Multiple scattering of waves from random rough surfaces

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(Received 21 April 1980)

A recent multiple-scattering theory of waves scattered from a random rough surface of Garcia *et al.* [Opt. Commun. 30, 279 (1979)] is modified by the use of cumulant techniques to yield an expression for the mean scattered intensity that can be separated explicitly into a specular and a diffuse contribution, and possesses a simple physical interpretation.

In a recent paper[1] Garcia *et al.* have presented an exact multiple-scattering theory of waves scattered from a random rough surface. In this paper we present a variant of this theory that appears to have certain formal and conceptual advantages.

We consider scattering of a particle of mass m, incident from above, on a random rough hard wall described by the potential

$$V(\vec{x}) = \begin{cases} 0, & x_3 > \zeta(\vec{x}_\parallel) \\ \infty, & x_3 < \zeta(\vec{x}_\parallel), \end{cases} \tag{1}$$

where $\zeta(\vec{x}_\parallel)$ is the surface-roughness profile function. It is a function of the two-dimensional position vector $\vec{x}_\parallel = \hat{x}_1 x_1 + \hat{x}_2 x_2$, where $\hat{x}_1$ and $\hat{x}_2$ are two mutually perpendicular unit vectors in the plane $x_3 = 0$.

The function $\zeta(\vec{x}_\parallel)$ is assumed to be a stationary stochastic process, characterized by the following statistical properties. (1) The average over the ensemble of realizations of the surface profile function of the product of an odd number of $\zeta(\vec{x}_\parallel)$'s vanishes, e.g.,

$$\langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel')\zeta(\vec{x}_\parallel'')\rangle = 0 \ , \tag{2}$$

where $\vec{x}_\parallel$, $\vec{x}_\parallel'$, and $\vec{x}_\parallel''$ do not need to be different points; and (2) the average of the product of an even number of $\zeta(\vec{x}_\parallel)$'s is given by the sum of the products of the averages of the $\zeta(\vec{x}_\parallel)$'s taken two-by-two different in all possible ways, e.g.,

$$\begin{aligned}\langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel')\zeta(\vec{x}_\parallel'')\zeta(\vec{x}_\parallel''')\rangle &= \langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel')\rangle\langle \zeta(\vec{x}_\parallel'')\zeta(\vec{x}_\parallel''')\rangle \\ &+ \langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel'')\rangle\langle \zeta(\vec{x}_\parallel')\zeta(\vec{x}_\parallel''')\rangle \\ &+ \langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel''')\rangle\langle \zeta(\vec{x}_\parallel')\zeta(\vec{x}_\parallel'')\rangle \ . \end{aligned} \tag{3}$$

Each average of a pair of $\zeta(\vec{x}_\parallel)$'s on the right-hand side of this equation, called a *contraction*, is given by

$$\langle \zeta(\vec{x}_\parallel)\zeta(\vec{x}_\parallel')\rangle = \delta^2 W(|\vec{x}_\parallel - \vec{x}_\parallel'|) \ . \tag{4}$$

Here $\delta^2 = \langle \zeta^2(\vec{x}_\parallel)\rangle$ is the mean-square departure of the surface from flatness. In actual calculations a Gaussian form will be adopted for the correlation function $W(|\vec{x}_\parallel - \vec{x}_\parallel'|)$,

$$W(|\vec{x}_\parallel - \vec{x}_\parallel'|) = \exp(-a^{-2}|\vec{x}_\parallel - \vec{x}_\parallel'|^2) \ . \tag{5}$$

The parameter a appearing in this expression is called the *transverse correlation length*.

The exact wave function for this problem can be obtained by an application of Green's theorem and is given by[2]

$$\exp[i\vec{k}_\parallel\cdot\vec{x}_\parallel - i\alpha(k_\parallel)x_3] + \tfrac{1}{2}i\int \frac{d^2q_\parallel}{(2\pi)^2}\frac{\exp(i\vec{q}_\parallel\cdot\vec{x}_\parallel)}{\alpha(q_\parallel)} \times \int d^2x_\parallel' \exp(-i\vec{q}_\parallel\cdot\vec{x}_\parallel')\exp[i\alpha(q_\parallel)|x_3 - \zeta(\vec{x}_\parallel')|]L(\vec{x}_\parallel') = \begin{cases}\psi(\vec{x}), & x_3 > \zeta(\vec{x}_\parallel) \\ 0, & x_3 < \zeta(\vec{x}_\parallel), \end{cases} \tag{6}$$

where $\vec{k}_\parallel = \hat{x}_1 k_1 + \hat{x}_2 k_2$ is a two-dimensional wave vector parallel to the plane $x_3 = 0$, and

$$\alpha(k_\parallel) = \begin{cases}(k_0^2 - k_\parallel^2)^{1/2}, & k_\parallel < k_0 \\ i(k_\parallel^2 - k_0^2)^{1/2}, & k_\parallel > k_0 \ . \end{cases} \tag{7}$$

Here $k_0=(2mE/\hbar^2)^{1/2}$, where $E(>0)$ is the energy of the incident particle. The function $L(\vec{x}_\parallel)$ is defined by

$$L(\vec{x}_\parallel)=\left[1+\left(\frac{\partial\zeta}{\partial x_1}\right)^2+\left(\frac{\partial\zeta}{\partial x_2}\right)^2\right]^{1/2}\frac{\partial}{\partial n}\psi(\vec{x})\bigg|_{x_3=\zeta(\vec{x}_\parallel)} . \tag{8}$$

In the present case the normal derivative is given by

$$\frac{\partial}{\partial n}=\left[1+\left(\frac{\partial\zeta}{\partial x_1}\right)^2+\left(\frac{\partial\zeta}{\partial x_2}\right)^2\right]^{-1/2}\left(\frac{\partial\zeta}{\partial x_1}\frac{\partial}{\partial x_1}+\frac{\partial\zeta}{\partial x_2}\frac{\partial}{\partial x_2}-\frac{\partial}{\partial x_3}\right) . \tag{9}$$

The scattered wave function is obtained from the second term on the left-hand side of Eq. (6) in the limit that $x_3 >> \zeta_{\max}$:

$$\psi_s(\vec{x})=\int\frac{d^2q_\parallel}{(2\pi)^2}R(\vec{k}_\parallel|\vec{q}_\parallel)\exp[i\vec{q}_\parallel\cdot\vec{x}_\parallel+i\alpha(q_\parallel)x_3] , \tag{10}$$

where

$$R(\vec{k}_\parallel|\vec{q}_\parallel)=\frac{i}{2\alpha(q_\parallel)}\int d^2x_\parallel\exp[-i\vec{q}_\parallel\cdot\vec{x}_\parallel-i\alpha(q_\parallel)\zeta(\vec{x}_\parallel)]L(\vec{x}_\parallel) . \tag{11}$$

The three-component of the scattered flux of particles, averaged over the ensemble of realizations of the surface roughness, is

$$\begin{aligned}\langle J_3^{(s)}(\vec{x})\rangle&=\frac{\hbar}{2im}\left\langle\psi_s^*(\vec{x})\frac{\partial}{\partial x_3}\psi_s(\vec{x})-\psi_s(\vec{x})\frac{\partial}{\partial x_3}\psi_s^*(\vec{x})\right\rangle\\&=\frac{\hbar}{m}\int\frac{d^2q_\parallel}{(2\pi)^2}\int\frac{d^2p_\parallel}{(2\pi)^2}\langle R^*(\vec{k}_\parallel|\vec{q}_\parallel)R(\vec{k}_\parallel|\vec{p}_\parallel)\rangle\exp[-i(\vec{q}_\parallel-\vec{p}_\parallel)\cdot\vec{x}_\parallel]\\&\qquad\times\exp\{-i[\alpha^*(q_\parallel)-\alpha(p_\parallel)]x_3\}\tfrac{1}{2}[\alpha^*(q_\parallel)+\alpha(p_\parallel)] .\end{aligned} \tag{12}$$

The three-component of the incident flux is

$$J_3^{(i)}(\vec{x})=-\frac{\hbar}{m}\alpha(k_\parallel) . \tag{13}$$

Equating the magnitudes of the normal components of the incident and scattered particle fluxes, we obtain the unitarity condition on the scattered wave in the form

$$\int\frac{d^2q_\parallel}{(2\pi)^2}\int\frac{d^2p_\parallel}{(2\pi)^2}\frac{\alpha^*(q_\parallel)+\alpha(p_\parallel)}{2\alpha(k_\parallel)}\langle R^*(\vec{k}_\parallel|\vec{q}_\parallel)R(\vec{k}_\parallel|\vec{p}_\parallel)\rangle\exp[-i(\vec{q}_\parallel-\vec{p}_\parallel)\cdot\vec{x}_\parallel]\exp\{-i[\alpha^*(q_\parallel)-\alpha(p_\parallel)]x_3\}=1 . \tag{14}$$

We will return to this condition below.

To proceed farther we require the function $L(\vec{x}_\parallel)$. It can be obtained from Eq. (6) in one of two ways. We can let $x_3\to\zeta(\vec{x}_\parallel)$ from above in the first of Eqs. (6). The right-hand side of this equation vanishes and we obtain the following integral equation for $L(\vec{x}_\parallel)$:

$$\begin{aligned}-\exp[i\vec{k}_\parallel\cdot\vec{x}_\parallel-i\alpha(k_\parallel)\zeta(\vec{x}_\parallel)]&=\tfrac{1}{2}i\int\frac{d^2q_\parallel}{(2\pi)^2}\frac{\exp(i\vec{q}_\parallel\cdot\vec{x}_\parallel)}{\alpha(q_\parallel)}\\&\qquad\times\int d^2x'_\parallel\exp(-i\vec{q}_\parallel\cdot\vec{x}'_\parallel)\exp[i\alpha(q_\parallel)|\zeta(\vec{x}_\parallel)-\zeta(\vec{x}'_\parallel)|]L(\vec{x}'_\parallel) .\end{aligned} \tag{15}$$

Alternatively, we can use the second of Eqs. (6). We require that it be satisfied for all $x_3<\zeta_{\min}$. In this way we obtain the equation

$$-\exp[i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}-i\alpha(k_{\parallel})x_3]=\tfrac{1}{2}i\int\frac{d^2q_{\parallel}}{(2\pi)^2}\frac{\exp[i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}-i\alpha(q_{\parallel})x_3]}{\alpha(q_{\parallel})}\int d^2x'_{\parallel}\exp[-i\vec{q}_{\parallel}\cdot\vec{x}'_{\parallel}+i\alpha(q_{\parallel})\zeta(\vec{x}'_{\parallel})]L(\vec{x}'_{\parallel}) \ . \tag{16}$$

We see that his equation is satisfied if $L(\vec{x}_{\parallel})$ is a solution of the integral equation

$$\int d^2x_{\parallel}\exp[-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}+i\alpha(q_{\parallel})\zeta(\vec{x}_{\parallel})]L(\vec{x}_{\parallel})=2i\alpha(q_{\parallel})(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{k}_{\parallel}) \ . \tag{17}$$

To illustrate the method for obtaining the scattered wave function we are proposing in this paper we will work with the simpler equation for $L(\vec{x}_{\parallel})$, Eq. (17). We begin by simplifying this equation. If we expand $L(\vec{x}_{\parallel})$ formally as

$$L(\vec{x}_{\parallel})=\sum_{n=0}^{\infty}\frac{L^{(n)}(\vec{x}_{\parallel})}{n!} \ , \tag{18}$$

where the index n denotes the order of the corresponding term in $\zeta(\vec{x}_{\parallel})$, substitute this expansion into Eq. (17), and equate the terms of the same order in $\zeta(\vec{x}_{\parallel})$ on both sides of the resulting equation, we obtain a series of equations for the determination of the $\{L^{(n)}(\vec{x}_{\parallel})\}$, the first three of which are

$$\int d^2x_{\parallel}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel})L^{(0)}(\vec{x}_{\parallel})=2i\alpha(q_{\parallel})(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{k}_{\parallel}) \ , \tag{19a}$$

$$\int d^2x_{\parallel}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel})[L^{(1)}(\vec{x}_{\parallel})+i\alpha(q_{\parallel})\zeta(\vec{x}_{\parallel})L^{(0)}(\vec{x}_{\parallel})]=0 \ , \tag{19b}$$

$$\int d^2x_{\parallel}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel})[\tfrac{1}{2}L^{(2)}(\vec{x}_{\parallel})+i\alpha(q_{\parallel})\zeta(\vec{x}_{\parallel})L^{(1)}(\vec{x}_{\parallel})-\tfrac{1}{2}\alpha^2(q_{\parallel})\zeta^2(\vec{x}_{\parallel})L^{(0)}(\vec{x}_{\parallel})]=0 \ . \tag{19c}$$

These equations can be solved successively with the aid of Fourier's inversion theorem, with the result that

$$L^{(0)}(\vec{x}_{\parallel})=2i\alpha(k_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}) \ , \tag{20a}$$

$$L^{(1)}(\vec{x}_{\parallel})=2i\alpha(k_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})(-i)\int\frac{d^2P_{\parallel}}{(2\pi)^2}\exp(i\vec{P}_{\parallel}\cdot\vec{x}_{\parallel})\hat{\zeta}(\vec{P}_{\parallel})\alpha(|\vec{P}_{\parallel}+\vec{k}_{\parallel}|) \ , \tag{20b}$$

$$L^{(2)}(\vec{x}_{\parallel})=2i\alpha(k_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})(-i)^2\int\frac{d^2P_{\parallel}}{(2\pi)^2}\int\frac{d^2Q_{\parallel}}{(2\pi)^2}\exp(i\vec{P}_{\parallel}\cdot\vec{x}_{\parallel})\hat{\zeta}(\vec{P}_{\parallel}-\vec{Q}_{\parallel})\hat{\zeta}(\vec{Q}_{\parallel})$$
$$\times\alpha(|\vec{P}_{\parallel}+\vec{k}_{\parallel}|)[2\alpha(|\vec{Q}_{\parallel}+\vec{k}_{\parallel}|)-\alpha(|\vec{P}_{\parallel}+\vec{k}_{\parallel}|)] \ . \tag{20c}$$

In obtaining these results we have introduced the Fourier transform of $\zeta(\vec{x}_{\parallel})$,

$$\zeta(\vec{x}_{\parallel})=\int\frac{d^2q_{\parallel}}{(2\pi)^2}\exp(i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel})\hat{\zeta}(\vec{q}_{\parallel}) \ . \tag{21}$$

The results given by Eqs. (20) suggest that we express $L(\vec{x}_{\parallel})$ in the form

$$L(\vec{x}_{\parallel})=2i\alpha(k_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})f(\vec{k}_{\parallel}|\vec{x}_{\parallel}) \ , \tag{22}$$

where $f(\vec{k}_{\parallel}|\vec{x}_{\parallel})$ obeys the integral equation

$$\int d^2x_{\parallel}\exp[-i(\vec{q}_{\parallel}-\vec{k}_{\parallel})\cdot\vec{x}_{\parallel}+i\alpha(q_{\parallel})\zeta(\vec{x}_{\parallel})]f(\vec{k}_{\parallel}|\vec{x}_{\parallel})=(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{k}_{\parallel}) \ . \tag{23}$$

The point of our approach is that we seek $f(\vec{k}_{\parallel}|\vec{x}_{\parallel})$ in an exponential form

$$f(\vec{k}_{\parallel}|\vec{x}_{\parallel})=\exp[g(\vec{k}_{\parallel}|\vec{x}_{\parallel})] \ , \tag{24}$$

where the function $g(\vec{k}_{\parallel}|\vec{x}_{\parallel})$ will be expanded in powers of $\zeta(\vec{x}_{\parallel})$ according to

$$g(\vec{k}_{\parallel}|\vec{x}_{\parallel})=\sum_{n=1}^{\infty}(-i)^n\frac{g^{(n)}(\vec{k}_{\parallel}|\vec{x}_{\parallel})}{n!} \ , \tag{25}$$

where, again, the superscript denotes the order of the corresponding term in $\zeta(\vec{x}_{\parallel})$. To obtain the $\{g^{(n)}(\vec{k}_{\parallel}|\vec{x}_{\parallel})\}$ we use, as did Garcia *et al.*,[1] the method of Lopez *et al.*[3] Thus we expand $f(\vec{k}_{\parallel}|\vec{x}_{\parallel})$ formally as

$$f(\vec{k}_{\parallel}|\vec{x}_{\parallel})=\sum_{n=0}^{\infty}(-i)^n\frac{f^{(n)}(\vec{k}_{\parallel}|\vec{x}_{\parallel})}{n!} \ , \tag{26}$$

where from Eqs. (20a) and (22) $f^{(0)}(\vec{k}_{\parallel}|\vec{x}_{\parallel})\equiv 1$. It is easy to see that the relation between $g^{(n)}(\vec{k}_\parallel|\vec{x}_\parallel)$ and the $\{f^{(m)}(\vec{k}_\parallel|\vec{x}_\parallel)\}$ for $0 \leq m \leq n$ is exactly that between the cumulant average $\langle x^n\rangle_c$ of a random variable x and the moments $\{\langle x^m\rangle\}$ for $0\leq m\leq n$.[4] Thus we have that the first few $\{g^{(n)}(\vec{k}_\parallel|\vec{x}_\parallel)\}$ are given by

$$g^{(1)}=f^{(1)} , \tag{27a}$$

$$g^{(2)}=f^{(2)}-f^{(1)^2} , \tag{27b}$$

$$g^{(3)}=f^{(3)}-3f^{(2)}f^{(1)}+2f^{(1)^3} , \tag{27c}$$

$$g^{(4)}=f^{(4)}-4f^{(3)}f^{(1)}-3f^{(2)^2}+12f^{(2)}f^{(1)^2}-6f^{(1)^4} , \tag{27d}$$

and in general[4]

$$g^{(n)}=n!\sum_{m=0}^{n}\sum\left[\frac{f^{(p_1)}}{p_1!}\right]^{\pi_1}\cdots\left[\frac{f^{(p_m)}}{p_m!}\right]^{\pi_m}\times\frac{(-1)^{\rho-1}(\rho-1)!}{\pi_1!\cdots\pi_m!} , \tag{28}$$

where the second summation extends over all nonnegative π's and ρ's subject to the two conditions

$$p_1\pi_1+p_2\pi_2+\cdots+p_m\pi_m=n , \tag{29a}$$

$$\pi_1+\pi_2+\cdots+\pi_m=\rho . \tag{29b}$$

To obtain the $\{f^{(n)}(\vec{k}_\parallel|\vec{x}_\parallel)\}$ we substitute the expansion (26) into Eq. (23) and equate the different powers of $\zeta(\vec{x}_\parallel)$ on both sides of the equation. In this way we obtain the results that

$$\hat{f}^{(0)}(\vec{k}_\parallel|\vec{q}_\parallel)=(2\pi)^2\delta(\vec{q}_\parallel) , \tag{30a}$$

$$\hat{f}^{(n)}(\vec{k}_\parallel|\vec{q}_\parallel)=-\sum_{m=1}^{n}(-1)^m\binom{n}{m}\alpha(|\vec{q}_\parallel+\vec{k}_\parallel|)^m\times\int\frac{d^2Q_\parallel}{(2\pi)^2}\hat{f}^{(n-m)}(\vec{k}_\parallel|\vec{q}_\parallel-\vec{Q}_\parallel)\times\hat{\zeta}^{(m)}(\vec{Q}_\parallel),\quad n\geq 1 \tag{30b}$$

where we have introduced the Fourier representations

$$f^{(n)}(\vec{k}_\parallel|\vec{x}_\parallel)=\int\frac{d^2q_\parallel}{(2\pi)^2}\exp(i\vec{q}_\parallel\cdot\vec{x}_\parallel)\hat{f}^{(n)}(\vec{k}_\parallel|\vec{q}_\parallel) , \tag{31}$$

$$[\zeta(\vec{x}_\parallel)]^m=\int\frac{d^2q_\parallel}{(2\pi)^2}\exp(i\vec{q}_\parallel\cdot\vec{x}_\parallel)\hat{\zeta}^{(m)}(\vec{q}_\parallel) . \tag{32}$$

The Fourier coefficient $\hat{\zeta}^{(m)}(\vec{q}_\parallel)$ can be obtained recursively from the relation

$$\hat{\zeta}^{(m)}(\vec{q}_\parallel)=\int\frac{d^2Q_\parallel}{(2\pi)^2}\hat{\zeta}^{(m-1)}(\vec{q}_\parallel-\vec{Q}_\parallel)\,\hat{\zeta}(\vec{Q}_\parallel),\quad m\geq 1 \tag{33a}$$

with

$$\hat{\zeta}^{(0)}(\vec{q}_\parallel)=(2\pi)^2\delta(\vec{q}_\parallel) , \tag{33b}$$

$$\hat{\zeta}^{(1)}(\vec{q}_\parallel)=\hat{\zeta}(\vec{q}_\parallel) . \tag{33c}$$

Combining Eqs. (11), (22), and (24) we can write the scattering amplitude $R(\vec{k}_\parallel|\vec{q}_\parallel)$ in the form

$$R(\vec{k}_\parallel|\vec{q}_\parallel)=-\frac{\alpha(k_\parallel)}{\alpha(q_\parallel)}\int d^2x_\parallel\exp[i(\vec{k}_\parallel-\vec{q}_\parallel)\cdot\vec{x}_\parallel]\times\exp[G(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)] , \tag{34}$$

where

$$G(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)=-i\alpha(q_\parallel)\zeta(\vec{x}_\parallel)+g(\vec{k}_\parallel|\vec{x}_\parallel) . \tag{35}$$

Thus, if we expand $G(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)$ in the form

$$G(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)=\sum_{n=1}^{\infty}(-i)^n\frac{G^{(n)}(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)}{n!} \tag{36}$$

we have

$$G^{(n)}(\vec{k}_\parallel\vec{q}_\parallel|\vec{x}_\parallel)=\begin{cases}\alpha(q_\parallel)\zeta(\vec{x}_\parallel)+g^{(1)}(\vec{k}_\parallel|\vec{x}_\parallel), & n=1 \quad (37a)\\ g^{(n)}(\vec{k}_\parallel|\vec{x}_\parallel), & n\geq 2 . \quad (37b)\end{cases}$$

The average appearing in the scattered flux, Eq. (12), and in the unitarity condition, Eq. (14), now takes the form

$$\langle R^*(\vec{k}_\parallel|\vec{q}_\parallel)R(\vec{k}_\parallel|\vec{p}_\parallel)\rangle=\frac{\alpha^2(k_\parallel)}{\alpha^*(q_\parallel)\alpha(p_\parallel)}\int d^2x_\parallel\int d^2x_\parallel'\exp(i\vec{q}_\parallel\cdot\vec{x}_\parallel-i\vec{p}_\parallel\cdot\vec{x}_\parallel')\times\exp[-i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')]\langle\exp[G^*(\vec{x}_\parallel)+G(\vec{x}_\parallel')]\rangle , \tag{38}$$

where, to simplify the notation, we have dropped the arguments $\vec{k}_\parallel$ and $\vec{q}_\parallel$ in writing $G(\vec{x}_\parallel)$. The average appearing in this expression will be evaluated in terms of cumulant averages.[4] We begin with the identity

$$\langle\exp[G^*(\vec{x}_\parallel)+G(\vec{x}_\parallel')]\rangle=\exp[\langle\exp G^*(\vec{x}_\parallel)-1\rangle_c]\exp[\langle\exp G(\vec{x}_\parallel')-1\rangle_c]\times\frac{\exp\{\langle\exp[G^*(\vec{x}_\parallel)+G(\vec{x}_\parallel')]-1\rangle_c\}}{\exp[\langle\exp G^*(\vec{x}_\parallel)-1\rangle_c]\exp[\langle\exp G(\vec{x}_\parallel')-1\rangle_c]} , \tag{39}$$

where $\langle \cdots \rangle_c$ denotes the cumulant average. The first factor on the right-hand side of this equation gives that part of the average on the left-hand side that is independent of $\vec{x}'_\parallel$; the second factor gives that part that is independent of $\vec{x}_\parallel$; the third factor gives the correlated part, i.e., the part that depends on both $\vec{x}_\parallel$ and $\vec{x}'_\parallel$. We next introduce the definitions

$$M(\vec{k}_\parallel;\vec{q}_\parallel) = -\langle \exp G(\vec{x}_\parallel) - 1 \rangle_c \ , \tag{40}$$

$$C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{x}_\parallel - \vec{x}'_\parallel) = \langle \exp[G^*(\vec{x}_\parallel) + G(\vec{x}'_\parallel)] - 1 \rangle_c - \langle \exp G^*(\vec{x}_\parallel) - 1 \rangle_c - \langle \exp G(\vec{x}'_\parallel) - 1 \rangle_c \ . \tag{41}$$

The fact that $M(\vec{k}_\parallel;\vec{q}_\parallel)$ is independent of $\vec{x}_\parallel$ is due to the stationarity of $\zeta(\vec{x}_\parallel)$, as is the fact that $C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{x}_\parallel - \vec{x}'_\parallel)$ depends on $\vec{x}_\parallel$ and $\vec{x}'_\parallel$ only through their difference. Thus we are led to the result that

$$\langle \exp[G^*(\vec{x}_\parallel) + G(\vec{x}'_\parallel)] \rangle = \exp[-2\overline{M}(\vec{k}_\parallel;\vec{q}_\parallel)] \exp[C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{x}_\parallel - \vec{x}'_\parallel)] \ , \tag{42}$$

where

$$\overline{M}(\vec{k}_\parallel;\vec{q}_\parallel) = \mathrm{Re} M(\vec{k}_\parallel;\vec{q}_\parallel) \ . \tag{43}$$

When the result given by Eq. (42) is substituted into Eq. (38) we obtain the result that

$$\langle R^*(\vec{k}_\parallel|\vec{q}_\parallel) R(\vec{k}_\parallel|\vec{p}_\parallel) \rangle = (2\pi)^2 \delta(\vec{p}_\parallel - \vec{q}_\parallel) |\alpha(k_\parallel)/\alpha(q_\parallel)|^2 \exp[-2\overline{M}(\vec{k}_\parallel;\vec{q}_\parallel)] \times \int d^2y_\parallel \exp[-i(\vec{k}_\parallel - \vec{q}_\parallel)\cdot\vec{y}_\parallel] \exp[C(\vec{k}_\parallel;\vec{q}|\vec{y}_\parallel)] \ . \tag{44}$$

It follows that the scattered flux is given by

$$\langle J_3^{(s)}(\vec{x}) \rangle = \frac{\hbar}{m} \alpha(k_\parallel) \int_{q_\parallel < k_0} \frac{d^2 q_\parallel}{(2\pi)^2} \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle \ , \tag{45}$$

where the integral is restricted to such values of $q_\parallel$ that $\alpha(q_\parallel)$ is real, and where the mean scattered intensity corresponding to the wave vector $\vec{q}_\parallel$ is

$$\langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle = \frac{\alpha(k_\parallel)}{\alpha(q_\parallel)} \exp[-2\overline{M}(\vec{k}_\parallel;\vec{q}_\parallel)] \times \int d^2y_\parallel \exp[-i(\vec{k}_\parallel - \vec{q}_\parallel)\cdot\vec{y}_\parallel] \times \exp[C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{y}_\parallel)] \ . \tag{46}$$

With this definition the unitarity condition (14) takes the form

$$\int_{q_\parallel < k_0} \frac{d^2 q_\parallel}{(2\pi)^2} \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle = 1 \ . \tag{47}$$

Using the identity

$$e^x = 1 + (e^x - 1) \tag{48}$$

we can separate the mean scattered intensity into the specular contribution and the diffuse contribution,

$$\langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle = \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_s + \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_d \ , \tag{49}$$

where

$$\langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_s = (2\pi)^2 \delta(\vec{q}_\parallel - \vec{k}_\parallel) \exp[-2\overline{M}(\vec{k}_\parallel;\vec{k}_\parallel)] \ , \tag{50}$$

$$\langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_d = \frac{\alpha(k_\parallel)}{\alpha(q_\parallel)} \exp[-2\overline{M}(\vec{k}_\parallel;\vec{q}_\parallel)] \times \int d^2y_\parallel \exp[-i(\vec{k}_\parallel - \vec{q}_\parallel)\cdot\vec{y}_\parallel] \times \{\exp[C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{y}_\parallel)] - 1\} \ . \tag{51}$$

We see from Eq. (50) that the mean scattered intensity in the specular direction is reduced from its value for a flat surface by the factor $\exp[-2\overline{M}(\vec{k}_\parallel;\vec{k}_\parallel)]$, that describes the effects of scattering in directions other than the specular by the surface roughness.

From the results given by Eqs. (47), (49), and (50) we can establish the following sum rules:

$$\int_{q_\parallel < k_0} \frac{d^2 q_\parallel}{(2\pi)^2} \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_s = \exp[-2\overline{M}(\vec{k}_\parallel;\vec{k}_\parallel)] \ , \tag{52a}$$

$$\int_{q_\parallel < k_0} \frac{d^2 q_\parallel}{(2\pi)^2} \langle I(\vec{k}_\parallel;\vec{q}_\parallel) \rangle_d = 1 - \exp[-2\overline{M}(\vec{k}_\parallel;\vec{k}_\parallel)] \ . \tag{52b}$$

If we now use the definitions (40) and (41), the expansion (36), and the rules for evaluating cumulant averages,[4] we obtain the following expressions for $M(\vec{k}_\parallel;\vec{q}_\parallel)$ and $C(\vec{k}_\parallel;\vec{q}_\parallel|\vec{x}_\parallel - \vec{x}'_\parallel)$ to $O(\delta^4)$:

$$M(\vec{k}_{\parallel};\vec{q}_{\parallel}) = \tfrac{1}{2}(\langle G^{(2)}\rangle + \langle G^{(1)^2}\rangle) - \tfrac{1}{24}(\langle G^{(4)}\rangle + 4\langle G^{(3)}G^{(1)}\rangle + 3\langle G^{(2)^2}\rangle + 6\langle G^{(2)}G^{(1)^2}\rangle + \langle G^{(1)^4}\rangle - 6\langle G^{(2)}\rangle\langle G^{(1)^2}\rangle - 3\langle G^{(1)^2}\rangle^2 - 3\langle G^{(2)}\rangle^2) + O(\delta^6) \; , \tag{53}$$

$$\begin{aligned} C(\vec{k}_{\parallel};\vec{q}_{\parallel}|\vec{x}_{\parallel}-\vec{x}'_{\parallel}) = \langle G^{(1)}G^{(1)*}\rangle + \tfrac{1}{12}(&-2\langle G^{(1)}G^{(3)*}\rangle - 2\langle G^{(1)*}G^{(3)}\rangle + 3\langle G^{(2)}G^{(2)*}\rangle + 3\langle G^{(1)^2}G^{(2)*}\rangle \\ &+3\langle G^{(1)*^2}G^{(2)}\rangle - 6\langle G^{(1)}G^{(1)*}G^{(2)}\rangle - 6\langle G^{(1)}G^{(1)*}G^{(2)*}\rangle - 2\langle G^{(1)^3}G^{(1)*}\rangle \\ &-2\langle G^{(1)}G^{(1)*^3}\rangle + 3\langle G^{(1)^2}G^{(1)*^2}\rangle - 3\langle G^{(2)}\rangle\langle G^{(2)*}\rangle + 6\langle G^{(2)}\rangle\langle G^{(1)}G^{(1)*}\rangle \\ &+6\langle G^{(2)*}\rangle\langle G^{(1)}G^{(1)*}\rangle - 3\langle G^{(2)}\rangle\langle G^{(1)*^2}\rangle - 3\langle G^{(2)*}\rangle\langle G^{(1)^2}\rangle - 6\langle G^{(1)}G^{(1)*}\rangle^2 \\ &-3\langle G^{(1)^2}\rangle\langle G^{(1)*^2}\rangle + 6\langle G^{(1)^2}\rangle\langle G^{(1)}G^{(1)*}\rangle + 6\langle G^{(1)*^2}\rangle\langle G^{(1)}G^{(1)*}\rangle) + O(\delta^6) \; . \end{aligned} \tag{54}$$

In Eq. (54) the argument of $G^{(n)}$ is $\vec{x}'_{\parallel}$, while the argument of $G^{(n)*}$ is $\vec{x}_{\parallel}$.

The explicit results for $M(\vec{k}_{\parallel};\vec{q}_{\parallel})$ and $C(\vec{k}_{\parallel};\vec{q}_{\parallel}|\vec{y}_{\parallel})$ to $O(\delta^2)$ are

$$M(\vec{k}_{\parallel};\vec{q}_{\parallel}) = \tfrac{1}{2}\delta^2(k_{\parallel}^2 - q_{\parallel}^2) + \delta^2[\alpha(k_{\parallel}) + \alpha(q_{\parallel})] \times \int \frac{d^2Q_{\parallel}}{(2\pi)^2} g(Q_{\parallel})\alpha(|\vec{Q}_{\parallel}+\vec{k}_{\parallel}|) \; , \tag{55}$$

$$C(\vec{k}_{\parallel};\vec{q}_{\parallel}|\vec{y}_{\parallel}) = \delta^2 \int \frac{d^2Q_{\parallel}}{(2\pi)^2} \exp(-i\vec{Q}_{\parallel}\cdot\vec{y}_{\parallel}) g(Q_{\parallel}) \times \left|\alpha(q_{\parallel}) + \alpha(|\vec{Q}_{\parallel}+\vec{k}_{\parallel}|)\right|^2 \; . \tag{56}$$

In obtaining these expressions we have used the results that

$$\langle \hat{\zeta}(\vec{k}_{\parallel})\hat{\zeta}(\vec{k}'_{\parallel})\rangle = \delta^2 g(k_{\parallel})(2\pi)^2\delta(\vec{k}_{\parallel}+\vec{k}'_{\parallel}) \; , \tag{57}$$

where

$$\begin{aligned} g(k_{\parallel}) &= \int d^2x_{\parallel} \exp(-i\vec{k}\cdot\vec{x}_{\parallel}) W(|\vec{x}_{\parallel}|) \; , \\ &= \pi a^2 \exp(-\tfrac{1}{4}a^2k_{\parallel}^2) \; , \end{aligned} \tag{58}$$

where the second form for $g(k_{\parallel})$ follows from the choice for $W(|\vec{x}_{\parallel}|)$ expressed by Eq. (5).

When the expressions given by Eqs. (55)–(56) are used in Eq. (46), and the result is expanded to second order in δ, we obtain for the mean scattered intensity

$$\begin{aligned} \langle I(\vec{k}_{\parallel};\vec{q}_{\parallel})\rangle &= (2\pi)^2\delta(\vec{k}_{\parallel}-\vec{q}_{\parallel}) \\ &\quad - 2\overline{M}(\vec{k}_{\parallel};\vec{k}_{\parallel})(2\pi)^2\delta(\vec{k}_{\parallel}-\vec{q}_{\parallel}) \\ &\quad + \frac{\alpha(k_{\parallel})}{\alpha(q_{\parallel})} \int d^2y_{\parallel} \exp[-i(\vec{k}_{\parallel}-\vec{q}_{\parallel})\cdot\vec{y}_{\parallel}] \\ &\quad \times C(\vec{k}_{\parallel};\vec{q}_{\parallel}|\vec{y}_{\parallel}) + O(\delta^4) \; . \end{aligned} \tag{59}$$

When this expression is substituted into the unitarity integral, Eq. (47), the integrals of the second and third terms cancel, and we conclude that the expression for $\langle I(\vec{k}_{\parallel};\vec{q}_{\parallel})\rangle$ given by Eq. (46) satisfies unitarity through terms of $O(\delta^2)$ when the expressions for $\overline{M}(\vec{k}_{\parallel};\vec{q}_{\parallel})$ and $C(\vec{k}_{\parallel};\vec{q}_{\parallel}|\vec{y}_{\parallel})$ given by Eqs. (55) and (56) are used in it. This is as it should be, since the expression for $\langle I(\vec{k}_{\parallel};\vec{q}_{\parallel})\rangle$ given by Eq. (59) is equivalent to that obtained to the same order in δ by Garcia *et al.*[1] and shown by them to satisfy unitarity to the same degree.

A closed form expression can be obtained for the quantity $2\overline{M}(\vec{k}_{\parallel};\vec{k}_{\parallel})$ that appears in the expression (50) for the specular contribution to the mean scattered intensity for the special case of normal incidence ($\vec{k}_{\parallel}=0$). In general we have that

$$2\overline{M}(\vec{k}_{\parallel};\vec{k}_{\parallel}) = 4\delta^2\alpha(k_{\parallel}) \int \frac{d^2Q_{\parallel}}{(2\pi)^2} g(Q_{\parallel}) \,\mathrm{Re}\,\alpha(|\vec{Q}_{\parallel}+\vec{k}_{\parallel}|) + O(\delta^4) \; . \tag{60}$$

At normal incidence we find that

$$\begin{aligned} 2\overline{M}(\vec{0};\vec{0}) &= \frac{2}{3}\frac{\delta^2}{a^2}(k_0a)^4 \exp[-\tfrac{1}{4}(k_0a)^2] \times M\left(\frac{3}{2},\frac{5}{2},\frac{k_0^2a^2}{4}\right) \\ &= \frac{2}{3}\frac{\delta^2}{a^2}(k_0a)^4 M\left(1,\frac{5}{2},-\frac{k_0^2a^2}{4}\right) \; , \end{aligned} \tag{61}$$

where $M(a,b,z)$ is Kummer's function,[5] and Kummer's transformation[5] has been employed in going from the first to the second equation.

The result given by the second of Eqs. (61) is equivalent to that given in Eq. (13) of Ref. 1. Alternative forms of this expression that may be better suited to its numerical evaluation are

$$2\overline{M}(\vec{0};\vec{0}) = 4\frac{\delta^2}{a^2}(k_0a)^2\left\{1 - \frac{\pi^{1/2}}{ik_0a}\exp[-\tfrac{1}{4}(k_0a)^2] \times \mathrm{erf}(\tfrac{1}{2}ik_0a)\right\} \tag{62a}$$

$$= 4\frac{\delta^2}{a^2}(k_0a)^2\left\{1 - \frac{2}{k_0a}F(\tfrac{1}{2}k_0a)\right\} \; , \tag{62b}$$

where erf(z) is the error function,[6] and $F(x)$ is Dawson's integral,[7]

$$F(x)=e^{-x^2}\int_0^x e^{t^2}\,dt \ . \tag{63}$$

At the beginning of this paper we stated that we believed that the approach to multiple scattering of waves from random rough surfaces outlined here has formal and conceptual advantages over that presented in the note by Garcia *et al.*[1] The formal advantage we see in the present approach is that it provides an explicit separation of the mean scattered intensity $\langle I(\vec{k}_{\parallel};\vec{q}_{\parallel})\rangle$ into the specular and diffuse components, according to Eqs. (49)–(51). The conceptual advantage it possesses in our view is the analogy it permits us to draw between multiple scattering of waves from a random rough surface and the multiple scattering of waves from another well-known random system—the thermal vibrations of atoms in a crystal—as exemplified by the diffraction of low-energy electrons by the thermal vibrations of a semi-infinite crystal.[8] In the latter theory it is found that the positions of the Bragg peaks in the scattered intensity (the analogs of the specular beam in the present context) are not displaced by the atomic vibrations from their positions for a static lattice. Their intensities, however, are reduced by the atomic vibrations through the Debye-Waller factor, that describes the scattering out of the Bragg beams caused by the thermal motions of the atoms. The decrease in the intensity of the Bragg peaks is compensated by the appearance of a nonzero scattered intensity in directions away from the Bragg directions, the so-called thermal diffuse scattering. If one regards the surface roughness profile function $\zeta(\vec{x}_{\parallel})$ as a continuous analog of the displacements from equilibrium of the atoms in the surface layer of a crystal, we expect by analogy with the theory of low-energy electron diffraction that the intensity of the specular beam in the present case should be decreased by surface roughness by a Debye-Waller-type factor, and that there should be diffuse scattering in directions away from the specular. The analogy between the two theories becomes even closer if we recall that the atomic displacements in the theory of low-energy electron diffraction are random variables distributed in a Gaussian manner, in the harmonic approximation. The statistical properties of the $\{\zeta(\vec{x}_{\parallel})\}$ described by Eqs. (2)–(5) define them also as random variables distributed in a Gaussian manner. In the theory of low-energy electron diffraction the atomic displacements appear in the analog of $R(\vec{k}_{\parallel}|\vec{q}_{\parallel})$ in the exponential fashion in which $\zeta(\vec{x}_{\parallel})$ appears in Eq. (34) [note that $G(\vec{k}_{\parallel}\vec{q}_{\parallel}|\vec{x}_{\parallel})$ is linear in $\zeta(\vec{x}_{\parallel})$ in first approximation], and it is this fact that leads to the appearance of displacement correlation functions in exponential factors in that theory, just as correlation functions of the $\zeta(\vec{x}_{\parallel})$'s appear in the same form, for the same reason, in the present theory.

Thus, we conclude that the simple variant of the theory of Garcia *et al.*[1] presented here offers distinct advantages over that theory, with no significant increase in the computational effort required to implement it.

ACKNOWLEDGMENT

This research was supported in part by U.S. Army Research Grant No. DAAG-29-78-G0108.

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