual $m(p_i|p_j)$ which stand to the left of the factor $m(p_i|p_j)$ which is paired with a second factor $m(p_i'|p_j')$ which stands to its right; the series in powers of $-X(p)$ is associated with the product of the averages of the individual $m(p_i|p_j)$ which stand between the paired factors; the series in powers of $-X(k)$ is associated with the product of the averages of the individual factors, including $A(p_{n-1}|k)$, which stand to the right of the second factor $m(p_i'|p_j')$ in the pair.

Using the definitions of $A(q|k)$ and $m(q|k)$ given by (2.19), the definitions of $X(k)$ and $a(k)$ given by equations (2.27*b*) and (2.28*b*), respectively, and the result that

$$\{J(\gamma_1|Q_1)J(\gamma_2|Q_2)\} = 2\pi\delta(Q_1 + Q_2)\mathrm{e}^{-\frac{1}{2}(\gamma_1^2+\gamma_2^2)\delta^2} \int_{-\infty}^{\infty} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}Q_1 u}(\mathrm{e}^{-\gamma_1\gamma_2\delta^2 W(|u|)} - 1) \qquad (2.32)$$

we can rewrite equations (2.30) and (2.31) compactly as

$$\langle B(q|k)\rangle_{(21)} = 2\pi\delta(q-k)\eta^2[\mathrm{e}^{-2\alpha_0(k)\alpha(k)\delta^2}N_{\mathrm{p}}(k) + R_0(k)M_{\mathrm{p}}(k)] \qquad (2.33a)$$

and

$$\langle B(q|k)\rangle_{(22)} = 2\pi\delta(q-k)\eta^2[\mathrm{e}^{-2\alpha_0(k)\alpha(k)\delta^2} - 1]R_0(k)M_{\mathrm{p}}(k) \qquad (2.33b)$$

respectively, where the subscript p denotes p-polarization, and

$$M_{\rm p}(k) = \int_{-\infty}^{\infty} \frac{{\rm d}p}{2\pi} \hat{m}(k|p)\hat{m}(p|k){\rm e}^{-(\alpha(p)-\alpha(k))(\alpha_0(p)-\alpha_0(k))\delta^2} \times \int_{-\infty}^{\infty} {\rm d}u\, {\rm e}^{-{\rm i}(k-p)u}[{\rm e}^{-(\alpha(k)-\alpha_0(p))(\alpha(p)-\alpha_0(k))\delta^2 W(|u|)} - 1] \qquad (2.34a)$$

$$N_{\rm p}(k) = \int_{-\infty}^{\infty} \frac{{\rm d}p}{2\pi} \hat{m}(k|p)\hat{n}(p|k){\rm e}^{-(\alpha(p)-\alpha(k))(\alpha_0(p)+\alpha_0(k))\delta^2} \times \int_{-\infty}^{\infty} {\rm d}u\, {\rm e}^{-{\rm i}(k-p)u}[{\rm e}^{-(\alpha(k)-\alpha_0(p))(\alpha(p)+\alpha_0(k))\delta^2 W(|u|)} - 1]. \qquad (2.34b)$$

Thus, the total contribution to $\langle B(q|k)\rangle$ of second order in η is

$$\langle B(q|k)\rangle_{(2)} = 2\pi\delta(q-k)\eta^2 {\rm e}^{-2\alpha_0(k)\alpha(k)\delta^2}\left[N_{\rm p}(k) + R_0(k)M_{\rm p}(k)\right]. \qquad (2.35)$$

Using equations (2.21), (2.29), and (2.35), we obtain the result that

$$\langle R(q|k)\rangle = 2\pi\delta(q-k)r_{\rm p}(\theta_0), \qquad (2.36)$$

where

$$r_{\rm p}(\theta_0) = \exp\left[-2\left(\frac{\omega\delta}{c}\right)^2 \cos\theta_0(\cos^2\theta_0-\eta)^{1/2}\right]\left\{\frac{\epsilon\cos\theta_0 - (\cos^2\theta_0-\eta)^{1/2}}{\epsilon\cos\theta_0 + (\cos^2\theta_0-\eta)^{1/2}} + \eta^2\left[N_{\rm p}\left(\frac{\omega}{c}\sin\theta_0\right) + \frac{\epsilon\cos\theta_0 - (\cos^2\theta_0-\eta)^{1/2}}{\epsilon\cos\theta_0 + (\cos^2\theta_0-\eta)^{1/2}} M_{\rm p}\left(\frac{\omega}{c}\sin\theta_0\right)\right] + {\rm o}(\eta^2)\right\} \qquad (2.37)$$

and we have used the fact that $k = (\omega/c)\sin\theta_0$. When the result given by equation (2.36) is substituted into equation (2.8), and use is made of the relations

$$[2\pi\delta(q-k)]^2 = 2\pi\delta(0)2\pi\delta(q-k) = L_1 2\pi\delta(q-k) \qquad (2.38a)$$

$$\delta(q-k) = \frac{c}{\omega}\frac{\delta(\theta_{\rm s}-\theta_0)}{\cos\theta_0} \qquad (2.38b)$$

the contribution to the mean DRC from the coherent component of the scattered electromagnetic field becomes

$$\left\langle\frac{\partial R}{\partial\theta_{\rm s}}\right\rangle_{\rm coh} = \delta(\theta_{\rm s}-\theta_0)R_{\rm p}(\theta_0) \qquad (2.39)$$

where the reflectivity $R_{\rm p}(\theta_0)$ is given by

$$R_{\rm p}(\theta_0) = |r_{\rm p}(\theta_0)|^2. \qquad (2.40)$$

Up to now we have dealt only with the scattering of p-polarized x-rays. For completeness we note that in the case where the random surface is illuminated by an s-polarized electromagnetic wave the integral equation for the scattering amplitude $R(q|k)$ analogous to equation (2.10) has the form [26]:

$$\int_{-\infty}^{\infty}\frac{{\rm d}p}{2\pi}\frac{I(\alpha(q)-\alpha_0(p)|q-p)}{\alpha(q)-\alpha_0(p)}R(p|k) = -\frac{I(\alpha(q)+\alpha_0(k)|q-k)}{\alpha(q)+\alpha_0(k)}. \qquad (2.41)$$

The analysis presented here can be easily repeated starting from this equation. In this case we obtain for the reflectivity

$$R_{\rm s}(\theta_0) = |r_{\rm s}(\theta_0)|^2 \qquad (2.42)$$

where

$$r_s(\theta_0) = \exp\left[-2\left(\frac{\omega\delta}{c}\right)^2 \cos\theta_0(\cos^2\theta_0 - \eta)^{1/2}\right]\left\{\frac{\cos\theta_0 - (\cos^2\theta_0 - \eta)^{1/2}}{\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}} + \eta^2\left[N_s\left(\frac{\omega}{c}\sin\theta_0\right) + \frac{\cos\theta_0 - (\cos^2\theta_0 - \eta)^{1/2}}{\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}} M_s\left(\frac{\omega}{c}\sin\theta_0\right)\right] + \mathrm{o}(\eta^2)\right\} \tag{2.43}$$

and the functions $M_s(k)$ and $N_s(k)$ are given by equations (2.34) in which $\hat{m}(q|k)$ and $\hat{n}(q|k)$ are replaced by

$$\hat{m}_s(q|k) = \frac{\omega^2}{c^2}\frac{1}{[\alpha(q) + \alpha_0(q)][\alpha(q) - \alpha_0(k)]} \tag{2.44a}$$

$$\hat{n}_s(q|k) = \frac{\omega^2}{c^2}\frac{1}{[\alpha(q) + \alpha_0(q)][\alpha(q) + \alpha_0(k)]}. \tag{2.44b}$$

2.2. *Incoherent scattering*

When we substitute equation (2.17) into equation (2.9) we find that the contribution to the mean DRC from the incoherent component of the scattered field can be expressed equivalently as

$$\left\langle\frac{\partial R}{\partial\theta_s}\right\rangle_{\mathrm{incoh}} = \frac{1}{L_1}\frac{\omega}{2\pi c}\frac{\cos^2\theta_s}{\cos\theta_0}[\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2]. \tag{2.45}$$

To obtain $\langle|B(q|k)|^2\rangle$ we square the modulus of the right-hand side of equation (2.20), and average the resulting series term by term:

$$\langle|B(q|k)|^2\rangle = \eta^2\langle A(q|k)A^*(q|k)\rangle + \eta^3\left[\left\langle A(q|k)\int_{-\infty}^{\infty}\frac{\mathrm{d}r_1}{2\pi}m^*(q|r_1)A^*(r_1|k)\right\rangle + \left\langle\int_{-\infty}^{\infty}\frac{\mathrm{d}p_1}{2\pi}m(q|p_1)A(p_1|k)A^*(q|k)\right\rangle\right] + \cdots. \tag{2.46}$$

From the explicit expressions for $A(q|k)$ and $m(q|k)$ obtained from equations (2.19*a*)–(2.19*c*), we see that the coefficient of η^n on the right-hand side of equation (2.46), where $n \geqslant 2$, is the sum of $n-1$ terms, the mth of which contains the average of a product of m $J(\gamma|Q)$'s and $n-m$ $J^*(\gamma|Q)$'s. These averages are very similar to the average of a product of n $J(\gamma|Q)$'s encountered in obtaining the average $\langle B(q|k)\rangle$. They consist of the product of the averages of the n individual factors, plus the sum of terms in which two factors are paired, and the correlated part of the average of their product is multiplied by the product of the averages of the remaining $n-2$ factors, and so on. Since what we really need is not $\langle|B(q|k)|^2\rangle$ but the difference $\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2$, the first category of averages described can be omitted, since it does not contribute to this difference. The second category of averages does, but only if one of the factors in the pair whose correlated average is evaluated is unconjugated while the second is a complex conjugate. The $n-2$ delta functions associated with the product of the averages of the remaining $n-2$ factors that are unpaired yield a result that is proportional to $\eta^{-(n-2)}$ which, combined with the factor of η^n multiplying the nth-order term produces a contribution of order $\mathrm{O}(\eta^2)$ to $\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2$ from each term on the right-hand side of equation (2.46). Thus, an infinite series of terms must be summed to obtain the contribution to $\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2$ of the lowest non-zero order in η, namely the second.

Four classes of terms contribute to $\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2$ in this order, defined by the two factors that appear in the pair whose correlated average is evaluated. They can be written schematically as $\{AA^*\}$, $\{mA^*\}$, $\{Am^*\}$, and $\{mm^*\}$. These four categories of terms can be summed to yield the result that to $O(\eta^2)$

$$
\begin{aligned}
&\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2 \\
&\quad = \eta^2[[1 - X(q) + X(q)^2 - \cdots]\{A(q|k)[1 - X^*(q) + X^*(q)^2 - \cdots]A^*(q|k)\} \\
&\qquad +[1 - X(q) + X(q)^2 - \cdots]\{m(q|k)[1 - X(k) + X(k)^2 - \cdots]a(k) \\
&\qquad \times[1 - X^*(q) + X^*(q)^2 - \cdots]A^*(q|k)\} \\
&\qquad +[1 - X(q) + X(q)^2 - \cdots]\{A(q|k)[1 - X^*(q) + X^*(q)^2 - \cdots]m^*(q|k)\} \\
&\qquad \times[1 - X^*(k) + X^*(k)^2 - \cdots]a^*(k) \\
&\qquad +[1 - X(q) + X(q)^2 - \cdots]\{m(q|k)[1 - X(k) + X(k)^2 - \cdots]a(k) \\
&\qquad \times[1 - X^*(q) + X^*(q)^2 - \cdots]m^*(q|k)\}[1 - X^*(k) + X^*(k)^2 - \cdots]a^*(k)] \\
&\quad = \eta^2 \frac{1}{|1 + X(q)|^2} \frac{1}{|1 + X(k)|^2} \{[A(q|k)(1 + X(k)) + m(q|k)a(k)] \\
&\qquad \times[A^*(q|k)(1 + X^*(k)) + m^*(q|k)a^*(k)]\}
\end{aligned} \tag{2.47}
$$

where the curly bracket symbol has been defined in equation (2.24). The interpretation of the various series that appear in these expressions is identical to that of the series appearing in equations (2.30) and (2.31) in our calculations of $\langle B(q|k)\rangle_{(21)}$ and $\langle B(q|k)\rangle_{(22)}$. Using the explicit expressions for $X(k)$ and $a(k)$, equations (2.27*b*) and (2.28*b*), respectively, we can rewrite equation (2.47) in the form

$$
\begin{aligned}
\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2 &= \eta^2\, e^{\mathrm{Re}\,(\alpha(q)-\alpha_0(q))^2\delta^2} e^{\mathrm{Re}\,(\alpha(k)-\alpha_0(k))^2\delta^2} \\
&\quad \times\{[e^{-\frac{1}{2}(\alpha^2(k)+\alpha_0^2(k))\delta^2} b(q|k)][e^{-\frac{1}{2}(\alpha^2(k)+\alpha_0^2(k))\delta^2} b(q|k)]^*\}
\end{aligned} \tag{2.48a}
$$

where

$$
\begin{aligned}
b(q|k) &= \cosh(\alpha(k)\alpha_0(k)\delta^2)[n(q|k) + m(q|k)R_0(k)] \\
&\quad + \sinh(\alpha(k)\alpha_0(k)\delta^2)[n(q|k) - m(q|k)R_0(k)].
\end{aligned} \tag{2.48b}
$$

As it stands, the result given by equation (2.48) is not reciprocal. Reciprocity, which is a consequence of the Lorentz reciprocity theorem [27], requires that the scattering matrix $S(q|k)$ defined by

$$
S(q|k) = \frac{\alpha_0^{1/2}(q)}{\alpha_0^{1/2}(k)} R(q|k) \tag{2.49}
$$

satisfies the relation [28]

$$
S(q|k) = S(-k|-q). \tag{2.50}
$$

In view of equation (2.17) this condition requires that

$$
\langle|B(-k|-q)|^2\rangle - |\langle B(-k|-q)\rangle|^2 = \frac{\alpha_0^2(q)}{\alpha_0^2(k)}[\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2]. \tag{2.51}
$$

The result given by equation (2.48) does not satisfy this condition.

However, it is possible to transform equation (2.48) into a form that is manifestly reciprocal. It is shown in appendix A that

$$
n(q|k) + m(q|k)R_0(k) = \frac{qk - \alpha(q)\alpha(k)}{d(q)d(k)} \frac{J(\alpha(q) + \alpha(k)|q - k)}{\alpha(q) + \alpha(k)} 2\alpha_0(k) + O(\eta) \tag{2.52a}
$$

$$
n(q|k) - m(q|k)R_0(k) = \frac{qk - \alpha(q)\alpha(k)}{d(q)d(k)} \frac{J(\alpha(q) + \alpha(k)|q - k)}{\alpha(q) + \alpha(k)} 2\alpha(k) + O(\eta). \tag{2.52b}
$$

Since we seek a result correct to the lowest order in η, we neglect the corrections to these results of order $O(\eta)$. When these results are used in equation (2.48*b*), we find that

$$\begin{aligned} e^{-\frac{1}{2}(\alpha^2(k)+\alpha_0^2(k))\delta^2} b(q|k) &= \frac{qk - \alpha(q)\alpha(k)}{d(q)d(k)} \frac{J(\alpha(q)+\alpha(k)|q-k)}{\alpha(q)+\alpha(k)} \\ &\quad \times [(\alpha_0(k)+\alpha(k)) e^{-\frac{1}{2}(\alpha(k)-\alpha_0(k))^2\delta^2} + (\alpha_0(k)-\alpha(k)) e^{-\frac{1}{2}(\alpha(k)+\alpha_0(k))^2\delta^2}] \\ &= \frac{qk - \alpha(q)\alpha(k)}{d(q)d(k)} \frac{J(\alpha(q)+\alpha(k)|q-k)}{\alpha(q)+\alpha(k)} \Bigg[2\alpha_0(k) - (\alpha_0^2(k) - \alpha^2(k)) \\ &\quad \times \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\delta^2}{2}\right)^n [(\alpha(k)-\alpha_0(k))^{2n-1} - (\alpha(k)+\alpha_0(k))^{2n-1}] \Bigg]. \end{aligned} \tag{2.53}$$

However, since $\alpha_0^2(k) - \alpha^2(k) = \eta(\omega^2/c^2)$, the second term in brackets is of order $O(\eta)$ and we neglect it. Thus, finally,

$$\begin{aligned} \langle |B(q|k)|^2 \rangle - |\langle B(q|k) \rangle|^2 &= \eta^2 e^{\mathrm{Re}\,(\alpha(q)-\alpha_0(q))^2\delta} e^{\mathrm{Re}\,(\alpha(k)-\alpha_0(k))^2\delta^2} \\ &\quad \times \left| 2\alpha_0(k) \frac{qk - \alpha(q)\alpha(k)}{d(q)d(k)} \right|^2 \left\{ \frac{J(\alpha(q)+\alpha(k)|q-k)}{\alpha(q)+\alpha(k)} \frac{J^*(\alpha(q)+\alpha(k)|q-k)}{\alpha^*(q)+\alpha^*(k)} \right\}. \end{aligned} \tag{2.54}$$

In this form, the reciprocity condition (2.51) is manifestly satisfied.

Using the result that

$$\{J(\gamma|Q)J^*(\gamma|Q)\} = L_1\, e^{-\frac{1}{2}(\gamma^2+\gamma^{*2})\delta^2} \int_{-\infty}^{\infty} du\, e^{-iQu} [e^{|\gamma|^2\delta^2 W(|u|)} - 1] \tag{2.55}$$

together with the result given by equation (2.45), we can write the contribution to the mean DRC from the incoherent component of the scattered x-rays to $O(\eta^2)$ as

$$\left\langle \frac{\partial R}{\partial \theta_s} \right\rangle_{\mathrm{incoh}} = \eta^2 \frac{1}{8\sqrt{\pi}} \left(\frac{\omega a}{c}\right) \frac{1}{\cos\theta_0} \sum_{n=1}^{\infty} \left(\frac{\omega\delta}{c}\right)^{2n} \frac{e^{-(q-k)^2a^2/(4n)}}{n!\sqrt{n}} |\tilde{b}_n^{\mathrm{p}}(\theta_s,\theta_0)|^2 \tag{2.56a}$$

where

$$\begin{aligned} \tilde{b}_n^{\mathrm{p}}(\theta_s,\theta_0) &= \exp\left[-\frac{1}{2} \left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_s - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^2 \right] \\ &\quad \times \exp\left[\frac{1}{2} \left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_s - \eta)^{1/2} - \cos^2\theta_s]^2 \right] \\ &\quad \times \exp\left[\frac{1}{2} \left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_0 - \eta)^{1/2} - \cos\theta_0]^2 \right] \\ &\quad \times 2\cos\theta_s \frac{\sin\theta_s \sin\theta_0 - (\cos^2\theta_s - \eta)^{1/2}(\cos^2\theta_0 - \eta)^{1/2}}{[\epsilon\cos\theta_s + (\cos^2\theta_s - \eta)^{1/2}][\epsilon\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}]} 2\cos\theta_0 \\ &\quad \times [(\cos^2\theta_s - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^{n-1}. \end{aligned} \tag{2.56b}$$

In obtaining the result given by equation (2.56) we have used the Gaussian form for the surface height autocorrelation function given by $W(|u|) = \exp(-u^2/a^2)$.

We can simplify equation (2.56) somewhat if we note that

$$(\cos^2\theta_{0,s} - \eta)^{1/2} - \cos\theta_{0,s} = \frac{-\eta}{(\cos^2\theta_{0,s} - \eta)^{1/2} + \cos\theta_{0,s}}. \tag{2.57}$$

Consequently, we can replace the second and third exponential factors on the right-hand side of equation (2.56*b*) by unity, in the approximation we are maintaining here. These replacements are equivalent to the assumption that $(\omega\delta/c)\sqrt{\eta(\omega)} \ll 1$. We can also replace the explicit factor of ϵ in the denominator of equation (2.56*b*) by unity to the same degree of approximation. As a result, we obtain, finally,

$$\tilde{b}_n^{\mathrm{p}}(\theta_{\mathrm{s}}, \theta_0) = \exp\left[-\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^2\right] \times 2\cos\theta_{\mathrm{s}} \frac{\sin\theta_{\mathrm{s}}\sin\theta_0 - (\cos^2\theta_{\mathrm{s}} - \eta)^{1/2}(\cos^2\theta_0 - \eta)^{1/2}]}{[\epsilon\cos\theta_{\mathrm{s}} + (\cos^2\theta_{\mathrm{s}} - \eta)^{1/2}][\epsilon\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}]} 2\cos\theta_0 \times [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^{n-1}. \tag{2.58}$$

In the case of the scattering of x-rays of s-polarization we can repeat the calculations presented in this subsection starting from equation (2.41). As a result we obtain for $\tilde{b}_n^{\mathrm{s}}(\theta_{\mathrm{s}}, \theta_0)$ instead of equation (2.56*b*)

$$\tilde{b}_n^{\mathrm{s}}(\theta_{\mathrm{s}}, \theta_0) = \exp\left[-\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^2\right] \times \exp\left[\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} - \cos^2\theta_{\mathrm{s}}]^2\right] \times \exp\left[\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_0 - \eta)^{1/2} - \cos\theta_0]^2\right] \times \frac{2\cos\theta_{\mathrm{s}}}{\cos\theta_{\mathrm{s}} + (\cos^2\theta_{\mathrm{s}} - \eta)^{1/2}} \frac{2\cos\theta_0}{\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}} \times [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^{n-1}. \tag{2.59}$$

As in the case of the scattering of p-polarized x-rays, we can replace the second and third exponential factors on the right-hand side of equation (2.59) by unity and finally obtain

$$\tilde{b}_n^{\mathrm{s}}(\theta_{\mathrm{s}}, \theta_0) = \exp\left[-\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2 [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^2\right] \times \frac{2\cos\theta_{\mathrm{s}}}{\cos\theta_{\mathrm{s}} + (\cos^2\theta_{\mathrm{s}} - \eta)^{1/2}} \frac{2\cos\theta_0}{\cos\theta_0 + (\cos^2\theta_0 - \eta)^{1/2}} \times [(\cos^2\theta_{\mathrm{s}} - \eta)^{1/2} + (\cos^2\theta_0 - \eta)^{1/2}]^{n-1}. \tag{2.60}$$

When both θ_0 and θ_{s} are close to $\pi/2$, i.e. for small grazing angles of incidence and scattering, the factor $\sin\theta_{\mathrm{s}}\sin\theta_0 - (\cos^2\theta_{\mathrm{s}} - \eta)^{1/2}(\cos^2\theta_0 - \eta)^{1/2}$ is close to unity, and the expressions for the contribution to the mean DRC from the incoherent component of the scattered x-rays of p- and s-polarizations coincide.

3. A two-dimensional random surface

With the results for the one-dimensional surface as a guide, we can obtain the corresponding results for a two-dimensional randomly rough surface quite directly. The physical system we consider in this section consists of vacuum in the region $x_3 > \zeta(\boldsymbol{x}_\parallel)$, where $\boldsymbol{x}_\parallel = (x_1, x_2, 0)$ is a position vector in the mean scattering plane $x_3 = 0$, and the scattering medium, which is characterized by an isotropic, complex, frequency-dependent dielectric function $\epsilon(\omega)$, in the region $x_3 < \zeta(\boldsymbol{x}_\parallel)$. The surface profile function $\zeta(\boldsymbol{x}_\parallel)$ is assumed to be a single-valued function of $\boldsymbol{x}_\parallel$ that is differentiable with respect to x_1 and x_2 as many times as necessary.

It also constitutes a stationary, zero-mean, isotropic Gaussian random process, which is defined by the properties

$$\langle \zeta(\boldsymbol{x}_\parallel)\rangle = 0 \tag{3.1}$$

$$\langle \zeta(\boldsymbol{x}_\parallel)\zeta(\boldsymbol{x}'_\parallel)\rangle = \delta^2 W(|\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel|) \tag{3.2}$$

$$\delta^2 = \langle \zeta^2(\boldsymbol{x}_\parallel)\rangle. \tag{3.3}$$

For the surface height autocorrelation function $W(|\boldsymbol{x}_\parallel|)$ we shall again assume a Gaussian form

$$W(|\boldsymbol{x}_\parallel|) = \exp(-x_\parallel^2/a^2). \tag{3.4}$$

The contribution to the mean DRC when an incident electromagnetic wave of β-polarization, whose wavevector $\boldsymbol{k}$ has the projection $\boldsymbol{k}_\parallel = (k_1, k_2, 0)$ on the mean scattering surface, is scattered into an electromagnetic wave of α-polarization, within an element of solid angle $\mathrm{d}\Omega_\mathrm{s}$ about a wavevector $\boldsymbol{q}$ whose projection on the mean scattering surface is $\boldsymbol{q}_\parallel = (q_1, q_2, 0)$, is given in terms of the corresponding scattering amplitude $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ by

$$\left\langle \frac{\partial R}{\partial \Omega_\mathrm{s}} \right\rangle_{\alpha\beta} = \frac{1}{S}\left(\frac{\omega}{2\pi c}\right)^2 \frac{\cos^2\theta_\mathrm{s}}{\cos\theta_0} \langle |R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\rangle \tag{3.5}$$

where S is the area of the x_1x_2-plane covered by the rough surface, while

$$\boldsymbol{k}_\parallel = (\omega/c)\sin\theta_0 \times (\cos\phi_0, \sin\phi_0, 0)$$

$$\boldsymbol{q}_\parallel = (\omega/c)\sin\theta_\mathrm{s}(\cos\phi_\mathrm{s}, \sin\phi_\mathrm{s}, 0)$$

where (θ_0, ϕ_0) and $(\theta_\mathrm{s}, \phi_\mathrm{s})$ are the polar and azimuthal angles of incidence and scattering, respectively (see figure 2). The contributions to the mean DRC from the coherent and incoherent components of the scattered electromagnetic field are

$$\left\langle \frac{\partial R}{\partial \Omega_\mathrm{s}} \right\rangle_{\substack{\alpha\beta\\ \mathrm{coh}}} = \frac{1}{S}\left(\frac{\omega}{2\pi c}\right)^2 \frac{\cos^2\theta_\mathrm{s}}{\cos\theta_0} |\langle R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle|^2 \tag{3.6}$$

and

$$\left\langle \frac{\partial R}{\partial \Omega_\mathrm{s}} \right\rangle_{\substack{\alpha\beta\\ \mathrm{incoh}}} = \frac{1}{S}\left(\frac{\omega}{2\pi c}\right)^2 \frac{\cos^2\theta_\mathrm{s}}{\cos\theta_0} \left[\langle |R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\rangle - |\langle R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle|^2\right] \tag{3.7}$$

respectively.

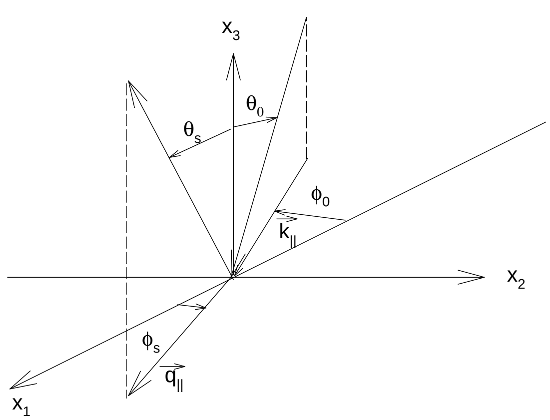

Figure 2. The scattering geometry for scattering from a two-dimensional random surface.

By the use of the method of reduced Rayleigh equations it is found that the scattering amplitudes $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ satisfy the matrix integral equation [15]

$$\int \frac{d^2 p_\parallel}{(2\pi)^2} \frac{I(\alpha(q_\parallel) - \alpha_0(p_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{p}_\parallel)}{\alpha(q_\parallel) - \alpha_0(p_\parallel))} \mathbf{M}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{R}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) = -\frac{I(\alpha(q_\parallel) + \alpha_0(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)}{\alpha(q_\parallel) + \alpha_0(k_\parallel)} \mathbf{N}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel), \tag{3.8}$$

where

$$I(\gamma|\boldsymbol{Q}_\parallel) = \int d^2 x_\parallel e^{-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel} e^{-i\gamma\zeta(\boldsymbol{x}_\parallel)} \tag{3.9}$$

while the matrices $\mathbf{M}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)$ and $\mathbf{N}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ are given by

$$\mathbf{M}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel) = \begin{pmatrix} [q_\parallel p_\parallel + \alpha(q_\parallel)\hat{q}_\parallel \cdot \hat{p}_\parallel \alpha_0(p_\parallel)] & -(\omega/c)\alpha(q_\parallel)(\hat{q}_\parallel \times \hat{p}_\parallel)_3 \\ (\omega/c)(\hat{q}_\parallel \times \hat{p}_\parallel)_3 \alpha_0(p_\parallel) & (\omega^2/c^2)\hat{q}_\parallel \cdot \hat{p}_\parallel \end{pmatrix} \tag{3.10}$$

$$\mathbf{N}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \begin{pmatrix} [q_\parallel k_\parallel - \alpha(q_\parallel)\hat{q}_\parallel \cdot \hat{k}_\parallel \alpha_0(k_\parallel)] & -(\omega/c)\alpha(q_\parallel)(\hat{q}_\parallel \times \hat{k}_\parallel)_3 \\ -(\omega/c)(\hat{q}_\parallel \times \hat{k}_\parallel)_3 \alpha_0(k_\parallel) & (\omega^2/c^2)\hat{q}_\parallel \cdot \hat{k}_\parallel \end{pmatrix}. \tag{3.11}$$

In these expressions $\hat{k}_\parallel = \boldsymbol{k}_\parallel/k_\parallel$, $\alpha_0(q_\parallel) = [(\omega^2/c^2) - q_\parallel^2]^{1/2}$, with $\mathrm{Re}\,\alpha_0(q_\parallel) > 0$, $\mathrm{Im}\,\alpha_0(q_\parallel) > 0$, and $\alpha(q_\parallel) = [\epsilon(\omega^2/c^2) - q_\parallel^2]^{1/2}$, with $\mathrm{Re}\,\alpha(q_\parallel) > 0$, $\mathrm{Im}\,\alpha(q_\parallel) > 0$. In equations (3.10) and (3.11) the rows and columns of the matrices are labelled by p and s, with the pp-element in the upper left-hand corner.

To solve equation (3.8), we begin by rewriting the function $I(\gamma|\boldsymbol{Q}_\parallel)$ in the form

$$I(\gamma|\boldsymbol{Q}_\parallel) = (2\pi)^2\delta(\boldsymbol{Q}_\parallel) + J(\gamma|\boldsymbol{Q}_\parallel) \tag{3.12}$$

where

$$J(\gamma|\boldsymbol{Q}_\parallel) = \int d^2 x_\parallel\, e^{-i\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel}(e^{-i\gamma\zeta(\boldsymbol{x}_\parallel)} - 1). \tag{3.13}$$

When equation (3.12) is substituted into equation (3.8), the result can be rearranged into

$$\mathbf{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel) + \eta\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) + \eta\int \frac{d^2 p_\parallel}{(2\pi)^2}\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{R}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) \tag{3.14}$$

where

$$\mathbf{R}^{(0)}(k_\parallel) = \begin{pmatrix} \dfrac{\epsilon\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)} & 0 \\ 0 & \dfrac{\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\alpha_0(k_\parallel) + \alpha(k_\parallel)} \end{pmatrix} \tag{3.15}$$

$$\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \begin{pmatrix} \dfrac{N_{pp}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\epsilon\alpha_0(q_\parallel) + \alpha(q_\parallel)} & \dfrac{N_{ps}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\epsilon\alpha_0(q_\parallel) + \alpha(q_\parallel)} \\ \dfrac{N_{sp}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\alpha_0(q_\parallel) + \alpha(q_\parallel)} & \dfrac{N_{ss}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\alpha_0(q_\parallel) + \alpha(q_\parallel)} \end{pmatrix} \frac{J(\alpha(q_\parallel) + \alpha_0(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)}{\alpha(q_\parallel) + \alpha_0(p_\parallel)} \tag{3.16a}$$

$$\equiv \hat{\mathbf{n}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)J(\alpha(q_\parallel) + \alpha_0(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \tag{3.16b}$$

$$\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \begin{pmatrix} \dfrac{M_{pp}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\epsilon\alpha_0(q_\parallel) + \alpha(q_\parallel)} & \dfrac{M_{ps}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\epsilon\alpha_0(q_\parallel) + \alpha(q_\parallel)} \\ \dfrac{M_{sp}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\alpha_0(q_\parallel) + \alpha(q_\parallel)} & \dfrac{M_{ss}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)}{\alpha_0(q_\parallel) + \alpha(q_\parallel)} \end{pmatrix} \frac{J(\alpha(q_\parallel) - \alpha_0(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)}{\alpha(q_\parallel) - \alpha_0(k_\parallel)} \tag{3.17a}$$

$$\equiv \hat{\mathbf{m}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)J(\alpha(q_\parallel)) - \alpha_0(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel). \tag{3.17b}$$

We shall seek a solution of equation (3.14) in the form

$$\mathbf{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel) + \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \tag{3.18}$$

where the 2×2 matrix $\mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ is the solution of the equation

$$\mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \eta\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) + \eta\int\frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{B}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel) \tag{3.19}$$

where

$$\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) + \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel). \tag{3.20}$$

The iterative solution of equation (3.19) is

$$\begin{aligned}\mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) &= \eta\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) + \eta^2\int\frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{A}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\\ &\quad+\eta^3\int\frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\int\frac{\mathrm{d}^2p'_\parallel}{(2\pi)^2}\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{m}(\boldsymbol{p}_\parallel|\boldsymbol{p}'_\parallel)\mathbf{A}(\boldsymbol{p}'_\parallel|\boldsymbol{k}_\parallel) + \cdots.\end{aligned} \tag{3.21}$$

3.1. Coherent scattering

We see from equation (3.6) that the calculation of the contribution to the mean DRC from the coherent component of the scattered electromagnetic field requires the calculation of the average of the matrix $\mathbf{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ over the ensemble of realizations of the surface profile function. From equation (3.18) we see that, in turn, this requires the determination of the ensemble average of the matrix $\mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$. The latter is given formally by

$$\begin{aligned}\langle\mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle &= \eta\langle\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle + \eta^2\int\frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\langle\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{A}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\rangle\\ &\quad+\eta^3\int\frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\int\frac{\mathrm{d}^2p'_\parallel}{(2\pi)^2}\langle\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)\mathbf{m}(\boldsymbol{p}_\parallel|\boldsymbol{p}'_\parallel)\mathbf{A}(\boldsymbol{p}'_\parallel|\boldsymbol{k}_\parallel)\rangle + \cdots.\end{aligned} \tag{3.22}$$

From the forms of the matrices $\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ and $\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ given by equations (3.15)–(3.17) and (3.20), we see that the nth term in this expansion contains the average of a product of n $J(\gamma|\boldsymbol{Q}_\parallel)$ functions. This average is given by

$$\begin{aligned}\langle J(\gamma_1|\boldsymbol{Q}_\parallel^{(1)})J(\gamma_2|\boldsymbol{Q}_\parallel^{(2)})\cdots J(\gamma_n|\boldsymbol{Q}_\parallel^{(n)})\rangle &= \prod_{i=1}^{n}(2\pi)^2\delta(\boldsymbol{Q}_\parallel^{(i)})(\mathrm{e}^{-\frac{1}{2}\gamma_i^2\delta^2}-1)\\ &\quad+\theta(n-2)\sum_{\substack{i,j=1\\(i>j)}}^{n}(2\pi)^2\delta(\boldsymbol{Q}_\parallel^{(i)}+\boldsymbol{Q}_\parallel^{(j)})\mathrm{e}^{-\frac{1}{2}(\gamma_i^2+\gamma_j^2)\delta^2}\\ &\quad\times\int\mathrm{d}^2u_\parallel\,\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}_\parallel^{(i)}\cdot\boldsymbol{u}_\parallel}(\mathrm{e}^{-\gamma_i\gamma_j\delta^2W(|\boldsymbol{u}_\parallel|)}-1)\prod_{\substack{k=1\\(k\neq i,j)}}^{n}(2\pi)^2\delta(\boldsymbol{Q}_\parallel^{(k)})(\mathrm{e}^{-\frac{1}{2}\gamma_k^2\delta^2}-1)\\ &\quad+\text{ terms containing } n-2 \text{ or few delta functions}\end{aligned} \tag{3.23a}$$

$$\begin{aligned}&= \prod_{i=1}^{n}\langle J(\gamma_i|\boldsymbol{Q}_\parallel^{(i)})\rangle + \theta(n-2)\sum_{\substack{i,j=1\\(i>j)}}^{n}\{J(\gamma_i|\boldsymbol{Q}_\parallel^{(i)})J(\gamma_j|\boldsymbol{Q}_\parallel^{(j)})\}\prod_{\substack{k=1\\(k\neq i,j)}}^{n}\langle J(\gamma_k|\boldsymbol{Q}_\parallel^{(k)})\rangle\\ &\quad+\text{ terms containing } n-2 \text{ or fewer delta functions.}\end{aligned} \tag{3.23b}$$

We now note that the averages of the matrices $\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ and $\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ are diagonal and inversely proportional to η,

$$\langle\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle = (2\pi)^2\delta(\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel)\left[\frac{\mathbf{a}(k_\parallel)}{\eta}\right] \tag{3.24a}$$

where

$$\mathbf{a}(k_\parallel) = \left[\mathrm{e}^{-\frac{1}{2}(\alpha(k_\parallel)+\alpha_0(k_\parallel))^2\delta^2} - \mathrm{e}^{-\frac{1}{2}(\alpha(k_\parallel)-\alpha_0(k_\parallel))^2\delta^2}\right]\mathbf{R}^{(0)}(k_\parallel) \tag{3.24b}$$

while

$$\langle \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\mathbf{I}\left[-\frac{X(k_\parallel)}{\eta}\right] \tag{3.25a}$$

with

$$X(k_\parallel) = \mathrm{e}^{-\frac{1}{2}(\alpha(k_\parallel)-\alpha_0(k_\parallel))^2\delta^2} - 1. \tag{3.25b}$$

These results, together with the result expressed by the first term on the right-hand side of equation (3.23), have the consequence that the contribution to $\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle$ of zero order in η is obtained by replacing each average on the right-hand side of equation (3.22) by the product of the averages of the individual factors appearing in it. In this way we find that

$$\begin{aligned}\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(0)} &= (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)[1 - X(k_\parallel) + X(k_\parallel)^2 - \cdots]\mathbf{a}(k_\parallel)\\ &= (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)[\mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2} - 1]\mathbf{R}^{(0)}(k_\parallel).\end{aligned} \tag{3.26}$$

To obtain the leading contribution to $\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle$ that is of non-zero order in η, according to the second term on the right-hand side of equation (3.23), we must pair two of the factors in each of the averages on the right-hand side of equation (3.22) in all possible ways, evaluate the correlated average of that pair, and multiply the result by the product of the averages of each of the remaining factors. As in the case of a one-dimensional surface, there are two types of terms that arise in nth order. In the first, the final factor $\mathbf{A}(\boldsymbol{p}_\parallel^{(n-1)}|\boldsymbol{k}_\parallel)$ is paired with one of the factors $\mathbf{m}(\boldsymbol{p}_\parallel^{(i)}|\boldsymbol{p}_\parallel^{(j)})$ and the correlated average of their product is evaluated. In the second, the final factor $\mathbf{A}(\boldsymbol{p}_\parallel^{(n-1)}|\boldsymbol{k}_\parallel)$ is unpaired with any of the $\mathbf{m}(\boldsymbol{p}_\parallel^{(i)}|\boldsymbol{p}_\parallel^{(j)})$, and only its average appears. The contribution to $\langle \boldsymbol{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle$ from all terms of the first type is

$$\begin{aligned}\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(21)} &= \eta^2[1 - X(q_\parallel) + X(q_\parallel)^2 - \cdots]\\ &\times\int \frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\{\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)[1 - X(p_\parallel) + X(p_\parallel)^2 - \cdots]\mathbf{A}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\}.\end{aligned} \tag{3.27}$$

The contribution to $\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle$ from all terms of the second type is

$$\begin{aligned}\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(22)} &= \eta^2[1 - X(q_\parallel) + X(q_\parallel)^2 - \cdots]\\ &\times\int \frac{\mathrm{d}^2p_\parallel}{(2\pi)^2}\{\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{p}_\parallel)[1 - X(p_\parallel) + X(p_\parallel)^2 - \cdots]\mathbf{m}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\}\\ &\times[1 - X(k_\parallel) + X(k_\parallel)^2 - \cdots]\mathbf{a}(k_\parallel).\end{aligned} \tag{3.28}$$

In obtaining these results we have exploited the fact that the average of the matrix $\mathbf{m}(\boldsymbol{p}_\parallel^{(i)}|\boldsymbol{p}_\parallel^{(j)})$ is a multiple of the unit matrix.

Using the explicit expressions for the function $X(k_\parallel)$ and the matrices $\mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, $\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, $\mathbf{A}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, and $\mathbf{a}(k_\parallel)$, given by equations (3.25*b*), (3.17), (3.16), (3.20), and (3.24*b*), respectively, together with the result that

$$\begin{aligned}\{J(\gamma_1|\boldsymbol{Q}_\parallel^{(1)})J(\gamma_2|\boldsymbol{Q}_\parallel^{(2)})\} &= (2\pi)^2\delta(\boldsymbol{Q}_\parallel^{(1)} + \boldsymbol{Q}_\parallel^{(2)})\\ &\times\mathrm{e}^{-\frac{1}{2}(\gamma_1^2+\gamma_2^2)\delta^2}\int \mathrm{d}^2u_\parallel\,\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}_\parallel^{(1)}\cdot\boldsymbol{u}_\parallel}(\mathrm{e}^{-\gamma_1\gamma_2\delta^2W(|\boldsymbol{u}_\parallel|)} - 1)\end{aligned} \tag{3.29}$$

we can rewrite equations (3.27) and (3.28) in the forms

$$\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(21)} = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\eta^2[\mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2}\mathbf{N}(k_\parallel) + \mathbf{M}(k_\parallel)\mathbf{R}^{(0)}(k_\parallel)] \tag{3.30}$$

and

$$\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(22)} = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\eta^2[\mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2} - 1]\mathbf{M}(k_\parallel)\mathbf{R}^{(0)}(k_\parallel) \tag{3.31}$$

respectively, where

$$\mathbf{N}(k_\parallel) = \int \frac{\mathrm{d}^2 p_\parallel}{(2\pi)^2}\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{n}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\mathrm{e}^{-(\alpha(p_\parallel)-\alpha(k_\parallel))(\alpha_0(k_\parallel)+\alpha_0(p_\parallel))\delta^2} \times \int \mathrm{d}^2 u_\parallel\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}_\parallel-\boldsymbol{p}_\parallel)\cdot\boldsymbol{u}_\parallel}(\mathrm{e}^{-(\alpha(k_\parallel)-\alpha_0(p_\parallel))(\alpha(p_\parallel)+\alpha_0(k_\parallel))\delta^2 W(|\boldsymbol{u}_\parallel|)} - 1) \tag{3.32}$$

$$\mathbf{M}(k_\parallel) = \int \frac{\mathrm{d}^2 p_\parallel}{(2\pi)^2}\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{m}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)\mathrm{e}^{-(\alpha(p_\parallel))-\alpha(k_\parallel))(\alpha_0(p_\parallel)-\alpha_0(k_\parallel))\delta^2} \times \int \mathrm{d}^2 u_\parallel\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}_\parallel-\boldsymbol{p}_\parallel)\cdot\boldsymbol{u}_\parallel}(\mathrm{e}^{-(\alpha(k_\parallel)-\alpha_0(p_\parallel))(\alpha(p_\parallel))-\alpha_0(k_\parallel))\delta^2 W(|\boldsymbol{u}_\parallel|)} - 1). \tag{3.33}$$

The total contribution to $\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle$ of second order in η is the sum of the contributions given by equations (3.30) and (3.31), and is given by

$$\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(2)} = (2\pi)^2\delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)\eta^2\mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2}[\mathbf{N}(k_\parallel) + \mathbf{M}(k_\parallel)\mathbf{R}^{(0)}(k_\parallel)]. \tag{3.34}$$

We now note that the elements of the matrix $\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{n}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ are given by

$$\mathrm{pp}: \quad \frac{[k_\parallel p_\parallel + \alpha(k_\parallel)\hat{k}_\parallel\cdot\hat{p}_\parallel\alpha_0(p_\parallel)][p_\parallel k_\parallel - \alpha(p_\parallel)\hat{p}_\parallel\cdot\hat{k}_\parallel\alpha_0(k_\parallel)]}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel)) - \alpha_0(p_\parallel))d_\mathrm{p}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} - \frac{\omega^2 c^{-2}\alpha(k_\parallel)(\hat{k}_\parallel\times\hat{p}_\parallel)_3^2\alpha_0(k_\parallel)}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} \tag{3.35a}$$

$$\mathrm{ps}: \quad \frac{\omega}{c}(\hat{k}_\parallel\times\hat{p}_\parallel)_3\left\{\frac{[k_\parallel p_\parallel + \alpha(k_\parallel)\hat{k}_\parallel\cdot\hat{p}_\parallel\alpha_0(p_\parallel)]\alpha(p_\parallel)}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{p}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} - \frac{\omega^2 c^{-2}\alpha(k_\parallel)\hat{p}_\parallel\cdot\hat{k}_\parallel}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))}\right\} \tag{3.35b}$$

$$\mathrm{sp}: \quad \frac{\omega}{c}(\hat{k}_\parallel\times\hat{p}_\parallel)_3\left\{\frac{\alpha_0(p_\parallel)[p_\parallel k_\parallel - \alpha(p_\parallel)\hat{p}_\parallel\cdot\hat{k}_\parallel\alpha_0(k_\parallel)]}{d_\mathrm{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{p}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} + \frac{\omega^2 c^{-2}\hat{k}_\parallel\cdot\hat{p}_\parallel\alpha_0(k_\parallel)}{d_\mathrm{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))}\right\} \tag{3.35c}$$

$$\mathrm{ss}: \quad \frac{\omega^2 c^{-2}\alpha_0(p_\parallel)(\hat{k}_\parallel\times\hat{p}_\parallel)_3^2\alpha(p_\parallel)}{d_\mathrm{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} + \frac{\omega^4 c^{-4}(\hat{k}_\parallel\cdot\hat{p}_\parallel)^2}{d_\mathrm{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) + \alpha_0(k_\parallel))} \tag{3.35d}$$

while the elements of the matrix $\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{m}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ are

$$\mathrm{pp}: \quad \frac{[k_\parallel p_\parallel + \alpha(k_\parallel)\hat{k}_\parallel\cdot\hat{p}_\parallel\alpha_0(p_\parallel)][p_\parallel k_\parallel - \alpha(p_\parallel)\hat{p}_\parallel\cdot\hat{k}_\parallel\alpha_0(k_\parallel)]}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{p}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} + \frac{\omega^2 c^{-2}\alpha(k_\parallel)(\hat{k}_\parallel\times\hat{p}_\parallel)_3^2\alpha_0(k_\parallel)}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(k_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} \tag{3.36a}$$

$$\mathrm{ps}: \quad \frac{\omega}{c}(\hat{k}_\parallel\times\hat{p}_\parallel)_3\left\{\frac{[k_\parallel p_\parallel + \alpha(k_\parallel)\hat{k}_\parallel\cdot\hat{p}_\parallel\alpha_0(p_\parallel)]\alpha(p_\parallel)}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{p}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} - \frac{\omega^2 c^{-2}\alpha(k_\parallel)\hat{p}_\parallel\cdot\hat{k}_\parallel}{d_\mathrm{p}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\mathrm{s}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))}\right\} \tag{3.36b}$$

$$\text{sp}: \quad \frac{\omega}{c}(\hat{k}_\parallel \times \hat{p}_\parallel)_3 \left\{ \frac{\alpha_0(p_\parallel)[p_\parallel k_\parallel + \alpha(p_\parallel)\hat{p}_\parallel \cdot \hat{k}_\parallel \alpha_0(k_\parallel)]}{d_\text{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\text{p}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} - \frac{\omega^2 c^{-2}\hat{k}_\parallel \cdot \hat{p}_\parallel \alpha_0(k_\parallel)}{d_\text{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\text{s}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} \right\} \tag{3.36c}$$

$$\text{ss}: \quad \frac{\omega^2 c^{-2}\alpha_0(p_\parallel)(\hat{k}_\parallel \times \hat{p}_\parallel)_3^2 \alpha(p_\parallel)}{d_\text{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\text{s}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} + \frac{\omega^4 c^{-4}(\hat{k}_\parallel \cdot \hat{p}_\parallel)^2}{d_\text{s}(k_\parallel)(\alpha(k_\parallel) - \alpha_0(p_\parallel))d_\text{s}(p_\parallel)(\alpha(p_\parallel) - \alpha_0(k_\parallel))} \tag{3.36d}$$

where $d_\text{p}(k_\parallel) = \epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)$ and $d_\text{s}(k_\parallel) = \alpha_0(k_\parallel) + \alpha(k_\parallel)$. With the aid of these results and the definitions (3.32) and (3.33) we can see that the matrices $\mathbf{N}(k_\parallel)$ and $\mathbf{M}(k_\parallel)$ are diagonal and depend on the wavevector $\boldsymbol{k}_\parallel$ only through its magnitude. This follows from the results that when the integrals over the azimuthal angle of $\boldsymbol{u}_\parallel$ are carried out in equations (3.32) and (3.33), the integrals over the magnitude of $\boldsymbol{u}_\parallel$ become

$$2\pi \int_0^\infty \mathrm{d}u_\parallel\, u_\parallel J_0(u_\parallel[k_\parallel^2 - 2k_\parallel p_\parallel \hat{k}_\parallel \cdot \hat{p}_\parallel + p_\parallel^2]^{1/2}) \times \left(\exp[-(\alpha(k_\parallel) - \alpha_0(p_\parallel))(\alpha(p_\parallel) + \alpha_0(k_\parallel))\delta^2 W(u_\parallel)] - 1\right) \tag{3.37a}$$

and

$$2\pi \int_0^\infty \mathrm{d}u_\parallel\, u_\parallel J_0(u_\parallel[k_\parallel^2 - 2k_\parallel p_\parallel \hat{k}_\parallel \cdot \hat{p}_\parallel + p_\parallel^2]^{1/2}) \times \left(\exp[-(\alpha(k_\parallel) - \alpha_0(p_\parallel))(\alpha(p_\parallel) - \alpha_0(k_\parallel))\delta^2 W(u_\parallel)] - 1\right) \tag{3.37b}$$

respectively, where $J_0(x)$ is a Bessel function. Thus they depend on the azimuthal angles of $\boldsymbol{k}_\parallel$ and $\boldsymbol{p}_\parallel$, ϕ_0 and ϕ_p, respectively, only through the combination $\hat{k}_\parallel \cdot \hat{p}_\parallel = \cos(\phi_0 - \phi_\text{p})$. At the same time, the ps and sp elements of the matrices $\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{n}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ and $\hat{\mathbf{m}}(\boldsymbol{k}_\parallel|\boldsymbol{p}_\parallel)\hat{\mathbf{m}}(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel)$ are proportional to $(\hat{k}_\parallel \times \hat{p}_\parallel)_3 = -\sin(\phi_0 - \phi_\text{p})$, in addition to containing a dependence on $\cos(\phi_0 - \phi_\text{p})$. As a result, the integral over the azimuthal angle of $\boldsymbol{p}_\parallel$ appearing in the definitions of these elements in equations (3.32) and (3.33) vanishes, because it is an odd function of $\phi_0 - \phi_\text{p}$. Consequently the matrix $\langle \mathbf{B}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle_{(2)}$ is diagonal, as it should be. After the corresponding integrals in the expressions for the diagonal elements of the matrices $\mathbf{N}(k_\parallel)$ and $\mathbf{M}(k_\parallel)$ have been carried out, their remaining dependence on the wavevector $\boldsymbol{k}_\parallel$ is only through its magnitude.

It follows from this result, equation (3.18), and equation (3.26) that to order $\mathrm{O}(\eta^2)$

$$\langle \mathbf{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle = (2\pi)^2 \delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \begin{pmatrix} r_\text{p}(k_\parallel) & 0 \\ 0 & r_\text{s}(k_\parallel) \end{pmatrix} \tag{3.38}$$

where

$$r_\text{p}(k_\parallel) = \mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2} \left[\frac{\epsilon\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)} + \eta^2 (N_\text{pp}(k_\parallel) + \frac{\epsilon\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)} M_\text{pp}(k_\parallel)) \right] \tag{3.39a}$$

$$r_\text{s}(k_\parallel) = \mathrm{e}^{-2\alpha_0(k_\parallel)\alpha(k_\parallel)\delta^2} \left[\frac{\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\alpha_0(k_\parallel) + \alpha(k_\parallel)} + \eta^2 (N_\text{ss}(k_\parallel) + \frac{\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\alpha_0(k_\parallel) + \alpha(k_\parallel)} M_\text{ss}(k_\parallel)) \right]. \tag{3.39b}$$

When the result given by equations (3.38) is substituted into equation (3.6), and use is made of the results that in two dimensions

$$[(2\pi)^2 \delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)]^2 = (2\pi)^2 \delta(\mathbf{0})(2\pi)^2 \delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) = S(2\pi)^2 \delta(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \tag{3.40a}$$

and that

$$\delta(\boldsymbol{q}_{\|} - \boldsymbol{k}_{\|}) = \left(\frac{c}{\omega}\right)^2 \frac{\delta(\theta_s - \theta_0)\delta(\phi_s - \phi_0)}{\cos\theta_0 \sin\theta_0} \tag{3.40b}$$

we obtain

$$\left\langle \frac{\partial R}{\partial \Omega_s} \right\rangle_{\substack{\mathrm{pp}\\ \mathrm{coh}}} = \frac{\delta(\theta_s - \theta_0)\delta(\phi_s - \phi_0)}{\sin\theta_0} R_p(\theta_0) \tag{3.41a}$$

$$\left\langle \frac{\partial R}{\partial \Omega_s} \right\rangle_{\substack{\mathrm{ss}\\ \mathrm{coh}}} = \frac{\delta(\theta_s - \theta_0)\delta(\phi_s - \phi_0)}{\sin\theta_0} R_s(\theta_0) \tag{3.41b}$$

where the reflectivities for p- and s-polarized electromagnetic radiation, $R_p(\theta_0)$ and $R_s(\theta_0)$, respectively, are given by

$$R_{p,s}(\theta_0) = \left| r_{p,s}\left(\frac{\omega}{c}\sin\theta_0\right)\right|^2. \tag{3.42}$$

3.2. Incoherent scattering

We now turn to the study of the incoherent scattering of x-rays from a two-dimensional, randomly rough surface. If we substitute equation (3.18) into equation (3.7) we find that we can express the contribution to the mean DRC from the incoherent component of the scattered field in the form

$$\left\langle \frac{\partial R}{\partial \Omega_s} \right\rangle_{\substack{\alpha\beta\\ \mathrm{incoh}}} = \frac{1}{S}\left(\frac{\omega}{2\pi c}\right)^2 \frac{\cos^2\theta_s}{\cos\theta_0} [\langle |B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})|^2\rangle - |\langle B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\rangle|^2]. \tag{3.43}$$

The average $\langle |B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})|^2\rangle$ is given formally by

$$\begin{aligned}\langle |B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})|^2\rangle &= \eta^2 \langle A_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|}) A^*_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\rangle \\ &\quad + \eta^3 \Bigg[\Bigg\langle A_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|}) \int \frac{\mathrm{d}^2 r^{(1)}_{\|}}{(2\pi)^2} [\mathbf{m}^*(\boldsymbol{q}_{\|}|\boldsymbol{r}^{(1)}_{\|})\mathbf{A}^*(\boldsymbol{r}^{(1)}_{\|}|\boldsymbol{k}_{\|})]_{\alpha\beta}\Bigg\rangle \\ &\quad + \Bigg\langle \int \frac{\mathrm{d}^2 p^{(1)}_{\|}}{(2\pi)^2} [\mathbf{m}(\boldsymbol{q}_{\|}|\boldsymbol{p}^{(1)}_{\|})\mathbf{A}(\boldsymbol{p}^{(1)}_{\|}|\boldsymbol{k}_{\|})]_{\alpha\beta} A^*_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\Bigg\rangle\Bigg] + \cdots.\end{aligned} \tag{3.44}$$

To obtain the difference $\langle |B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})|^2\rangle - |\langle B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\rangle|^2$ to the lowest non-zero order in η, the second, in each term on the right-hand side of equation (3.44) we must pair one of the unconjugated matrix elements with one of the elements in complex conjugate form in all possible ways, calculate the correlated average of their product, and then multiply the result by the product of the average of each of the remaining matrix elements. In so doing we recall that the average of $\mathbf{m}(\boldsymbol{p}^{(i)}_{\|}|\boldsymbol{p}^{(j)}_{\|})$ is diagonal in $\boldsymbol{p}^{(i)}_{\|}$ and $\boldsymbol{p}^{(j)}_{\|}$ and is a multiple of the unit matrix, and that the average of the matrix $\mathbf{A}(\boldsymbol{p}^{(i)}_{\|}|\boldsymbol{k}_{\|})$ is diagonal in $\boldsymbol{p}^{(i)}_{\|}$ and $\boldsymbol{k}_{\|}$ and is a diagonal matrix. In this way we find that

$$\begin{aligned}&\langle |B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})|^2\rangle - |\langle B_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\rangle|^2 \\ &\qquad = \eta^2 \Big[[1 - X(q_{\|}) + X(q_{\|})^2 - \cdots]\{A_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})[1 - X^*(q_{\|}) \\ &\qquad\quad + X^*(q_{\|})^2 - \cdots] A^*_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\} \\ &\qquad\quad + [1 - X(q_{\|}) + X(q_{\|})^2 - \cdots]\{m_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})[1 - X(k_{\|}) \\ &\qquad\quad + X(k_{\|})^2 - \cdots] a_{\beta\beta}(k_{\|})[1 - X^*(q_{\|}) + X^*(q_{\|})^2 - \cdots] A^*_{\alpha\beta}(\boldsymbol{q}_{\|}|\boldsymbol{k}_{\|})\}\end{aligned}$$

$$+[1 - X(q_\parallel) + X(q_\parallel)^2 - \cdots]\{A_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[1 - X^*(q_\parallel) + X^*(q_\parallel)^2 - \cdots]$$
$$\times m^*_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\}[1 - X^*(k_\parallel) + X^*(k_\parallel)^2 - \cdots]a^*_{\beta\beta}(k_\parallel)$$
$$+[1 - X(q_\parallel) + X(q_\parallel)^2 - \cdots]\{m_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[1 - X(k_\parallel) + X(k_\parallel)^2 - \cdots]$$
$$\times a_{\beta\beta}(k_\parallel)[1 - X^*(q_\parallel) + X^*(q_\parallel)^2 - \cdots]m^*_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\}$$
$$\left.\times[1 - X^*(k_\parallel) + X^*(k_\parallel)^2 - \cdots]a^*_{\beta\beta}(k_\parallel)\right]$$
$$= \eta^2 \frac{1}{|1 + X(q_\parallel)|^2} \frac{1}{|1 + X(k_\parallel)|^2} \{[A_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)(1 + X(k_\parallel)) + m_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)a_{\beta\beta}(k_\parallel)]$$
$$\times[A^*_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)(1 + X^*(k_\parallel)) + m^*_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)a^*_{\beta\beta}(k_\parallel)]\}. \tag{3.45}$$

Using the explicit expressions for $X(k_\parallel)$ and $a_{\beta\beta}(k_\parallel)$ given by equations (3.25*b*) and (3.24*b*), respectively, we can rewrite equation (3.45) in the form

$$\langle|B_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\rangle - |\langle B_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle|^2 = \eta^2 \mathrm{e}^{\mathrm{Re}\,(\alpha(q_\parallel)-\alpha_0(q_\parallel))^2\delta^2} \mathrm{e}^{\mathrm{Re}\,(\alpha(k_\parallel)-\alpha_0(k_\parallel))^2}\delta^2$$
$$\times\{[\mathrm{e}^{-\frac{1}{2}(\alpha^2(k_\parallel)+\alpha_0^2(k_\parallel))\delta^2} b_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)][\mathrm{e}^{-\frac{1}{2}(\alpha^2(k_\parallel)+\alpha_0^2(k_\parallel))\delta^2} b_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)]^*\} \tag{3.46}$$

where

$$b_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \cosh(\alpha(k_\parallel)\alpha_0(k_\parallel)\delta^2)[n_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) + m_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)R^{(0)}_\beta(k_\parallel)]$$
$$+ \sinh(\alpha(k_\parallel)\alpha_0(k_\parallel)\delta^2)[n_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) - m_{\alpha\beta}(q_\parallel|k_\parallel)R^{(0)}_\beta(k_\parallel)] \tag{3.47}$$

and

$$R^{(0)}_{\mathrm{p}}(k_\parallel) = \frac{\epsilon\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)} \tag{3.48a}$$
$$R^{(0)}_{\mathrm{s}}(k_\parallel) = \frac{\alpha_0(k_\parallel) - \alpha(k_\parallel)}{\alpha_0(k_\parallel) + \alpha(k_\parallel)}. \tag{3.48b}$$

The result given by equation (3.46) is not manifestly reciprocal.

In scattering from a two-dimensional rough surface the elements of the scattering matrix $S_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ defined by

$$S_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \frac{\alpha_0^{1/2}(q_\parallel)}{\alpha_0^{1/2}(k_\parallel)} R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \tag{3.49}$$

satisfy the reciprocity relations [15]

$$S_{\mathrm{pp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = S_{\mathrm{pp}}(-\boldsymbol{k}_\parallel| - \boldsymbol{q}_\parallel) \tag{3.50a}$$
$$S_{\mathrm{ss}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = S_{\mathrm{ss}}(-\boldsymbol{k}_\parallel| - \boldsymbol{q}_\parallel) \tag{3.50b}$$
$$S_{\mathrm{ps}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = -S_{\mathrm{sp}}(-\boldsymbol{k}_\parallel| - \boldsymbol{q}_\parallel). \tag{3.50c}$$

These conditions require that

$$\langle|B_{\alpha\beta}(-\boldsymbol{k}_\parallel| - \boldsymbol{q}_\parallel)|^2\rangle - |\langle B_{\alpha\beta}(-\boldsymbol{k}_\parallel| - \boldsymbol{q}_\parallel)\rangle|^2$$
$$= \frac{\alpha_0^2(q_\parallel)}{\alpha_0^2(k_\parallel)}[\langle|B_{\beta\alpha}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\rangle - |\langle B_{\beta\alpha}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle|^2]. \tag{3.51}$$

The result given by equation (3.46) does not satisfy this condition.

However, as in the one-dimensional case, it is possible to transform equation (3.46) into a form that is manifestly reciprocal. It is shown in appendix B that

$$\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \pm \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel)$$
$$= \mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\frac{J(\alpha(q_\parallel) + \alpha(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)}{\alpha(q_\parallel) + \alpha(k_\parallel)} \begin{pmatrix} 2\alpha_0(k_\parallel) \\ 2\alpha(k_\parallel \end{pmatrix} + \mathrm{O}(\eta) \tag{3.52}$$

where

$$\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = \begin{pmatrix} \dfrac{q_\parallel k_\parallel - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha(k_\parallel)}{d_\mathrm{p}(q_\parallel)d_\mathrm{p}(k_\parallel)} & -\dfrac{\omega}{c}\dfrac{\alpha(q_\parallel)(\hat{q}_\parallel\times\hat{k}_\parallel)_3}{d_\mathrm{p}(q_\parallel)d_\mathrm{s}(k_\parallel)} \\ -\dfrac{\omega}{c}\dfrac{(\hat{q}_\parallel\times\hat{k}_\parallel)_3\alpha(k_\parallel)}{d_\mathrm{s}(q_\parallel)d_\mathrm{p}(k_\parallel)} & \dfrac{\omega^2}{c^2}\dfrac{\hat{q}_\parallel\cdot\hat{k}_\parallel}{d_\mathrm{s}(q_\parallel)d_\mathrm{s}(k_\parallel)} \end{pmatrix}. \tag{3.53}$$

Note that the matrix $\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ satisfies the reciprocity conditions (3.50). It follows, therefore, that

$$\begin{aligned} \mathrm{e}^{-\frac{1}{2}(\alpha^2(k_\parallel)+\alpha_0^2(k_\parallel))\delta^2}\mathbf{b}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) &= \Big[(\alpha_0(k_\parallel)+\alpha(k_\parallel))\mathrm{e}^{-\frac{1}{2}(\alpha_0(k_\parallel)+\alpha(k_\parallel))^2\delta^2} \\ &\quad +(\alpha_0(k_\parallel)-\alpha(k_\parallel))\mathrm{e}^{-\frac{1}{2}(\alpha_0(k_\parallel)+\alpha(k_\parallel))^2\delta^2}\Big]\frac{J(\alpha(q_\parallel)+\alpha(k_\parallel)|\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel)}{\alpha(q_\parallel)+\alpha(k_\parallel)}\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \\ &= \Big[2\alpha_0(k_\parallel) - (\alpha_0^2(k_\parallel)-\alpha^2(k_\parallel))\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-\delta^2}{2}\right)^n \\ &\quad \times[(\alpha(k_\parallel)-\alpha_0(k_\parallel))^{2n-1} - (\alpha(k_\parallel)+\alpha_0(k_\parallel))^{2n-1}]\Big] \\ &\quad \times\frac{J(\alpha(q_\parallel)+\alpha(k_\parallel)|\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel)}{\alpha(q_\parallel)+\alpha(k_\parallel)}\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel). \end{aligned} \tag{3.54}$$

However, in view of the relation

$$\alpha_0^2(k_\parallel) = \alpha^2(k_\parallel) + \eta(\omega^2/c^2) \tag{3.55}$$

the second term in brackets is of order $\mathrm{O}(\eta)$, and we neglect it. Thus, finally, we have the result that

$$\begin{aligned} \langle|B_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\rangle - |\langle B_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\rangle|^2 &= \eta^2\mathrm{e}^{\mathrm{Re}\,(\alpha(q_\parallel)-\alpha_0(q_\parallel))^2\delta^2}\mathrm{e}^{\mathrm{Re}\,(\alpha(k_\parallel)-\alpha_0(k_\parallel))^2\delta^2} \\ &\quad \times|2\alpha_0(k_\parallel)P_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)|^2\Bigg\{\frac{J(\alpha(q_\parallel)+\alpha(k_\parallel)|\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel)}{\alpha(q_\parallel)+\alpha(k_\parallel)} \\ &\quad \times\frac{J^*(\alpha(q_\parallel)+\alpha(k_\parallel)|\boldsymbol{q}_\parallel-\boldsymbol{k}_\parallel)}{\alpha^*(q_\parallel)+\alpha^*(k_\parallel)}\Bigg\}. \end{aligned} \tag{3.56}$$

In this form the reciprocity condition (3.51) is manifestly satisfied.

The result that

$$\begin{aligned} \{J(\gamma|\boldsymbol{Q}_\parallel)J^*(\gamma|\boldsymbol{Q}_\parallel)\} &= S\,\mathrm{e}^{-\delta^2\mathrm{Re}\,(\gamma^2)}\int \mathrm{d}^2u_\parallel\,\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}_\parallel\cdot\boldsymbol{u}_\parallel}[\mathrm{e}^{|\gamma|^2\delta^2W(|\boldsymbol{u}_\parallel|)}-1] \\ &= S\pi a^2\mathrm{e}^{-\delta^2\mathrm{Re}\,(\gamma^2)}\sum_{n=1}^{\infty}\frac{\delta^{2n}|\gamma|^{2n}}{n\,n!}\mathrm{e}^{-(a^2/4n)Q_\parallel^2} \end{aligned} \tag{3.57}$$

where we have used equations (3.4) and (3.40*a*), enables us to write the contribution to the mean DRC from the incoherent component of the scattered x-rays to order $\mathrm{O}(\eta^2)$ as

$$\begin{aligned} \left\langle\frac{\partial R}{\partial\Omega_\mathrm{s}}\right\rangle_{\substack{\alpha\beta\\ \mathrm{incoh}}} &= \frac{1}{4\pi}\left(\frac{\omega a}{2c}\right)^2\frac{1}{\cos\theta_0}\eta^2\sum_{n=1}^{\infty}\frac{1}{n\,n!}\left(\frac{\delta\omega}{c}\right)^{2n} \\ &\quad \times\exp\left\{-\frac{1}{n}\left(\frac{\omega a}{2c}\right)^2[\sin^2\theta_\mathrm{s} - 2\sin\theta_\mathrm{s}\sin\theta_0\cos(\phi_\mathrm{s}-\phi_0) + \sin^2\theta_0]\right\} \\ &\quad \times|\tilde{b}_{\alpha\beta}^{(n)}(\theta_\mathrm{s},\phi_\mathrm{s}|\theta_0,\phi_0)|^2 \end{aligned} \tag{3.58}$$

where

$$\tilde{b}^{(n)}_{\alpha\beta}(\theta_s, \phi_s|\theta_0, \phi_0) = e^{-\frac{1}{2}(\omega\delta/c)^2[(\cos^2\theta_s-\eta)^{1/2}+(\cos^2\theta_0-\eta)^{1/2}]^2} \times e^{\frac{1}{2}(\omega\delta/c)^2[(\cos^2\theta_s-\eta)^{1/2}-\cos\theta_s]^2} e^{\frac{1}{2}(\omega\delta/c)^2[(\cos^2\theta_0-\eta)^{1/2}-\cos\theta_0]^2} \times 2\cos\theta_s P_{\alpha\beta}(\theta_s, \phi_s|\theta_0, \phi_0) 2\cos\theta_0[(\cos^2\theta_s-\eta)^{1/2}+(\cos^2\theta_0-\eta)^{1/2}]^{n-1} \quad (3.59)$$

with

$$P_{pp}(\theta_s, \phi_s|\theta_0, \phi_0) = \frac{\sin\theta_s\sin\theta_0 - (\cos^2\theta_s-\eta)^{1/2}\cos(\phi_s-\phi_0)(\cos^2\theta_0-\eta)^{1/2}}{[\epsilon\cos\theta_s + (\cos^2\theta_s-\eta)^{1/2}][\epsilon\cos\theta_0+(\cos^2\theta_0-\eta)^{1/2}]} \quad (3.60a)$$

$$P_{ps}(\theta_s, \phi_s|\theta_0, \phi_0) = \frac{(\cos^2\theta_s-\eta)^{1/2}\sin(\phi_s-\phi_0)}{[\epsilon\cos\theta_s + (\cos^2\theta_s-\eta)^{1/2}][\cos\theta_0+(\cos^2\theta_0-\eta)^{1/2}]} \quad (3.60b)$$

$$P_{sp}(\theta_s, \phi_s|\theta_0, \phi_0) = \frac{\sin(\phi_s-\phi_0)(\cos^2\theta_0-\eta)^{1/2}}{[\cos\theta_s + (\cos^2\theta_s-\eta)^{1/2}][\epsilon\cos\theta_0+(\cos^2\theta_0-\eta)^{1/2}]} \quad (3.60c)$$

$$P_{ss}(\theta_s, \phi_s|\theta_0, \phi_0) = \frac{\cos(\phi_s-\phi_0)}{[\cos\theta_s + (\cos^2\theta_s-\eta)^{1/2}][\cos\theta_0+(\cos^2\theta_0-\eta)^{1/2}]}. \quad (3.60d)$$

As in the one-dimensional case we can simplify the result given by equations (3.58)–(3.60) using equation (2.57) and replacing the explicit factors of ϵ by unity in the denominators in the expressions (3.60) for the $P_{\alpha\beta}(\theta_s, \phi_s|\theta_0, \phi_0)$. In this way we obtain

$$\tilde{b}^{(n)}_{\alpha\beta}(\theta_s, \phi_s|\theta_0, \phi_0) = \exp\left\{-\frac{1}{2}\left(\frac{\omega\delta}{c}\right)^2[(\cos^2\theta_s-\eta)^{1/2}+(\cos^2\theta_0-\eta)^{1/2}]^2\right\} \times \frac{(2\cos\theta_s)p_{\alpha\beta}(\theta_s, \phi_s|\theta_0, \phi_0)(2\cos\theta_0)}{[\cos\theta_s+(\cos^2\theta_s-\eta)^{1/2}][\cos\theta_0+(\cos^2\theta_0-\eta)^{1/2}]} \times[(\cos\theta_s-\eta)^{1/2}+(\cos^2\theta_0-\eta)^{1/2}]^{n-1} \quad (3.61)$$

with

$$p_{pp}(\theta_s, \phi_s|\theta_0, \phi_0) = \sin\theta_s\sin\theta_0 - (\cos^2\theta_s-\eta)^{1/2}\cos(\phi_s-\phi_0)(\cos^2\theta_0-\eta)^{1/2} \quad (3.62a)$$

$$p_{ps}(\theta_s, \phi_s|\theta_0, \phi_0) = (\cos^2\theta_s-\eta)^{1/2}\sin(\phi_s-\phi_0) \quad (3.62b)$$

$$p_{sp}(\theta_s, \phi_s|\theta_0, \phi_0) = \sin(\phi_s-\phi_0)(\cos^2\theta_0-\eta)^{1/2} \quad (3.62c)$$

$$p_{ss}(\theta_s, \phi_s|\theta_0, \phi_0) = \cos(\phi_s-\phi_0). \quad (3.62d)$$

4. Results

In section 2 we have obtained explicit expressions for the contributions to the mean scattering amplitude $\langle R(q|k)\rangle$ for a one-dimensional random surface that are of zero and second order in $\eta(\omega)$. The contribution to the reflectivity from the zero-order term, for the scattering of p-polarized x-rays, given by the first term in equation (2.37), and for the scattering of s-polarized x-rays by the first term in equation (2.43),

$$R_p(\theta_0) = \left|\frac{\epsilon\cos\theta_0 - (\cos^2\theta_0-\eta)^{1/2}}{\epsilon\cos\theta_0 + (\cos^2\theta_0-\eta)^{1/2}}\right|^2 \exp\left[-4\left(\frac{\omega\delta}{c}\right)^2\cos\theta_0 \mathrm{Re}\,(\cos^2\theta_0-\eta)^{1/2}\right] \quad (4.1a)$$

$$R_s(\theta_0) = \left|\frac{\cos\theta_0 - (\cos^2\theta_0-\eta)^{1/2}}{\cos\theta_0 + (\cos^2\theta_0-\eta)^{1/2}}\right|^2 \exp\left[-4\left(\frac{\omega\delta}{c}\right)^2\cos\theta_0 \mathrm{Re}\,(\cos^2\theta_0-\eta)^{1/2}\right] \quad (4.1b)$$

has the form of the Fresnel reflectivity multiplied by a factor similar to the Debye–Waller factor, and coincides with the result obtained in [7, 10, 13]. However, while in [7, 13] this result was obtained in the first-order distorted-wave Born approximation as an approximate result, valid only for relatively weakly rough surfaces, $(\delta/\lambda)\cos\theta_0 \ll 1$, we have summed all the terms in the perturbation series for the mean scattering amplitude which are of zero order in $\eta(\omega)$ without imposing any restrictions on the RMS height of the surface beyond that implied by our adoption of the Rayleigh hypothesis.

For a lossless medium the reflectivities given by equations (4.1) become equal to unity when the angle of incidence θ_0 is equal to or greater than the critical angle for total internal reflection $\theta_c = \arccos\sqrt{\eta}$, at which the term $(\cos^2\theta_0 - \eta)^{1/2}$ goes to zero, and then becomes purely imaginary for $\theta_c < \theta_0 < \pi/2$. This is because the Fresnel reflectivity is unity in this range of angles of incidence, while the exponent of the Debye–Waller factor vanishes or is purely imaginary. In view of the smallness of $\eta(\omega)$ the difference between the Fresnel reflectivities for the scattering of p- and s-polarized x-rays is small. In figure 3(*a*) the reflectivity given by equation (4.1*a*), calculated for a one-dimensional, randomly rough gold surface, is plotted for different values of the roughness parameters as a function of the grazing angle of incidence $\bar{\theta}_0 = \pi/2 - \theta_0$. We see that it is equal to unity for $\bar{\theta}_0 < \bar{\theta}_c$, where $\bar{\theta}_c$ is the grazing critical angle for total internal reflection, and then decreases rapidly for $\bar{\theta}_0 > \bar{\theta}_c$, the rate of decrease increasing with increasing surface roughness.

The lowest-order correction to the reflectivity given by equations (4.1) is of second order in $\eta(\omega)$, and is given by the second term in equations (2.37) and (2.43). Although this correction is small, it is important because it describes the decrease of the reflectivity from unity in the regime of total internal reflection. In addition, since this correction depends on the surface height autocorrelation function $W(|x_1|)$, in contrast with the result given by equation (4.1) which does not, and which can therefore be used to determine only the RMS height of the surface, an experimental determination of it affords the possibility of determining $W(|x_1|)$, or at least the transverse correlation length a of the surface roughness.

To illustrate the content of this result it is necessary to calculate the integrals given by equations (2.34). The functions

$$g_1(p|k) = \mathrm{e}^{-(\alpha(p)-\alpha(k))(\alpha_0(p)-\alpha_0(k))\delta^2} \times \int_{-\infty}^{\infty} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}(k-p)u} \left[\mathrm{e}^{-(\alpha(k)-\alpha_0(p))(\alpha(p)-\alpha_0(k))\delta^2 W(|u|)} - 1\right] \qquad (4.2a)$$

$$g_2(p|k) = \mathrm{e}^{-(\alpha(p)-\alpha(k))(\alpha_0(p)+\alpha_0(k))\delta^2} \times \int_{-\infty}^{\infty} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}(k-p)u} \left[\mathrm{e}^{-(\alpha(k)-\alpha_0(p))(\alpha(p)+\alpha_0(k))\delta^2 W(|u|)} - 1\right] \qquad (4.2b)$$

appearing in the integrands are often encountered in scattering problems, and can be calculated in a standard manner by expanding the exponential in the integrand in a Taylor series and evaluating the Fourier transforms of the Gaussian height autocorrelation function:

$$g_{1,2}(p|k) = \mathrm{e}^{-(\alpha(p)-\alpha(k))(\alpha_0(p)\mp\alpha_0(k))\delta^2} \times \sum_{n=1}^{\infty} \frac{(-1)^n \delta^{2n}}{n!\sqrt{n}} (\alpha(k) - \alpha_0(p))^n (\alpha(p) \mp \alpha_0(k))^n \exp\left[-\frac{(p-k)^2 a^2}{4n}\right]. \qquad (4.3)$$

The resulting sums converge slowly even for comparatively weak roughnesses [29]. Several approaches to improve the convergence of the series have been proposed [29, 30]. We note that because the factor $\exp[-(\alpha(p) - \alpha(k))(\alpha_0(p) \pm \alpha_0(k))\delta^2]$ in the functions $g_{1,2}(p|k)$ becomes $\exp(p^2\delta^2)$ in the limit $|p| \to \infty$ it may appear that the integrals over p in equations (2.34) diverge. In fact, this is not the case. The sums in equations (4.3) cancel this exponential increase of $g_{1,2}(p|k)$. However, in order to effect this cancellation an infinite number of terms in the series must be summed, so that the poor convergence of the

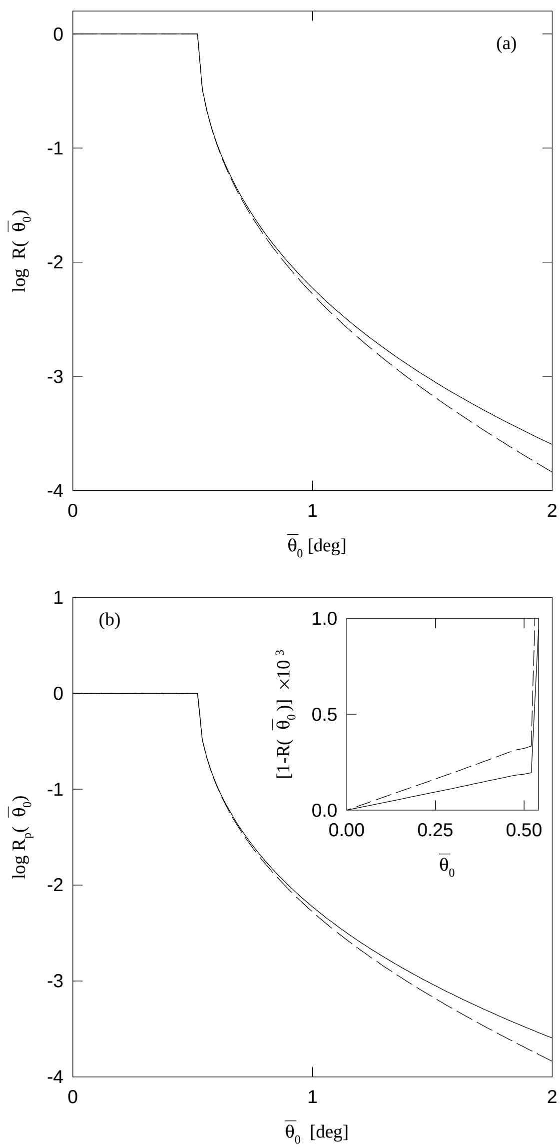

Figure 3. (*a*) The reflectivity (4.1*a*) of a one-dimensional randomly rough gold surface illuminated by p-polarized x-rays of wavelength $\lambda = 1.54$ Å, as a function of the grazing angle of incidence $\bar{\theta}_0 = \pi/2 - \theta_0$. The surface roughness is characterized by a transverse correlation length $a = 20\lambda$, and two values of the RMS height, $\delta = \lambda$ (solid line) and $\delta = 2\lambda$ (dashed line). (*b*) The reflectivity of a one-dimensional randomly rough gold surface illuminated by p-polarized x-rays of wavelength $\lambda = 1.54$ Å, calculated by including both the zero- and second-order terms in equation (2.43), as a function of the grazing angle of incidence $\bar{\theta}_0 = \pi/2 - \theta_0$. In the inset a plot of $1 - R(\bar{\theta}_0)$ is shown for grazing angles of incidence smaller than, and slightly larger than, $\bar{\theta}_c$. The surface roughness is characterized by a transverse correlation length $a = 20\lambda$, and two values of the RMS height, $\delta = \lambda$ (solid line) and $\delta = 2\lambda$ (dashed line). (*c*) The same as figure 3(*b*), but for the scattering of s-polarized x-rays.

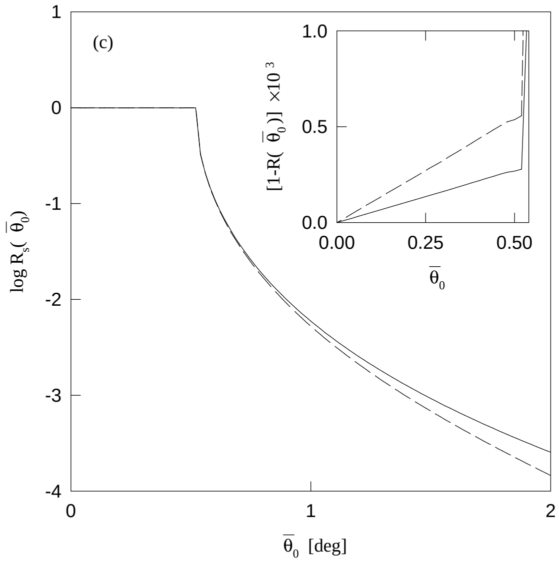

Figure 3. (Continued)

series makes the direct calculation of the integrals in equations (2.34) a difficult problem. To improve the behaviour of the functions $g_{1,2}(p|k)$ we rewrite them in the form

$$g_{1,2}(p|k) = \exp\left[-(\alpha(p)-\alpha(k))(\alpha_0(p)\mp\alpha_0(k))\delta^2\right]\exp\left[-(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2\right]$$
$$\times\int_{-\infty}^{\infty}\mathrm{d}u\,\exp[-\mathrm{i}(k-p)u]\Big\{\exp\left[(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2[1-W(|u|)]\right]$$
$$-\exp\left[(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2\right]\Big\}. \qquad (4.4)$$

As a result the exponential factor multiplying the integral does not grow with $p\to\infty$. To calculate the Fourier integral we now expand the exponentials in the integrand in a Taylor series

$$\exp\left[(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2[1-W(|u|)]\right]-\exp\left[(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2\right]$$
$$=\sum_{n=0}^{\infty}\frac{\delta^{2n}}{n!}(\alpha(k)-\alpha_0(p))^n(\alpha(p)\pm\alpha_0(k))^n\left\{[1-W(|u|)]^n-1\right\}. \qquad (4.5)$$

Making use of the binomial representation of $[1-W(|u|)]^n$ and integrating over u we obtain

$$g_{1,2}(p|k) = \exp\left[-(\alpha(p)-\alpha(k))(\alpha_0(p)\mp\alpha_0(k))\delta^2\right]\exp\left[-(\alpha(k)-\alpha_0(p))(\alpha(p)\mp\alpha_0(k))\delta^2\right]$$
$$\times\sum_{n=1}^{\infty}\sum_{m=1}^{n}\frac{\delta^{2n}}{(n-m)!m!\sqrt{m}}(\alpha(k)-\alpha_0(p))^n(\alpha(p)\pm\alpha_0(k))^n\mathrm{e}^{-(p-k)^2a^2/4m}. \qquad (4.6)$$

Despite the double summation, the series in equation (4.6) converges faster than that in equation (4.3). What is more important, the identical transformation we have used to calculate the integral (4.3) allows us to evaluate easily the integrals over p in equations (2.34).

In figures 3(*b*) and (*c*) we present the reflectivities of a one-dimensional random surface calculated for the case of the scattering of p-polarized x-rays from equation (2.40) with the use of equation (2.37) and for the case of the scattering of s-polarized x-rays from equation (2.42) with the use of equation (2.43), respectively. Although the contribution to the reflectivity of second order in $\eta(\omega)$ is small, it is important as it describes the losses in the regime of total internal reflection. Since the reflectivity drops from unity to almost zero in a very narrow range of angles of incidence, in the insets to figures 3(*b*) and (*c*) the deviation of the reflectivity from unity, $1 - R(\bar{\theta}_0)$, is shown for grazing angles of incidence smaller than the grazing critical angle for total reflection $\bar{\theta}_c$.

The reflectivity of a two-dimensional random surface has been obtained in section 3 and is given by equations (3.38) and (3.39). It has the form of a sum of the Fresnel reflectivity and the correction of the lowest order in $\eta(\omega)$, $\eta^2(\omega)$, multiplied by a Debye–Waller factor. As in the case of a one-dimensional random surface, the correction contains integrals, given by equations (3.32) and (3.33), which can be calculated in the manner described above or, in contrast to the one-dimensional case, by the method proposed in [30].

In figure 4 we present the reflectivity for p- and s-polarized x-rays scattered from a two-dimensional randomly rough gold surface. We note that, as pointed out in section 2, in the case of interest to us, namely that of grazing incidence, the difference between the results for p- and s-polarizations is unobservable.

We now turn to the contribution to the mean DRC from the incoherent component of the scattered x-rays of p- and s-polarizations, given for a one-dimensional random surface by equations (2.56), (2.58) and equations (2.59)–(2.60), respectively. It has been calculated to the lowest order in $\eta(\omega)$ (the second), and its reciprocal forms, given by equations (2.58) and (2.60), have been derived in the limit $(\delta/\lambda)\sqrt{\eta(\omega)} \ll 1$. In this case, our result for the contribution to the mean DRC from the incoherent component of the scattered x-rays of s-polarization, given by equation (2.60), coincides with the results obtained in the first-order distorted-wave Born approximation, or the modified Born approximation, in the limit of a weakly rough surface $(\delta/\lambda)\cos\theta_0 \ll 1$ [2, 7]. As in the case of the reflectivity, our results for the incoherent scattering are not limited by this condition. However, at small grazing angles of incidence and scattering where our results coincide with the results of the first-order distorted-wave Born approximation [7], or the modified Born approximation [2], the two limiting conditions are practically identical, because for such angles $\cos\theta_{0,s} \leqslant \sqrt{\eta(\omega)}$. We note, however, that the expressions (2.56*b*) and (2.59) remain valid even when the inequality $(\delta/\lambda)\sqrt{\eta(\omega)} \ll 1$ breaks down, and for arbitrary angles of incidence and scattering.

The contribution to the mean DRC from the incoherent component of the x-rays scattered from a one-dimensional random gold surface, plotted as a function of the grazing scattering angle for different grazing angles of incidence, is shown in figure 5(*a*), and for different values of the roughness parameters in figure 5(*b*) for a fixed grazing angle of incidence. In figure 6 the contribution to the mean DRC from the incoherent component of the scattered x-rays is plotted as a function of the angle of incidence for a fixed angle of scattering. The plots in figures 5 and 6 show the sharp asymmetric peak at $\theta_s = \theta_c$, and at $\theta_0 = \theta_c$, respectively, called the Yoneda peak [3]. This peak arises from the sharp feature at $\theta_{s,0} = \theta_c$ in the factors

$$\left| \frac{2\cos\theta_{0,s}}{\epsilon\cos\theta_{0,s} + \sqrt{\cos^2\theta_{0,s} - \eta(\omega)}} \right|^2 \tag{4.7}$$

present in the function $\tilde{b}_n(\theta_s, \theta_0)$, which are the Fresnel transmission coefficients that determine the electromagnetic field at the surface.

The contribution to the mean DRC from the incoherent component of the x-rays scattered from a two-dimensional random surface is given by equations (3.58)–(3.62). As in the case of a one-dimensional random surface, while the expressions (3.61) and (3.62) have been

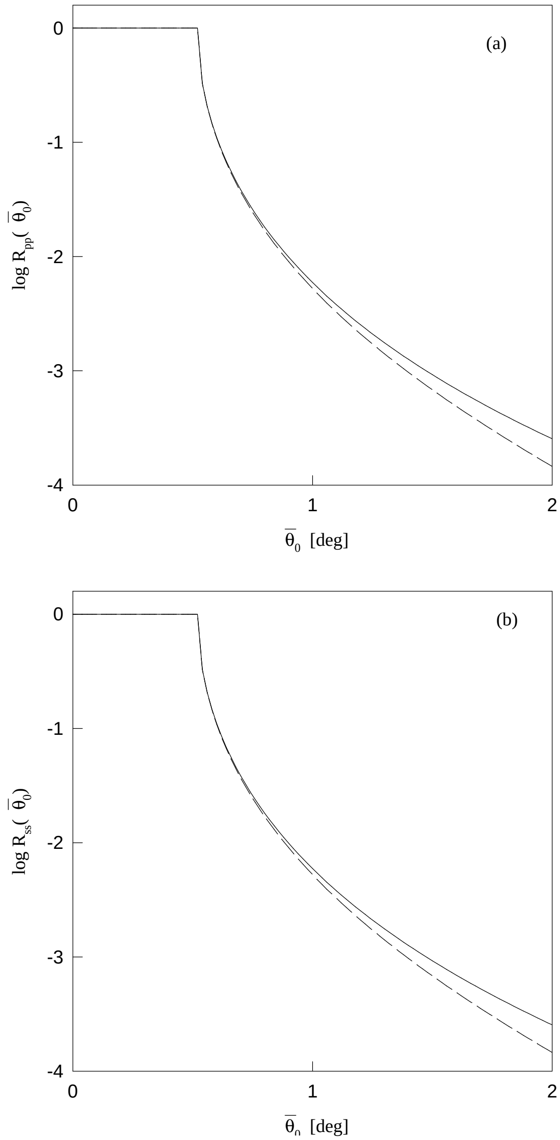

Figure 4. The reflectivity of a two-dimensional randomly rough gold surface illuminated by x-rays of wavelength $\lambda = 1.54$ Å, calculated by including both the zero- and second-order terms in equation (3.39), as a function of the grazing angle of incidence. The surface roughness is characterized by a transverse correlation length $a = 20\lambda$, and two values of the RMS height, $\delta = \lambda$ (solid line) and $\delta = 2\lambda$ (dashed line). (*a*) $R_{pp}(\bar{\theta}_0)$ and (*b*) $R_{ss}(\bar{\theta}_0)$.

obtained in the limit $(\delta/\lambda)\sqrt{\eta(\omega)} \ll 1$, the expressions (3.59) and (3.61) are valid when this inequality breaks down and for arbitrary angles of incidence and scattering.

In the in-plane ($\phi_s = \phi_0 = 0°$), co-polarized (p $\rightarrow$ p, s $\rightarrow$ s) scattering of x-rays from a two-dimensional random surface the contribution to the mean DRC from the incoherent component of the scattered x-rays, shown in figures 7(*a*) and (*b*), also displays a Yoneda peak when the grazing polar scattering angle $\bar{\theta}_s$ equals the grazing critical angle $\bar{\theta}_c$, and

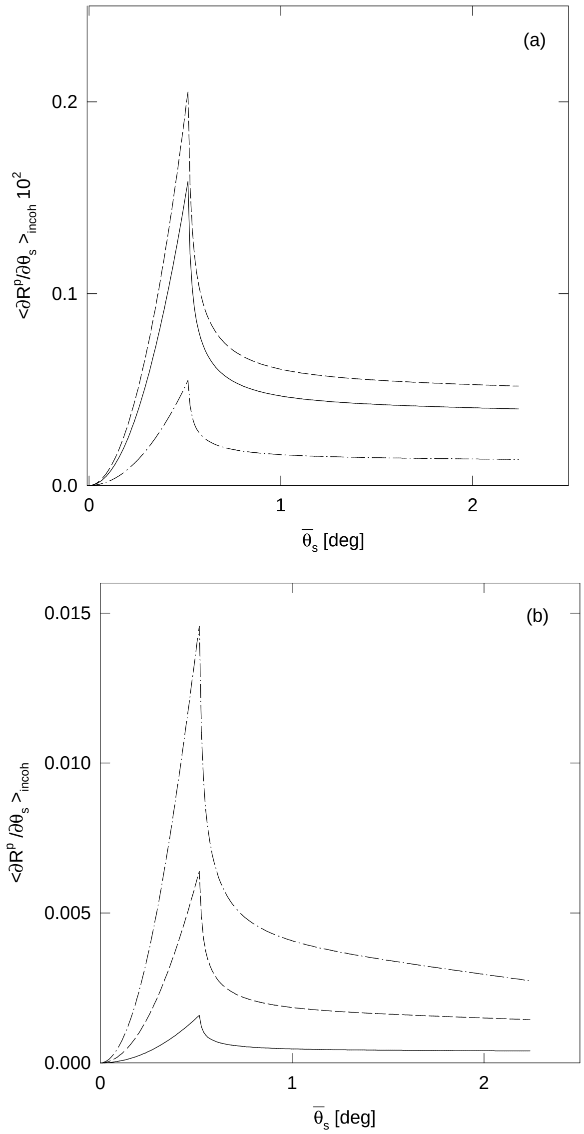

Figure 5. The contribution to the mean DRC from the incoherent component of the scattered x-rays as a function of the grazing scattering angle $\bar{\theta}_s = \pi/2 - \theta_s$, when p-polarized x-rays of wavelength $\lambda = 1.54$ Å are incident on a one-dimensional randomly rough gold surface characterized by a transverse correlation length $a = 10\lambda$. (*a*) For several grazing angles of incidence, $\bar{\theta}_0 = 0.4^\circ$ (solid line), $\bar{\theta}_0 = 0.52^\circ$ (dashed line), and $\bar{\theta}_0 = 0.7^\circ$ (dash-dotted line), and the RMS height $\delta = \lambda$. (*b*) For a fixed grazing angle of incidence $\bar{\theta}_0 = 0.4^\circ$, for three values of the RMS height; $\delta = \lambda$ (solid line), $\delta = 2\lambda$ (dashed line), and $\delta = 3\lambda$ (dash-dotted line).

the curves for p $\to$ p scattering coincide with those for s $\to$ s scattering. However, for slightly out-of-plane ($\phi_0 = 0^\circ$, $\phi_s = 2^\circ$), cross-polarized (p $\to$ s, s $\to$ p) scattering, the results are qualitatively different in the two cases. For p $\to$ s scattering (figure 8(*a*)) a Yoneda peak occurs for $\bar{\theta}_s = \bar{\theta}_c$ for grazing angles of incidence $\bar{\theta}_0$ smaller and greater than $\bar{\theta}_c$. The intensity of this peak, however, is nearly eight orders of magnitude lower

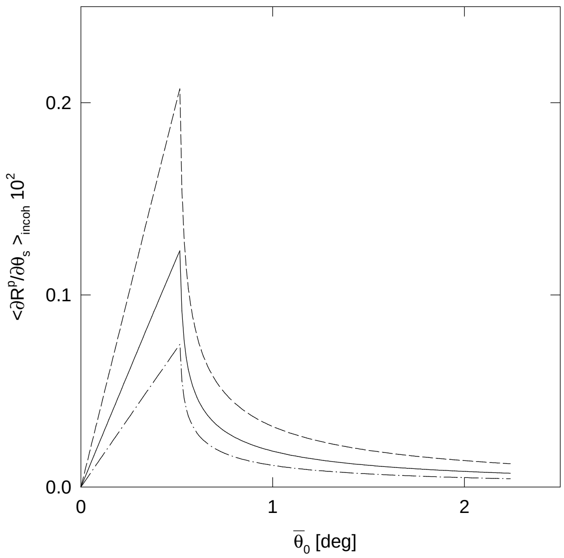

Figure 6. The contribution to the mean DRC from the incoherent component of the scattered x-rays as a function of the grazing angle of incidence $\bar{\theta}_0 = \pi/2 - \theta_0$, when p-polarized x-rays of wavelength $\lambda = 1.54$ Å are incident on a one-dimensional randomly rough gold surface characterized by the RMS height $\delta = 1\lambda$ and a transverse correlation length $a = 10\lambda$, for several grazing angles of scattering, $\bar{\theta}_s = 0.4^\circ$ (solid line), $\bar{\theta}_s = 0.52^\circ$ (dashed line), and $\bar{\theta}_s = 0.7^\circ$ (dash-dotted line).

than the intensity of the Yoneda peak observed in in-plane p $\to$ p and s $\to$ s scattering. When the grazing angle of incidence $\bar{\theta}_0$ exactly equals the grazing critical angle $\bar{\theta}_c$, the contribution to the mean DRC vanishes due to the presence of the factor $\sqrt{\cos^2\theta_0 - \eta}$ in equation (3.62*c*). In contrast, in s $\to$ p scattering (figure 8(*b*)), instead of a Yoneda peak when $\bar{\theta}_s$ equals $\bar{\theta}_c$, the contribution to the mean DRC vanishes there instead, for grazing angles of incidence smaller than, equal to, and greater than $\bar{\theta}_c$ due to the presence of the factor $\sqrt{\cos^2\theta_s - \eta}$ in equation (3.62*b*). The magnitude of this contribution to the mean DRC is lower by nearly seven orders of magnitude than the contribution from in-plane p $\to$ p and s $\to$ s scattering. In view of the weakness of the cross-polarized scattering, it will be a very difficult experimental problem to observe the features displayed by the corresponding contributions to the mean DRC.

5. Conclusions

We have presented in this paper a simple reciprocal theory of the scattering of x-rays from one- and two-dimensional, randomly rough surfaces. This has been accomplished by obtaining a solution of the reduced Rayleigh equation for the scattering of electromagnetic waves from such surfaces not as an expansion in powers of the surface profile function, but as an expansion in powers of the small parameter $\eta(\omega) = 1 - \epsilon(\omega)$. However, in carrying out this expansion we have been careful not to expand the functions $\alpha(k) = (\omega/c)(\cos^2\theta_0 - \eta(\omega))^{1/2}$ and $\alpha(q) = (\omega/c)(\cos^2\theta_s - \eta(\omega))^{1/2}$ appearing in the solution in powers of $\eta(\omega)$. This is because it is the vanishing of these functions when the angle of incidence θ_0 and the scattering angle θ_s equal the critical angle for total internal reflection, $\theta_c = \arccos\sqrt{\eta(\omega)}$, and their transformation into purely imaginary quantities for θ_0 or θ_s

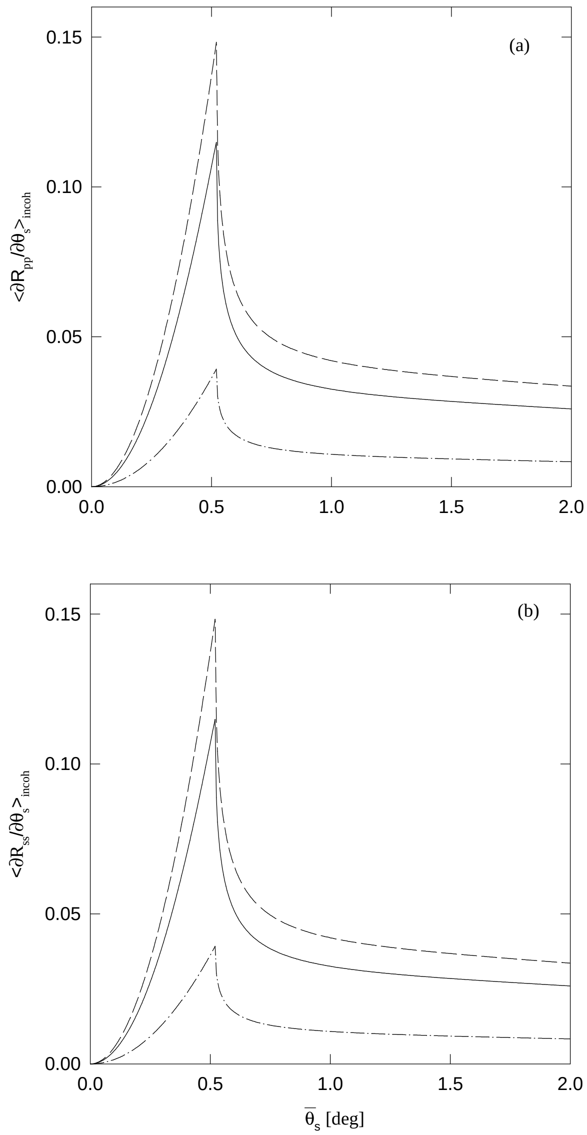

Figure 7. The contribution to the mean DRC from the incoherent component of the scattered x-rays as a function of the grazing scattering angle $\bar{\theta}_s = \pi/2 - \theta_s$, when x-rays of wavelength $\lambda = 1.54$ Å are incident on a two-dimensional randomly rough gold surface characterized by an RMS height $\delta = 2\lambda$ and a transverse correlation length $a = 20\lambda$, for several grazing angles of incidence, $\bar{\theta}_0 = 0.4^\circ$ (solid line), $\bar{\theta}_0 = 0.52^\circ$ (dashed line), and $\bar{\theta}_0 = 0.7^\circ$ (dash-dotted line), for in-plane co-polarized (*a*) p → p and (*b*) s → s scattering.

exceeding θ_c, that gives rise to the Yoneda peaks in the angular distribution of the intensity of the scattered x-rays.

For both one- and two-dimensional randomly rough surfaces our zero-order result for the reflectivity coincides with that obtained earlier by Nevot and Croce [10] by a rather different approach. It equals unity for grazing angles of incidence $\bar{\theta}_0$ smaller than the grazing critical angle for total internal reflection $\bar{\theta}_c$, and decreases rapidly as $\bar{\theta}_0$ increases beyond $\bar{\theta}_c$.

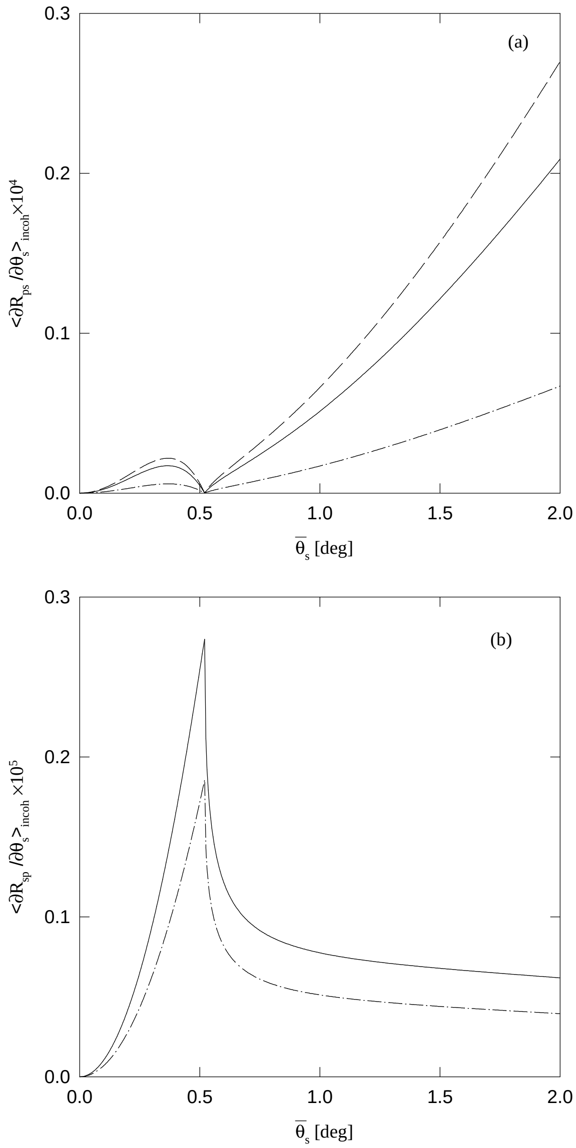

Figure 8. The contribution to the mean DRC from the incoherent component of the scattered x-rays as a function of the grazing scattering angle $\bar{\theta}_s = \pi/2 - \theta_s$, when x-rays of wavelength $\lambda = 1.54$ Å are incident on a two-dimensional randomly rough gold surface characterized by an RMS height $\delta = 2\lambda$ and a transverse correlation length $a = 20\lambda$, for several grazing angles of incidence, $\bar{\theta}_0 = 0.4^\circ$ (solid line), $\bar{\theta}_0 = 0.52^\circ$ (dashed line), and $\bar{\theta}_0 = 0.7^\circ$ (dash-dotted line), for out-of-plane ($\phi_0 = 0^\circ$, $\phi_s = 2^\circ$) cross-polarized (*a*) p → s and (*b*) s → p scattering.

However, we have also obtained the leading correction to this result, which is of $O(\eta(\omega)^2)$. It shows that for $0 < \bar{\theta}_0 < \bar{\theta}_c$ the surface roughness decreases the reflectivity slightly below unity, with the deviation of the reflectivity from unity increasing with increasing roughness. The surface roughness also shifts the grazing critical angle for total internal reflection to larger values. This latter result has also been obtained recently [31] by an application of self-energy perturbation theory [15], which will be reported elsewhere.

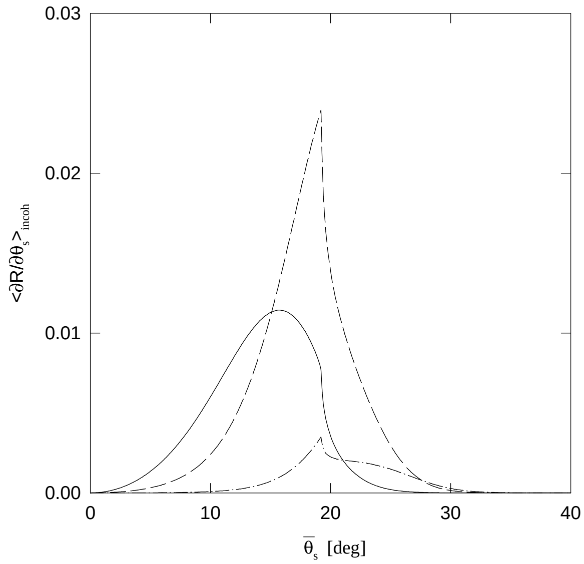

Figure 9. The contribution to the mean DRC from the incoherent component of the scattered light as a function of the grazing scattering angle $\bar{\theta}_s = \pi/2 - \theta_s$, when p-polarized light of wavelength $\lambda = 632.8$ nm is incident from a dielectric medium with an index of refraction $n_1 = 1.61$ onto the one-dimensional, randomly rough interface between it and a second dielectric medium with an index of refraction $n_2 = 1.52$. The RMS height $\delta = 0.1\lambda$, and the transverse correlation length $a = 5\lambda$ for several grazing angles of incidence, $\bar{\theta}_0 = 12^\circ$ (solid line), $\bar{\theta}_0 = 19.25^\circ$ (dashed line), and $\bar{\theta}_0 = 24^\circ$ (dash-dotted line). $\theta_c = 70.75^\circ$.

We note that our results for the contribution to the mean DRC from the incoherent component of the scattered x-rays, once the approximations given by equations (2.57) have been made, coincide with the results of the distorted-wave Born approximation [6]. Without these approximations the results given by equations (2.56), (2.59) and (3.58)–(3.60) should be more accurate than those of the distorted-wave Born approximation for larger values of $\eta(\omega)$ than those corresponding to the x-ray frequency range. Moreover, the approach used in the present work provides a direct and simple way of obtaining corrections to the results given by equations (2.56), (2.59) and (3.58)–(3.60) of higher order in $\eta(\omega)$, e.g. of order $O(\eta^3)$ and $O(\eta^4)$. Such calculations will be reported elsewhere.

The results obtained here are valid at small angles of incidence and scattering, like the results of the Born approximation but, unlike the Born approximation, are also valid in the vicinity of the critical angle for total internal reflection at the interface between vacuum and the scattering medium. In their validity for small grazing angles of incidence and scattering, our results also contrast with the results of the distorted-wave Born approximation.

Although the derivation of the results obtained here has been carried out in the context of the scattering of electromagnetic waves from solid surfaces, the results can also be applied to the scattering of x-rays from liquid surfaces, if the corresponding power spectrum for the surface roughness is used. The latter has the form [32]

$$g(|\boldsymbol{k}_\parallel|) = \int \mathrm{d}^2x_\parallel\, W(|\boldsymbol{x}_\parallel|)\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_\parallel\cdot\boldsymbol{x}_\parallel} = \frac{k_B T}{\gamma}\frac{\theta(k_c - |\boldsymbol{k}_\parallel|)}{\kappa^2 + k_\parallel^2} \tag{5.1}$$

where γ is the surface tension of the liquid at the absolute temperature T, k_B is Boltzmann's constant, and $\kappa = (g\rho/\gamma)^{1/2}$ is the gravitational cutoff, with ρ the mass density of the liquid and g the acceleration due to gravity. $\theta(x)$ is the Heaviside unit step function, and the wavenumber k_c is the upper wavevector cutoff for the thermally excited surface waves (surface ripplons) whose amplitudes roughen the liquid surface. The value of k_c is of the order of the reciprocal of a few atomic diameters [33].

Finally, it seems likely that the approach used here, namely the expansion of the scattering amplitude in powers of $\eta(\omega)$, may also be useful in theoretical studies of the multiple scattering of electromagnetic waves incident from one dielectric medium onto its randomly rough interface with a second dielectric medium, when the difference $\eta(\omega)$ between their dielectric constants is small, of the order of a few tenths. The function $\eta(\omega)$ would then serve as a new small parameter in the theory of the scattering of electromagnetic waves from such interfaces. As an illustration of this application of our approach, we present in figure 9 the contribution to the mean DRC from the incoherent component of the scattered light, when p-polarized light of wavelength $\lambda = 632.8$ nm is incident from a dielectric medium with an index of refraction $n_1 = 1.61$ onto the one-dimensional, randomly rough interface between it and a second dielectric medium with an index of refraction $n_2 = 1.52$, obtained from a second-order result analogous to the one given by equation (2.56). The critical angle for total internal reflection in this case is $\theta_c = 70.75°$. We see a well defined Yoneda peak at this value of the scattering angle. No evidence of enhanced backscattering is present in this result. However, the addition of the leading corrections (of order $O(\eta^3)$ and $O(\eta^4)$) to the terms of second order in $\eta(\omega)$ obtained here for the contribution to the mean DRC from the incoherent component of the scattered light may be sufficient to reproduce the enhanced backscattering of light from such interfaces that has been observed in the results of computer simulation studies of such scattering [34]. This possibility is now being explored.

Acknowledgment

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Appendix A.

In this appendix we show how the results given by equations (2.52) are obtained.

Using the following expansion of the function $J(\gamma|Q)$ defined by equation (2.14),

$$J(\gamma|Q) = \sum_{n=1}^{\infty} \frac{(-i\gamma)^n}{n!} \hat{\zeta}^{(n)}(Q) \tag{A.1}$$

where

$$\hat{\zeta}^{(n)}(Q) = \int_{-\infty}^{\infty} dx_1\, e^{-iQx_1} \zeta^n(x_1), \tag{A.2}$$

and the explicit expressions for $R_0(k)$ given by equation (2.16*a*) and for $m(q|k)$ and $n(q|k)$ given by equations (2.19*b*) and (2.19*c*), respectively, we find that

$$\begin{aligned} n(q|k) \pm m(q|k)R_0(k) = {} & \frac{1}{d(q)d(k)} \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \hat{\zeta}^{(n)}(q-k) \\ & \times \Big[(qk - \alpha(q)\alpha_0(k))(\epsilon\alpha_0(k) + \alpha(k,\omega))(\alpha(q) + \alpha_0(k))^{n-1} \\ & \pm (qk + \alpha(q)\alpha_0(k))(\epsilon\alpha_0(k) - \alpha(k,\omega))(\alpha(q) - \alpha_0(k))^{n-1} \Big]. \end{aligned} \tag{A.3}$$

We next note that

$$\alpha_0^2(k) = \alpha^2(k) + \eta(\omega^2/c^2) \tag{A.4}$$

and

$$\epsilon = 1 - \eta \tag{A.5}$$

so that

$$\begin{aligned}(qk-\alpha(q)\alpha_0(k))&(\epsilon\alpha_0(k)+\alpha(k,\omega))\\ &= qk(\epsilon\alpha_0(k)+\alpha(k,\omega))-\alpha(q)(\epsilon\alpha_0^2(k)+\alpha_0(k)\alpha(k,\omega))\\ &= qk(\alpha_0(k)+\alpha(k,\omega)) - \alpha(q)\alpha(k,\omega)(\alpha_0(k)+\alpha(k,\omega))\\ &\quad -\eta qk\alpha_0(k) + \eta\alpha(q)\alpha^2(k) - \eta(1-\eta)(\omega^2/c^2)\alpha(q).\end{aligned} \tag{A.6}$$

However, since the contribution to $\langle|B(q|k)|^2\rangle - |\langle B(q|k)\rangle|^2$ given by equation (2.47) is already proportional to η^2, we shall neglect all terms on the right-hand side of equation (A.6) that are explicitly proportional to η as of higher order in η than the order to which we are working. Thus, we find that

$$\begin{aligned}(qk-\alpha(q)\alpha_0(k))&(\epsilon\alpha_0(k)+\alpha(k,\omega))\\ &= (qk-\alpha(q)\alpha(k,\omega))(\alpha_0(k)+\alpha(k,\omega)) + \mathrm{O}(\eta).\end{aligned} \tag{A.7}$$

In exactly the same way we find that

$$\begin{aligned}(qk+\alpha(q)\alpha_0(k))&(\epsilon\alpha_0(k)-\alpha(k,\omega))\\ &= qk(\alpha_0(k)-\alpha(k,\omega))+\alpha(q)\alpha(k,\omega)(\alpha(k,\omega)-\alpha_0(k))\\ &\quad -\eta qk\alpha_0(k) - \eta\,\alpha(q)\alpha^2(k) + \eta(1-\eta)(\omega^2/c^2)\alpha(q)\\ &= (qk-\alpha(q)\alpha(k,\omega))(\alpha_0(k)-\alpha(k,\omega)) + \mathrm{O}(\eta).\end{aligned} \tag{A.8}$$

When the results given by equations (A.6)–(A.7) are substituted into equation (A.3), the latter becomes

$$\begin{aligned}n(q|k) \pm m(q|k)R_0(k) &= \frac{qk-\alpha(q)\alpha(k,\omega)}{d(q)d(k)}\sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\hat{\zeta}^{(n)}(q-k)\\ &\quad\times[(\alpha_0(k)+\alpha(k,\omega))(\alpha(q)+\alpha_0(k))^{n-1}\\ &\quad\pm(\alpha_0(k)-\alpha(k,\omega))(\alpha(q)-\alpha_0(k))^{n-1}] + \mathrm{O}(\eta).\end{aligned} \tag{A.9}$$

To simplify the notation we introduce the definitions

$$\alpha(q) = x \qquad \alpha(k,\omega) = y \qquad \alpha_0(k) = z \tag{A.10}$$

together with the functions ($n \geqslant 1$)

$$F_n = (z+y)(x+z)^{n-1} + (z-y)(x-z)^{n-1} \tag{A.11a}$$

$$G_n = (z+y)(x+z)^{n-1} - (z-y)(x-z)^{n-1}. \tag{A.11b}$$

The function F_n is associated with the + sign in parentheses on the right-hand side of equation (A.9), while G_n is associated with the − sign in these parentheses. The functions F_n and G_n satisfy a pair of coupled finite-difference equations:

$$F_{n+1} = xF_n + zG_n \qquad G_{n+1} = xG_n + zF_n \tag{A.12a}$$

with

$$F_1 = 2z \qquad G_1 = 2y. \tag{A.12b}$$

On the basis of these results we define new functions f_n and g_n by

$$F_n = 2zf_n \qquad G_n = 2g_n. \tag{A.13}$$

These functions satisfy the finite-difference equations

$$f_{n+1} = xf_n + g_n \tag{A.14a}$$
$$g_{n+1} = xg_n + z^2 f_n \tag{A.14b}$$

subject to $f_1 = 1$, $g_1 = y$. However, from the definitions (A.10) we find that

$$z^2 = y^2 + \eta(\omega^2/c^2). \tag{A.15}$$

We seek results for F_n and G_n that contain no terms explicitly proportional to η, for the reason given following equation (A.6).

We therefore drop the second term on the right-hand side of equation (A.15), and rewrite equation (A.14*b*) as

$$g_{n+1} = xg_n + y^2 f_n. \tag{A.16}$$

To solve equations (A.14*a*) and (A.16) we introduce the generating functions

$$f(t) = \sum_{n=1}^{\infty} t^n f_n \qquad g(t) = \sum_{n=1}^{\infty} t^n g_n. \tag{A.17}$$

They satisfy the pair of coupled equations

$$f(t) = xtf(t) + tg(t) + t \qquad g(t) = xtg(t) + y^2 tf(t) + yt \tag{A.18}$$

whose solutions are

$$f(t) = \frac{t}{1-(x+y)t} = \sum_{n=1}^{\infty} t^n (x+y)^{n-1} \tag{A.19a}$$

$$g(t) = \frac{yt}{1-(x+y)t} = \sum_{n=1}^{\infty} t^n y(x+y)^{n-1}. \tag{A.19b}$$

It follows from equations (A.10), (A.13), (A.17), and (A.19), that

$$F_n = 2z(x+y)^{n-1} = 2\alpha_0(k)(\alpha(q)+\alpha(k,\omega))^{n-1} \tag{A.20a}$$
$$G_n = 2y(x+y)^{n-1} = 2\alpha(k,\omega)(\alpha(q)+\alpha(k,\omega))^{n-1} \tag{A.20b}$$

where the terms neglected in obtaining these results are at least of order $O(\eta)$.

When the results given by equations (A.20) are used in equation (A.9), we find that

$$n(q|k) \pm m(q|k)R_0(k) = \frac{qk - \alpha(q)\alpha(k,\omega)}{d(q)d(k)}$$
$$\times \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} (\alpha(q)+\alpha(k,\omega))^{n-1} \hat{\zeta}^{(n)}(q-k) \begin{cases} 2\alpha_0(k) \\ 2\alpha(k,\omega) \end{cases} \tag{A.21a}$$
$$= \frac{qk - \alpha(q)\alpha(k,\omega)}{d(q)d(k)} \frac{J(\alpha(q)+\alpha(k,\omega)|q-k)}{\alpha(q)+\alpha(k,\omega)} \begin{cases} 2\alpha_0(k) \\ 2\alpha(k,\omega) \end{cases} \tag{A.21b}$$

where we have used equation (A.1) once more. These are the results given by equations (2.52).

Appendix B.

In this appendix we derive the result given by equation (3.52).

Our starting point is the expansion

$$J(\gamma|\boldsymbol{Q}_\parallel) = \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!}\gamma^n \hat{\zeta}^{(n)}(\boldsymbol{Q}_\parallel), \tag{B.1}$$

where

$$\hat{\zeta}^{(n)}(\boldsymbol{Q}_\parallel) = \int \mathrm{d}^2x_\parallel \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}_\parallel\cdot\boldsymbol{x}_\parallel}\zeta^n(\boldsymbol{x}_\parallel). \tag{B.2}$$

Using this we can write the matrices $\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \pm \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel)$ in the form

$$\begin{aligned}
\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \pm \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel) &= \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!}\hat{\zeta}^{(n)}(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \\
&\times \left[\begin{pmatrix} \dfrac{N_{\mathrm{pp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\epsilon\alpha_0(k_\parallel)+\alpha(k_\parallel)]}{d_{\mathrm{p}}(q_\parallel)d_{\mathrm{p}}(k_\parallel)} & \dfrac{N_{\mathrm{ps}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\alpha_0(k_\parallel)+\alpha(k_\parallel)]}{d_{\mathrm{p}}(q_\parallel)d_{\mathrm{s}}(k_\parallel)} \\ \dfrac{N_{\mathrm{sp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\epsilon\alpha_0(k_\parallel)+\alpha(k_\parallel)]}{d_{\mathrm{s}}(q_\parallel)d_{\mathrm{p}}(k_\parallel)} & \dfrac{N_{\mathrm{ss}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\alpha_0(k_\parallel)+\alpha(k_\parallel)]}{d_{\mathrm{s}}(q_\parallel)d_{\mathrm{s}}(k_\parallel)} \end{pmatrix} \right. \\
&\times[\alpha(q_\parallel)+\alpha_0(k_\parallel)]^{n-1} \\
&\pm \begin{pmatrix} \dfrac{M_{\mathrm{pp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\epsilon\alpha_0(k_\parallel)-\alpha(k_\parallel)]}{d_{\mathrm{p}}(q_\parallel)d_{\mathrm{p}}(k_\parallel)} & \dfrac{M_{\mathrm{ps}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\alpha_0(k_\parallel)-\alpha(k_\parallel)]}{d_{\mathrm{p}}(q_\parallel)d_{\mathrm{s}}(k_\parallel)} \\ \dfrac{M_{\mathrm{sp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\epsilon\alpha_0(k_\parallel)-\alpha(k_\parallel)]}{d_{\mathrm{s}}(q_\parallel)d_{\mathrm{p}}(k_\parallel)} & \dfrac{M_{\mathrm{ss}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[\alpha_0(k_\parallel)-\alpha(k_\parallel)]}{d_{\mathrm{s}}(q_\parallel)d_{\mathrm{s}}(k_\parallel)} \end{pmatrix} \\
&\left.\times[\alpha(q_\parallel)-\alpha_0(k_\parallel)]^{n-1} \right].
\end{aligned} \tag{B.3}$$

We examine the numerators of each of the matrix elements in turn, with the use of the results given by equations (3.10)–(3.11). In so doing we shall make repeated use of equation (3.55), and replace explicit factors of ϵ by unity, to obtain results to the lowest order in η. In what follows the first entry following $\alpha\beta$: is the numerator of the corresponding element of the first matrix on the right-hand side of equation (B.3); the second entry is the numerator of the corresponding element of the second matrix.

pp :

$$\begin{aligned}
&[q_\parallel k_\parallel - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha_0(k_\parallel)][\epsilon\alpha_0(k_\parallel)+\alpha(k_\parallel)] \\
&\quad = q_\parallel k_\parallel[\alpha_0(k_\parallel)+\alpha(k_\parallel)] - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel[\alpha_0^2(k_\parallel)+\alpha_0(k_\parallel)\alpha(k_\parallel)] + \mathrm{O}(\eta) \\
&\quad = q_\parallel k_\parallel[\alpha_0(k_\parallel)+\alpha(k_\parallel)] - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha(k_\parallel)[\alpha(k_\parallel)+\alpha_0(k_\parallel)] + \mathrm{O}(\eta) \\
&\quad = [q_\parallel k_\parallel - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha(k_\parallel)][\alpha(k_\parallel)+\alpha_0(k_\parallel)] + \mathrm{O}(\eta)
\end{aligned} \tag{B.4a}$$

$$\begin{aligned}
&[q_\parallel k_\parallel + \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha_0(k_\parallel)][\epsilon\alpha_0(k_\parallel)-\alpha(k_\parallel)] \\
&\quad = q_\parallel k_\parallel[\alpha_0(k_\parallel)-\alpha(k_\parallel)] + \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel[\alpha_0^2(k_\parallel)-\alpha_0(k_\parallel)\alpha(k_\parallel)] + \mathrm{O}(\eta) \\
&\quad = q_\parallel k_\parallel[\alpha_0(k_\parallel)-\alpha(k_\parallel)] + \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha(k_\parallel)[\alpha(k_\parallel)-\alpha_0(k_\parallel)] + \mathrm{O}(\eta) \\
&\quad = [q_\parallel k_\parallel - \alpha(q_\parallel)\hat{q}_\parallel\cdot\hat{k}_\parallel\alpha(k_\parallel)][\alpha_0(k_\parallel)-\alpha(k_\parallel)] + \mathrm{O}(\eta)
\end{aligned} \tag{B.4b}$$

$$\text{ps}: \quad -\frac{\omega}{c}(\alpha(q_\parallel)(\hat{q}_\parallel \times \hat{k}_\parallel)_3[\alpha_0(k_\parallel) + \alpha(k_\parallel)] \tag{B.5a}$$

$$-\frac{\omega}{c}\alpha(q_\parallel)(\hat{q}_\parallel \times \hat{k}_\parallel)_3[\alpha_0(k_\parallel) - \alpha(k_\parallel)] \tag{B.5b}$$

$$\begin{aligned}\text{sp}: \quad & -\frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3\alpha_0(k_\parallel)[\epsilon\alpha_0(k_\parallel) + \alpha(k_\parallel)] \\ &= -\frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3[\alpha_0^2(k_\parallel) + \alpha_0(k_\parallel)\alpha(k_\parallel)] + \mathrm{O}(\eta) \\ &= -\frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3\alpha(k_\parallel)[\alpha(k_\parallel) + \alpha_0(k_\parallel)] + \mathrm{O}(\eta)\end{aligned} \tag{B.6a}$$

$$\begin{aligned}& \frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3\alpha_0(k_\parallel)[\epsilon\alpha_0(k_\parallel) - \alpha(k_\parallel))] \\ &= \frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3[\alpha_0^2(k_\parallel) - \alpha_0(k_\parallel)\alpha(k_\parallel)] + \mathrm{O}(\eta) \\ &= \frac{\omega}{c}(\hat{q}_\parallel \times \hat{k}_\parallel)_3\alpha(k_\parallel)[\alpha(k_\parallel) - \alpha_0(k_\parallel)] + \mathrm{O}(\eta)\end{aligned} \tag{B.6b}$$

$$\text{ss}: \quad \frac{\omega^2}{c^2}\hat{q}_\parallel \cdot \hat{k}_\parallel[\alpha_0(k_\parallel) + \alpha(k_\parallel)] \tag{B.7a}$$

$$\frac{\omega^2}{c^2}\hat{q}_\parallel \cdot \hat{k}_\parallel[\alpha_0(k_\parallel) - \alpha(k_\parallel)]. \tag{B.7b}$$

Collecting these results, we can rewrite equation (B.3) in the form

$$\begin{aligned}\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \pm \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel) &= \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\hat{\zeta}^{(n)}(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \\ &\times\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)[(\alpha_0(k_\parallel) + \alpha(k_\parallel))(\alpha(q_\parallel) + \alpha_0(k_\parallel))^{n-1} \\ &\pm(\alpha_0(k_\parallel) - \alpha(k_\parallel))(\alpha(q_\parallel) - \alpha_0(k_\parallel))^{n-1}] + \mathrm{O}(\eta)\end{aligned} \tag{B.8}$$

where the matrix $\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ has been defined by equation (3.53). With the aid of the results given by equations (A.10), (A.11), and (A.20), equation (B.8) becomes

$$\begin{aligned}\mathbf{n}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \pm \mathbf{m}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\mathbf{R}^{(0)}(k_\parallel) &= \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\hat{\zeta}^{(n)}(\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel) \\ &\times\mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\begin{pmatrix}2\alpha_0(k_\parallel)\\ 2\alpha(k_\parallel)\end{pmatrix}(\alpha(q_\parallel) + \alpha(k_\parallel))^{n-1} + \mathrm{O}(\eta) \\ &= \mathbf{P}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)\frac{J(\alpha(q_\parallel) + \alpha(k_\parallel)|\boldsymbol{q}_\parallel - \boldsymbol{k}_\parallel)}{\alpha(q_\parallel) + \alpha(k_\parallel)}\begin{pmatrix}2\alpha_0(k_\parallel)\\ 2\alpha(k_\parallel)\end{pmatrix} + \mathrm{O}(\eta)\end{aligned} \tag{B.9}$$

where we have used equation (B.1) again. This is the result expressed by equation (3.52).

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