Resonant light scattering from a randomly rough surface

G. Brown, V. Celli, and M. Haller
University of Virginia, Charlottesville, Virginia 22901

A. A. Maradudin
University of California, Irvine, California 92717

A. Marvin
University of Trieste, I-34014, Trieste, Italy
(Received 2 July 1984)

A theory that describes the resonant scattering of light from a randomly rough surface is developed, based upon the rearranged vector Rayleigh equation obtained in previous work. Flux conservation in the intermediate states is ensured by deriving a Ward identity for the self-energy and irreducible vertex function. Approximate closed-form expressions for the differential reflection coefficients of a rough surface for p- and s-polarized light are given, and the results of numerical calculations are compared with some recent experimental results.

I. INTRODUCTION

The simplest of all optical phenomena involving the resonant excitation of surface polaritons is the scattering of light from rough surfaces. Experimental data for Ag and Au have been available for some time,[1-3] but a comprehensive and consistent theory of such scattering is still lacking, even for weakly corrugated surfaces. Lowest-order perturbation theory gives an adequate description of polarized scattering ($s\rightarrow s$ and $p\rightarrow p$), but cannot explain depolarized scattering ($s\rightarrow p$ and $p\rightarrow s$), which is due predominantly to the resonant excitation of surface polaritons. For stronger corrugations, the frequency dependence is not explained by perturbation theory, even for polarized scattering. Hunderi and Beaglehole[4] recognized that the inclusion of higher-order resonant effects was necessary in order to explain their data. The process which they describe phenomenologically as the excitation of surface currents can in fact be identified, as we shall see, with the excitation and subsequent reradiation of surface polaritons.

A theory of resonant excitation of surface polaritons on rough surfaces has been presented by Arya, Zeyher, and Maradudin.[5] The theory which we present here, and apply to scattering, is in many ways equivalent to theirs, but it is based on expansions that can be extended to all orders in the surface corrugation and satisfy, to each order, the requirements of reciprocity and unitarity (in the absence of dissipation). We find that it is important to satisfy these requirements in order that the transfer of electromagnetic energy into and out of the surface polaritons be taken into account correctly.

We have recently developed a vector theory of light scattering from rough surfaces;[6] here, we will begin with the expressions for the S matrix and T matrix from that work and treat the scattering from a randomly rough surface. In what follows the scattered beams are labeled by their momentum parallel to the mean surface, $\mathbf{K}$, and a polarization index α which specifies p polarization ($\alpha=1$) or s polarization ($\alpha=2$). Except where clarification of the polarization dependence of a certain quantity is necessary, we will omit α; it is to be assumed that each $\mathbf{K}$ is associated with a polarization index, and a sum over $\mathbf{K}$ implies a sum over α. For example, the S matrix, $S(\mathbf{K},\mathbf{K}_0)$, is a 2×2 matrix, and the fractional intensity scattered in the $p\rightarrow p$ transition is $|S_{11}(\mathbf{K},\mathbf{K}_0)|^2$.

The relevant formulas from Ref. 6 are

$$S(\mathbf{K}_f,\mathbf{K}_0)=R(\mathbf{K}_f,\mathbf{K}_0)-2i(p_f p_0)^{1/2}\times\sum_{\mathbf{K}_1,\mathbf{K}_2}G^{(0)}(\mathbf{K}_f,\mathbf{K}_2)T(\mathbf{K}_2,\mathbf{K}_1)\times G^{(0)}(\mathbf{K}_1,\mathbf{K}_0)\ , \tag{1.1}$$

$$T(\mathbf{K}_f,\mathbf{K}_0)=V(\mathbf{K}_f,\mathbf{K}_0)+\sum_{\mathbf{K}_1,\mathbf{K}_2}T(\mathbf{K}_f,\mathbf{K}_2)G^{(0)}(\mathbf{K}_2,\mathbf{K}_1)V(\mathbf{K}_1,\mathbf{K}_0)\ . \tag{1.2}$$

$R(\mathbf{K},\mathbf{K}')$ is the matrix of Fresnel reflection coefficients for a smooth surface:

$$R_{\alpha\alpha'}(\mathbf{K},\mathbf{K}')=\delta(\mathbf{K},\mathbf{K}')\delta_{\alpha\alpha'}R_\alpha(\mathbf{K}) \tag{1.3}$$

with

$$R_1(K)=R_p(K)=(\epsilon p-q)/(\epsilon p+q)$$

and

$$R_2(K)=R_s(K)=(p-q)/(p+q)\ .$$

$G^{(0)}(\mathbf{K},\mathbf{K}')$ is the surface matrix Green function, whose elements are defined by

$$G^{(0)}_{\alpha\alpha'}(\mathbf{K},\mathbf{K}')=\delta(\mathbf{K},\mathbf{K}')\delta_{\alpha\alpha'}G^{(0)}_\alpha(K) \tag{1.4}$$

with $G^{(0)}_1(K)=i\epsilon/(\epsilon p+q)$ and $G^{(0)}_2(K)=i/(p+q)$.

The momentum of a reflected beam perpendicular to the mean surface which appears in the above expressions is denoted by $p(K)$ or simply by p, and satisfies the kinematic condition, for frequency ω,

$$K^2+p^2=(\omega/c)^2 . \tag{1.5}$$

For the evanescent beams, it is convenient to define $p=i\beta$. Similarly, the perpendicular momentum of a refracted beam, denoted by q or by $i\gamma$, satisfies

$$K^2+q^2=\epsilon(\omega/c)^2 , \tag{1.6}$$

where $\epsilon=\epsilon_1+i\epsilon_2$ is the complex, frequency-dependent dielectric constant of the substrate. The momentum of the incident beam is $(\mathbf{K}_0, -p(K_0))=(\mathbf{K}_0,-p_0)$, and we define q_0 to be the solution of (1.6) when $K=K_0$. It should be noted that for a metallic substrate ($\epsilon_1<0$) the denominator of $G_1^{(0)}(K)$ can vanish; in fact, $\epsilon p+q=0$ gives the dispersion relation for surface polaritons on a smooth surface. The summations over $\mathbf{K}_1$ and $\mathbf{K}_2$ in (1.1) and (1.2) extend over all values of the parallel momenta, including evanescent states, and also states on the surface polariton "ring" (see Fig. 1).

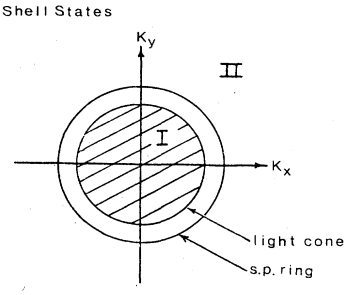

FIG. 1. At a given frequency ω, the polaritons having parallel momentum K lie on the surface polariton (s.p.) "ring."

The matrix $T(\mathbf{K},\mathbf{K}_0)$, defined by the integral equation (1.2), is the transition matrix. Only energy-conserving (on shell) elements enter, because we have been able to introduce the effective on-shell potential $V(\mathbf{K},\mathbf{K}_0)$, which is analogous to the K matrix in conventional scattering theory. The exact equation for $V(\mathbf{K},\mathbf{K}_0)$ in terms of the surface profile is given in Ref. 6, Eq. (3.8). In this paper we will use only the lowest-order approximation:

$$V(\mathbf{K},\mathbf{K}_0)\approx\zeta_{\mathbf{K}-\mathbf{K}_0}\left[\frac{\epsilon-1}{\epsilon}\right]\begin{bmatrix}[\epsilon KK_0-(\hat{\mathbf{K}}\cdot\hat{\mathbf{K}}_0)qq_0]/\epsilon & -(\omega/c)q(\hat{\mathbf{K}}\times\hat{\mathbf{K}}_0)_z \\ -(\omega/c)(\hat{\mathbf{K}}\times\hat{\mathbf{K}}_0)_z q_0 & \epsilon(\omega/c)^2(\hat{\mathbf{K}}\cdot\hat{\mathbf{K}}_0)\end{bmatrix} . \tag{1.7}$$

Here, $\hat{\mathbf{K}}$ and $\hat{\mathbf{K}}_0$ are unit vectors, and $\zeta_{\mathbf{K}-\mathbf{K}_0}$ is the Fourier transform of the two-dimensional surface corrugation function $\zeta(\mathbf{R})$:

$$\zeta_{\mathbf{K}-\mathbf{K}_0}=\frac{1}{L^2}\int d^2R\, e^{-i(\mathbf{K}-\mathbf{K}_0)\cdot\mathbf{R}}\zeta(\mathbf{R}) , \tag{1.8}$$

where L^2 is the area of the mean surface. As discussed in Ref. 6, $V(\mathbf{K},\mathbf{K}_0)$ is self-reciprocal, and for an opaque, nondissipative medium ($\epsilon_1<0$, $\epsilon_2=0$), it is also Hermitian. These formal properties hold to each order in the expansion for $V(\mathbf{K},\mathbf{K}_0)$ in powers of $\zeta(\mathbf{R})$.

Thus, we find that (1.2) is analogous to a two-dimensional scattering problem, and many results from conventional scattering theory can be utilized. In particular, a T matrix obeying Eq. (1.2) will automatically satisfy the generalized optical theorem (see Appendix B):

$$T-T^\dagger=T^\dagger[G^{(0)}-(G^{(0)})^\dagger]T + [1+T^\dagger(G^{(0)})^\dagger](V-V^\dagger)(1+G^{(0)}T) . \tag{1.9}$$

If V is Hermitian, the last term in (1.9) vanishes and the energy flux is explicitly conserved at all intermediate steps. This in turn leads to the unitarity of the S matrix, i.e., $S^\dagger S=1$.[6]

Since the surface is assumed to be randomly rough, the intensities $|S_{\alpha\alpha_0}(\mathbf{K},\mathbf{K}_0)|^2$ are statistically averaged over the surface profile. Diagrammatic techniques for computing these averages are developed in Sec. II, and Dyson's equation for the renormalized Green function is obtained. In Sec. III, a Bethe-Salpeter equation is written for the non-specularly-scattered intensity, and in Sec. IV this equation is used to derive the differential reflection coefficients for normal incidence.

II. SCATTERING FROM A RANDOMLY ROUGH SURFACE: DYSON'S EQUATION

The surface corrugation function $\zeta(\mathbf{R})$, or its Fourier transform (1.8), completely specifies our problem once the dielectric constant $\epsilon(\omega)$ is given. We take $\zeta(\mathbf{R})$ to be normally distributed with a correlation function

$$\langle\zeta(\mathbf{R}_1)\zeta(\mathbf{R}_2)\rangle=W(|\mathbf{R}_1-\mathbf{R}_2|) \tag{2.1}$$

that depends only on $|\mathbf{R}_1-\mathbf{R}_2|$. We will make use of a Gaussian two-point correlation

$$W(|\mathbf{R}_1-\mathbf{R}_2|)=\sigma^2\exp(-|\mathbf{R}_1-\mathbf{R}_2|^2/a^2) , \tag{2.2}$$

where σ^2 is the mean-square height

$$\sigma^2=\langle\zeta^2(\mathbf{R})\rangle \tag{2.3}$$

and a is the correlation length. Most of the treatment that follows, however, does not depend upon the particular form (2.2) for $W(R)$. The Fourier transform of (2.2) is

$$W(Q)=\frac{1}{L^2}\int d^2R\, e^{-i\mathbf{Q}\cdot\mathbf{R}}W(R)=\frac{\pi\sigma^2a^2}{L^2}e^{-Q^2a^2/4} . \tag{2.4}$$

In practice, we will be averaging products of the

Fourier coefficients $\zeta_{\mathbf{Q}}$. For these averages, the following rules apply.

(1) $\langle \zeta_{\mathbf{Q}}\zeta_{\mathbf{Q}'}\rangle = W(Q)\delta_{\mathbf{Q},-\mathbf{Q}'}$.

(2) The average of a product of an odd number of $\zeta_{\mathbf{Q}}$ vanishes.

(3) The average of a product containing an even number of $\zeta_{\mathbf{Q}}$ factors into a sum of a products of pair averages, with the pairing taken in all possible distinct combinations.

We apply these rules first to the averaging of the T matrix, or equivalently the exact Green-function matrix G, which satisfies

$$G(\mathbf{K},\mathbf{K}_0)=G^{(0)}(\mathbf{K},\mathbf{K}_0)+\sum_{\mathbf{K}_1,\mathbf{K}_2} G^{(0)}(\mathbf{K},\mathbf{K}_2)V(\mathbf{K}_2,\mathbf{K}_1) \times G(\mathbf{K}_1,\mathbf{K}_0) \tag{2.5}$$

or, symbolically

$$G=G^{(0)}+G^{(0)}VG =G^{(0)}+G^{(0)}VG^{(0)}+G^{(0)}VG^{(0)}VG^{(0)}+\cdots . \tag{2.6}$$

From a comparison of (1.2) and (2.5) it follows that

$$T=V+VGV \tag{2.7}$$

and

$$G^{(0)}T=GV , \qquad TG^{(0)}=VG . \tag{2.8}$$

When averaged, (2.5) gives

$$\langle G\rangle = G^{(0)}+G^{(0)}\langle VG\rangle . \tag{2.9}$$

If we now insert (2.5) for G, a series expansion for $\langle G\rangle$ is obtained. It is convenient to rewrite this series in terms of the self-energy operator M, defined in Appendix A. The important property is that from (A13)

$$\langle VG\rangle = \langle M\rangle\langle G\rangle , \tag{2.10}$$

so that $\langle G\rangle$ satisfies Dyson's equation

$$\langle G\rangle = G^{(0)}+G^{(0)}\langle M\rangle\langle G\rangle , \tag{2.11}$$

and also, using (2.8),

$$\langle T\rangle G^{(0)} = \langle M\rangle\langle G\rangle . \tag{2.12}$$

The explicit expansions for G, T, and M can be described graphically in terms of diagrams, in which $G(K)$ is represented by a line and $V(\mathbf{K},\mathbf{K}')$ is represented by a dot. For example, the second-order term in the expansion for G is given by the string

$$G^{(0)}VG^{(0)}VG^{(0)}=\sum_{\mathbf{K}_1} G^{(0)}(K_f)V(\mathbf{K}_f,\mathbf{K}_1)G^{(0)}(K_1) \times V(\mathbf{K}_1,\mathbf{K}_0)G^{(0)}(K_0) , \tag{2.13}$$

and is represented by the diagram shown in Fig. 2(a). These diagrams may be visualized as a succession of elementary scatterings beginning on the right-hand side with $\mathbf{K}_0$ and ending on the left-hand side with $\mathbf{K}_f$.

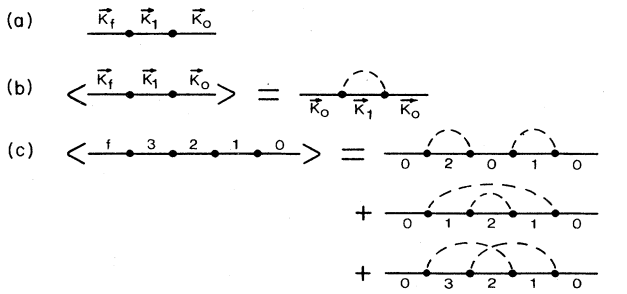

FIG. 2. Rules for averaging a pair of ζ are illustrated for the lowest-order strings; each line represents a free propagator $G^{(0)}$, a dot represents a factor of V, and a dashed line indicates a contraction.

The ensemble average of a given string is determined by rules (1)—(3). To apply these rules we note that $G^{(0)}(K)$ is a nonstochastic quantity [independent of $\zeta(\mathbf{R})$], while $V(\mathbf{K},\mathbf{K}')$ is proportional to $\zeta_{\mathbf{K}-\mathbf{K}'}$ and is stochastic. In the above example, the string average is found easily from the average of two $V(\mathbf{K},\mathbf{K}')$. According to rule (1), an averaged or "contracted" pair $\langle \zeta_{\mathbf{Q}}\zeta_{\mathbf{Q}'}\rangle$ vanishes unless the total momentum transferred is zero, $\mathbf{Q}+\mathbf{Q}'=\mathbf{0}$. This result is a consequence of the fact that the averaging restores translational invariance to the surface. The restriction on the momentum transfer associated with an averaged pair is indicated by joining the two $V(\mathbf{K},\mathbf{K}')$ by a dotted line, as shown in Fig. 2(b) for the string in (2.13). Furthermore, the average of a string containing an odd number of $V(\mathbf{K},\mathbf{K}')$ vanishes by rule (2), while the average of a string containing an even number of $V(\mathbf{K},\mathbf{K}')$ reduces to the sum of products of averaged pairs, where each term in the sum represents a distinct pairing combination. An illustration of this is given in Fig. 2(c). (Notice that the contractions in the last term give the additional restriction $\mathbf{K}_3=\mathbf{K}_0+\mathbf{K}_2-\mathbf{K}_1$.)

Because an averaged pair of $V(\mathbf{K},\mathbf{K}')$ can transfer no net momentum to the string, its initial and final momentum must be equal. The initial and final polarizations are also the same, as a consequence of the conservation of angular momentum. Thus we are led to define

$$\langle G(\mathbf{K}_f,\mathbf{K}_0)\rangle = \langle G(K_0)\rangle\delta(\mathbf{K}_f,\mathbf{K}_0) , \tag{2.14a}$$

$$\langle M(\mathbf{K}_f,\mathbf{K}_0)\rangle = \langle M(K_0)\rangle\delta(\mathbf{K}_f,\mathbf{K}_0) . \tag{2.14b}$$

In general, any contracted segment of a string in which all contractions are fully contained within that segment must begin and end with the same momentum and polarization. These segments, referred to as self-energy insertions, are a function of the initial momentum only. Thus, the averaged propagator $\langle G(K)\rangle$ consists of free propagators $G^{(0)}(K)$ which are linked together by self-energy insertions. The self-energy $\langle M(K)\rangle$ can be identified with the sum of all irreducible diagrams, which cannot be divided by a single cut of a propagator line [see Fig. 3(a)].

The sum of irreducible diagrams which define $\langle M(K)\rangle$ is generated by the integral equation (A8) for the self-energy operator (see Appendix A). The physical interpretation of Dyson's equation is obtained, as usual, by rewriting (2.11) as

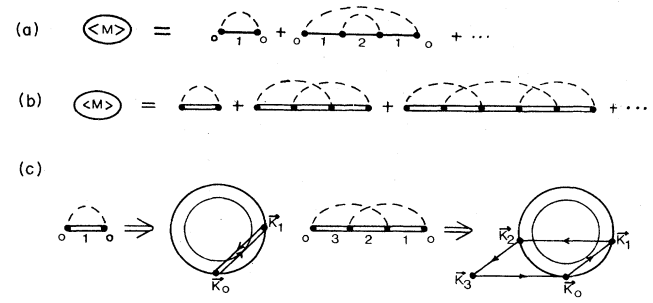

FIG. 3. (a) Self-energy $\langle M \rangle$ is the sum of all irreducible diagrams. (b) Series for $\langle M \rangle$ can be written in terms of skeleton diagrams by replacing the bare propagators $G^{(0)}$ with renormalized propagators $\langle G \rangle$; this series is generated by the integral equation (A17). (c) Crossed diagrams contain nonresonant factors in the intermediate states, as a consequence of the momentum restrictions that result from the averaging.

$$\langle G(K)\rangle=\{[G^{(0)}(K)]^{-1}-\langle M(K)\rangle\}^{-1} . \tag{2.15}$$

Recall that the poles of $G^{(0)}(K)$ determine the smooth surface eigenmodes; in particular,

$$[G_1^{(0)}(K)]^{-1}=\beta+\gamma/\epsilon=0$$

gives the dispersion relation for surface polaritons. Dyson's equation implies that the polariton modes on a rough surface behave as quasistates defined by the altered dispersion relation $\beta+\gamma/\epsilon-\langle M(K)\rangle=0$. The real part of $\langle M(K)\rangle$ shifts the location of the resonance, and the imaginary part of $\langle M(K)\rangle$ broadens the resonance. This broadening reflects the decreased lifetime of the polariton in a state with parallel momentum $\mathbf{K}$, due to its coupling with other polaritons and to outgoing radiation via the surface roughness.

As can be seen in Fig. 3(a), the self-energy insertions themselves may contain internal renormalizations; for example, the $\mathbf{K}_1$ line in Fig. 3(a) contains a renormalization part, which may be removed from the diagram by cutting two propagator lines. We thus can define the more basic "skeleton" diagrams which contain no internal renormalizations.

The self-energy $\langle M(K)\rangle$ is generated from the skeleton diagrams by replacing the bare propagator lines $G^{(0)}(K)$ with renormalized propagators $\langle G(K)\rangle$ [see Fig. 3(b)]. The complete expansion of $\langle M(K)\rangle$ in skeleton diagrams is generated by the integral equation (A17). In this paper we keep only the lowest skeleton diagram for $\langle M(K)\rangle$; the higher-order corrections are small by virtue of the fact that they contain nonresonant factors [see Fig. 3(c)]. The equation for $\langle M(K)\rangle$ then becomes

$$\langle M(K)\rangle\simeq\sum_{\mathbf{K}_1}\langle V(\mathbf{K},\mathbf{K}_1)V(\mathbf{K}_1,\mathbf{K})\rangle\langle G(K_1)\rangle . \tag{2.16}$$

This approximation for the self-energy, when used in Dyson's equation (2.11), yields a nonlinear integral equation for the averaged Green function $\langle G(K)\rangle$.

III. AVERAGED SCATTERED INTENSITY: THE BETHE-SALPETER EQUATION

In terms of the T matrix defined by (1.2), the nonspecular scattering intensity for incident polarization α_0 is given by

$$|S_{\alpha_f\alpha_0}(\mathbf{K}_f,\mathbf{K}_0)|^2=4p_fp_0|G^{(0)}_{\alpha_f}(K_f)|^2\times|T_{\alpha_f\alpha_0}(\mathbf{K}_f,\mathbf{K}_0)|^2|G^{(0)}_{\alpha_0}(K_0)|^2 . \tag{3.1}$$

The ensemble average of (3.1) reduces to the average of $|T_{\alpha_f\alpha_0}(\mathbf{K}_f,\mathbf{K}_0)|^2$. A general formalism for obtaining diagrammatic expansions of this quantity is discussed in Appendix A; here we summarize the important equations and describe the results graphically.

From the equation for the exact Green function G, written as

$$G-G^{(0)}=G^{(0)}TG^{(0)} \tag{3.2}$$

and its complex conjugate, along with Eq. (1.4), we find

$$|G(\mathbf{K}_f,\mathbf{K}_0)|^2=\delta(\mathbf{K}_f,\mathbf{K}_0)[G^*(\mathbf{K}_f,\mathbf{K}_0)G^{(0)}(K_0)+G^{(0)*}(K_f)G(\mathbf{K}_f,\mathbf{K}_0)-|G^{(0)}(K_0)|^2\delta(\mathbf{K}_f,\mathbf{K}_0)]+|G^{(0)}(K_f)|^2|T(\mathbf{K}_f,\mathbf{K}_0)|^2|G^{(0)}(K_0)|^2 . \tag{3.3}$$

Apart from terms that contribute only to specular scattering, the right-hand side of (3.3) is precisely what we need in (3.1). The averaged non-specularly-scattered intensity is then

$$\langle|S(\mathbf{K}_f,\mathbf{K}_0)|^2\rangle=4p_fp_0\langle|G(\mathbf{K}_f,\mathbf{K}_0)|^2\rangle . \tag{3.4}$$

In Appendix A we have derived a Bethe-Salpeter equation for the quantity

$$\langle G^*(\mathbf{K}'_f,\mathbf{K}'_0)G(\mathbf{K}_f,\mathbf{K}_0)\rangle .$$

If we set $\mathbf{K}'_0=\mathbf{K}_0$ and $\mathbf{K}'_f=\mathbf{K}_f$ in Eq. (A36) and define

$$\langle\Gamma(\mathbf{K}_f,\mathbf{K}'_f,\mathbf{K}_0,\mathbf{K}_0)\rangle=\delta(\mathbf{K}_f,\mathbf{K}'_f)\langle\Gamma(\mathbf{K}_f,\mathbf{K}_0)\rangle , \tag{3.5}$$

we then find that the quantity $\langle|G(\mathbf{K}_f,\mathbf{K}_0)|^2\rangle$, which appears in (3.4), satisfies the Bethe-Salpeter equation:

$$\langle|G(\mathbf{K}_f,\mathbf{K}_0)|^2\rangle=|\langle G(K_0)\rangle|^2\delta(\mathbf{K}_f,\mathbf{K}_0)+\sum_{\mathbf{K}_1}|\langle G(K_f)\rangle|^2\langle\Gamma(\mathbf{K}_f,\mathbf{K}_1)\rangle\times\langle|G(\mathbf{K}_1,\mathbf{K}_0)|^2\rangle . \tag{3.6}$$

Just as G may be represented by a series of strings, G^*G may be represented graphically by a series of two-line diagrams, where the upper line represents a complex conjugate string and the lower line is the usual string.

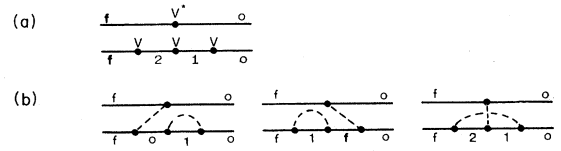

FIG. 4. (a) One of the lower-order two-line diagrams in the expansion of $G^*(f,0)G(f,0)$. (b) The average of the double string in (a). Note that the third diagram is irreducible, whereas the first two diagrams are not.

Figure 4(a) shows a typical diagram from this series. The same rules as before apply to the construction of the averaged diagrams, and in addition rule (1) implies

$$\langle \zeta_Q^* \zeta_{Q'} \rangle = W_Q \delta_{Q,Q'} , \tag{3.7}$$

because $\zeta_Q^* = \zeta_{-Q}$. If the two-line diagram contains an odd number of ζ_Q, its average vanishes according to rule 2. When averaging a diagram having an even number of ζ_Q, the ζ_Q are paired off in all possible distinct combinations. This will now include pairing ζ_Q on different lines. According to (3.7), ζ_Q that are paired on different lines transfer the same amount of momentum to each line. As before, we indicate this pairing, or contraction, by a dotted line connecting the ζ_Q. The average of the term in Fig. 4(a) is shown in Fig. 4(b).

The averaged two-line diagrams contain two basic features: interaction parts between lines and renormalization parts confined to a single line. For example, the first diagram in Fig. 4(b) shows a renormalization on the lower line, followed by a simple interaction between lines; the second diagram shows an interaction part followed by a renormalization; and the third diagram shows an interaction part only.

We note the further restriction that an interaction part consists of a closed set of pairings. Since any given contraction between lines must transfer the same momentum to each line, any interaction part transfers the same momentum to each line. Upon defining the irreducible interaction $\langle \Gamma(\mathbf{K}_f,\mathbf{K}_0) \rangle$ as the of all interaction parts which cannot be divided into two pieces by a cut on each line, the sum of diagrams for $\langle G^\dagger G \rangle$ can be represented schematically by the series in Fig. 5(a). The series is generated by the Bethe-Salpeter equation (3.6), which is represented diagrammatically in Fig. 5(b).

IV. SCATTERING CROSS SECTIONS FOR NORMAL INCIDENCE

As shown in Appendix A, the Bethe-Salpeter equation (3.6), which gives the non-specularly-scattered intensity, may also be written as the pair

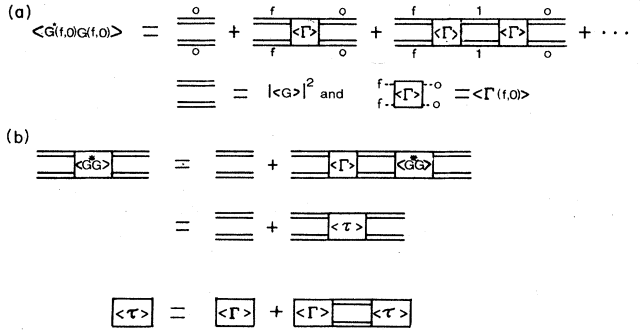

FIG. 5. (a) Expansion of the Bethe-Salpeter equation (3.6), with $\langle \Gamma \rangle$ defined as the sum of all irreducible two-line diagrams. (b) Bethe-Salpeter equation can be written in terms of the irreducible vertex function $\langle \Gamma \rangle$, or the reducible vertex function $\langle \tau \rangle$.

$$\langle |G(\mathbf{K}_f,\mathbf{K}_0)|^2 \rangle = |\langle G(K_0)\rangle|^2 \delta(\mathbf{K}_f,\mathbf{K}_0) + |\langle G(K_f)\rangle|^2 \langle \tau(\mathbf{K}_f,\mathbf{K}_0)\rangle \times |\langle G(K_0)\rangle|^2 \tag{4.1}$$

and

$$\langle \tau(\mathbf{K}_f,\mathbf{K}_0)\rangle = \langle \Gamma(\mathbf{K}_f,\mathbf{K}_0)\rangle + \sum_{\mathbf{K}_1} \langle \Gamma(\mathbf{K}_f,\mathbf{K}_1)\rangle |\langle G(K_1)\rangle|^2 \times \langle \tau(\mathbf{K}_1,\mathbf{K}_0)\rangle , \tag{4.2}$$

where $\langle \tau(\mathbf{K}_1,\mathbf{K}_0)\rangle$, the reducible vertex function, is defined in terms of the four-momentum quantity of Appendix A as [see also (3.5)]

$$\langle \tau(\mathbf{K}_1,\mathbf{K}_1';\mathbf{K}_0,\mathbf{K}_0)\rangle = \delta(\mathbf{K}_1,\mathbf{K}_1')\langle \tau(\mathbf{K}_1,\mathbf{K}_0)\rangle . \tag{4.3}$$

We can simplify the subsequent analysis by observing that for normal incidence, the light may be considered either p or s polarized; for convenience, we take the incident beam to always p polarized. We also noted earlier that $G_p^{(0)}(K)$ has a pole at the polariton resonance, and for $\epsilon_2 \ll \epsilon_1$ it is a strongly peaked function of K. On the other hand, $G_s^{(0)}(K)$ is a monotonically decreasing function of K. We therefore neglect the contribution due to $G_s^{(0)}$ in the summations over $\mathbf{K}$, which amounts to considering only p-polarized intermediate states. Furthermore, since the averaged Green function is diagonal in K and α, the first term in (4.1) does not contribute to the nonspecular intensity. What remains, then, are the following components of $\langle |G(\mathbf{K}_f,\mathbf{K}_0)|^2 \rangle$:

$$\langle |G(\mathbf{K}_f,\mathbf{K}_0)|^2 \rangle_{11} = |\langle G_p(K_f)\rangle|^2 \left[\langle \Gamma(\mathbf{K}_f,\mathbf{K}_0)\rangle_{11} + \sum_{\mathbf{K}_1} \langle \Gamma(\mathbf{K}_f,\mathbf{K}_1)\rangle_{11} |\langle G_p(K_1)\rangle|^2 \times \langle \tau(\mathbf{K}_1,\mathbf{K}_0)\rangle_{11} \right] |\langle G_p(K_0)\rangle|^2 , \tag{4.4}$$

$$\langle |G(\mathbf{K}_f,\mathbf{K}_0)|^2\rangle_{21}=|\langle G_s(K_f)\rangle|^2\left[\langle\Gamma(\mathbf{K}_f,\mathbf{K}_0)\rangle_{21}+\sum_{\mathbf{K}_1}\langle\Gamma(\mathbf{K}_f,\mathbf{K}_1)\rangle_{21}|\langle G_p(K_1)\rangle|^2\times\langle\tau(\mathbf{K}_1,\mathbf{K}_0)\rangle_{11}\right]|\langle G_p(K_0)\rangle|^2, \tag{4.5}$$

where

$$\langle\tau(\mathbf{K}_1,\mathbf{K}_0)\rangle_{11}=\langle\Gamma(\mathbf{K}_1,\mathbf{K}_0)\rangle_{11}+\sum_{\mathbf{K}_2}\langle\Gamma(\mathbf{K}_1,\mathbf{K}_2)\rangle_{11}|\langle G_p(K_2)\rangle|^2\langle\tau(\mathbf{K}_2,\mathbf{K}_0)\rangle_{11}. \tag{4.6}$$

In (4.4) and (4.5) the first term within large parens represents the direct scattering, and the second term includes the contributions of p-polarized intermediate states; these states are surface polariton modes which have been modified by the surface roughness.

Equations (4.4)—(4.6), along with (2.15), can be solved once $\langle\Gamma\rangle$ and $\langle M\rangle$ are specified. As is often the case in problems of this type, approximations for these functions cannot be made independently. In Appendix B we have derived a Ward identity which relates the irreducible vertex function $\langle\Gamma\rangle$ to the self-energy $\langle M\rangle$; this relation is a direct consequence of the optical theorem and ensures flux conservation in the intermediate states. In the calculation that follows we use the lowest-order approximations to $\langle\Gamma\rangle$ and $\langle M\rangle$ which satisfy the Ward identity when $\epsilon_2=0$. From (A39), (A22b), (A20), and (1.7) we find $\langle\Gamma\rangle\sim|V|^2$, or more explicitly,

$$\langle\Gamma(\mathbf{K},\mathbf{K}_1)\rangle_{11}\simeq|\xi_{\mathbf{K}-\mathbf{K}_1}|^2\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\times|\epsilon KK_1+(\hat{\mathbf{K}}\cdot\hat{\mathbf{K}}_1)\gamma(K)\gamma(K_1)|^2, \tag{4.7a}$$

$$\langle\Gamma(\mathbf{K},\mathbf{K}_1)\rangle_{21}\simeq|\xi_{\mathbf{K}-\mathbf{K}_1}|^2\left|\frac{\epsilon-1}{\epsilon}\right|^2\left[\frac{\omega}{c}\right]^2\times(\hat{\mathbf{K}}\times\hat{\mathbf{K}}_1)_z^2|\gamma(K_1)|^2. \tag{4.7b}$$

The self-energy, in turn, is approximated by (2.16). In order to carry out the computation required by (4.4)—(4.6) and (2.16), we first let

$$\sum_{\mathbf{K}'}\rightarrow\left[\frac{L}{2\pi}\right]^2\int d\phi\,dK'K'$$

and then carry out the angular integrations analytically. The details are given in Appendix C. In addition, we can replace the exact Green functions appearing outside the brackets in (4.4) and (4.5) by their zero-order approximations, because the main modifications to $\langle G\rangle$ occur near the polariton resonance.

Differential reflection coefficients for the scattering may be obtained by the correspondence

$$\sum_{\mathbf{K}}|S_{\alpha\alpha_0}(\mathbf{K},\mathbf{K}_0)|^2=\int d\Omega\left[\frac{dR}{d\Omega}\right]_{\alpha\alpha_0}. \tag{4.8}$$

We let

$$\sum_{\mathbf{K}}\rightarrow\left[\frac{L}{2\pi}\right]^2\int d\phi\,dK\,K$$

and then set $K=(\omega/c)\sin\theta$ and $dK=(\omega/c)\cos\theta\,d\theta$, where θ is the angle between the scattered wave vector and the outward normal of the mean surface. We find that

$$\sum_{\mathbf{K}}\rightarrow\left[\frac{\omega}{c}\right]^2\left[\frac{L}{2\pi}\right]^2\int d\Omega\cos\theta,$$

and it follows from (3.4) that the differential reflection coefficient for nonspecular scattering is obtained by multiplying (4.4) and (4.5) by

$$4p_fp_0\left[\frac{\omega}{c}\right]^2\left[\frac{L}{2\pi}\right]^2\cos\theta.$$

In addition, we will divide by the smooth surface reflection coefficient at normal incidence,

$$|R^{(0)}|^2=|(1-\sqrt{\epsilon})/(1+\sqrt{\epsilon})|^2.$$

The results are

$$\left[\frac{1}{|R^{(0)}|^2}\frac{dR}{d\Omega}\right]_{11}=\frac{\sigma^2a^2}{\pi}\left[\frac{\omega}{c}\right]^4|1+\sqrt{\epsilon}|^2\left|\frac{(\epsilon-\sin^2\theta)^{1/2}}{\epsilon\cos\theta+(\epsilon-\sin^2\theta)^{1/2}}\right|^2e^{-(\omega/c)^2a^2\sin^2\theta/4}\cos^2\theta\times\left[\cos^2\phi+\frac{\sigma^2a^2}{2}\left|\frac{1-\epsilon}{\epsilon^2}\right|^2\int dK'K'e^{-(K')^2a^2/4}|\gamma(K')|^2|\langle G_p(K')\rangle|^2H_1(K',\hat{\mathbf{K}}_0)\right], \tag{4.9}$$

$$\left[\frac{1}{|R^{(0)}|^2}\frac{dR}{d\Omega}\right]_{21}=\frac{\sigma^2a^2}{\pi}\left[\frac{\omega}{c}\right]^4|1+\sqrt{\epsilon}|^2\left|\frac{1}{\cos\theta+(\epsilon-\sin^2\theta)^{1/2}}\right|^2e^{-(\omega/c)^2a^2\sin^2\theta/4}\cos^2\theta\times\left[\sin^2\phi+\frac{\sigma^2a^2}{2}\left|\frac{1-\epsilon}{\epsilon^2}\right|^2\int dK'K'e^{-(K')^2a^2/4}|\gamma(K')|^2|\langle G_p(K')\rangle|^2H_2(K',\hat{\mathbf{K}}_0)\right] \tag{4.10}$$

with

$$H_1(K',\theta,\phi)=\chi^{(0)}(K')\{\tfrac{1}{2}I_2(\alpha)+2\mathrm{Re}(\eta)I_1(\alpha)+[\tfrac{1}{2}+|\eta|^2]I_0(\alpha)\}$$
$$+\chi^{(2)}(K')\cos(2\phi)\{\tfrac{1}{2}[I_4(\alpha)+I_0(\alpha)]+2\mathrm{Re}(\eta)[I_1(\alpha)+I_3(\alpha)]+2[\tfrac{1}{2}+|\eta|^2]I_2(\alpha)\}\ , \tag{4.11}$$

$$H_2(K',\theta,\phi)=\tfrac{1}{2}\chi^{(0)}(K')[I_0(\alpha)-I_2(\alpha)]+\chi^{(2)}(K')\cos(2\phi)\{I_2(\alpha)-\tfrac{1}{2}[I_4(\alpha)+I_0(\alpha)]\}\ , \tag{4.12}$$

where

$$\alpha=\frac{K'(\omega/c)a^2\sin\theta}{2},\quad \eta=\frac{\epsilon K'\sin\theta}{\gamma(K')(\sin^2\theta-\epsilon)^{1/2}}\ . \tag{4.13}$$

The function $\chi^{(m)}$ satisfies

$$\chi^{(m)}(K')=|\gamma(K')|^2e^{-(K')^2a^2/4}\left[\tfrac{1}{4}\delta_{m,\pm2}+\tfrac{1}{2}\delta_{m,0}+\frac{\sigma^2a^2}{2}\left|\frac{1-\epsilon}{\epsilon^2}\right|^2\int dK_1K_1e^{-K_1^2a^2/4}|\gamma(K_1)|^2|\langle G_p(K_1)\rangle|^2\right.$$
$$\left.\times h^{(m)}(K',K_1)\chi^{(m)}(K_1)\right] \tag{4.14}$$

with

$$h^{(m)}(K',K_1)=\tfrac{1}{4}[I_{m+2}(\alpha')+I_{m-2}(\alpha')]+\mathrm{Re}(\eta')[I_{m+1}(\alpha')+I_{m-1}(\alpha')]+(\tfrac{1}{2}+|\eta'|^2)I_m(\alpha')\ , \tag{4.15}$$

where

$$\alpha'=\frac{K'K_1a^2}{2},\quad \eta'=\frac{\epsilon K'K_1}{\gamma(K')\gamma(K_1)}\ . \tag{4.16}$$

The angle ϕ which appears in the above expressions is the angle between the final parallel wave vector, $\mathbf{K}_f$, and $\hat{\mathbf{K}}_0$, which in the limit $|\mathbf{K}_0|\to0$ (normal incidence) is the polarization vector for the incident beam. The quantities $I_n(\alpha)$ are modified Bessel functions.

We obtain the differential reflection coefficients for $p\to p$ and $s\to p$ scattering by setting $\phi=0$ and $\phi=\pi/2$ in (4.9). Similarly, by setting $\phi=0$ and $\phi=\pi/2$ in (4.10), we find the $p\to s$ and $s\to s$ scattering.

The averaged Green function appearing in (4.9)—(4.14) is the modulus squared of (2.15); $M(K)$ is determined by (2.16), which reduces to the following when the resonant contribution only is retained:

$$\langle M(K)\rangle=\left[\frac{1-\epsilon}{\epsilon^2}\right]^2\left[\frac{L}{2\pi}\right]^2\int d^2K'W(|\mathbf{K}-\mathbf{K}'|)\frac{[\epsilon KK'+(\hat{\mathbf{K}}\cdot\hat{\mathbf{K}}')\gamma(K)\gamma(K')]^2}{\beta(K')+\gamma(K')/\epsilon-\langle M(K')\rangle}\ . \tag{4.17a}$$

Using (2.4) and proceeding as in Appendix C, we obtain the one-dimensional equation

$$\langle M(K)\rangle=\frac{\sigma^2a^2}{2}\left[\frac{1-\epsilon}{\epsilon^2}\right]^2e^{-K^2a^2/4}\int dK'K'e^{-(K')^2a^2/4}$$
$$\times\{\tfrac{1}{2}\gamma^2(K)\gamma^2(K')I_2(\alpha'')+2\epsilon\gamma(K)\gamma(K')KK'I_1(\alpha'')$$
$$+[(\epsilon KK')^2+\tfrac{1}{2}\gamma^2(K)\gamma^2(K')]I_0(\alpha'')\}\frac{1}{\beta(K')+\gamma(K')/\epsilon-\langle M(K')\rangle}\ , \tag{4.17b}$$

where $\alpha''=KK'a^2/2$. We can find an approximate closed-form solution to (4.9)—(4.17b) by noting that in the evanescent region

$$\mathrm{Im}\langle G(K')\rangle=\mathrm{Im}[\beta(K')+\gamma(K')/\epsilon-\langle M(K')\rangle]^{-1}$$

is strongly peaked about the polariton resonance. If we expand $[G^{(0)}(K')]^{-1}$ about

$$K_{sp}=[\epsilon_1/(\epsilon_1+1)]^{1/2}(\omega/c)$$

we find that

$$[G_p^{(0)}(K')]^{-1}=\beta(K')+\gamma(K')/(\epsilon_1+i\epsilon_2)$$
$$\approx C^{-1}[(K'-K_{sp})-i\Delta_\epsilon]\ , \tag{4.18a}$$

where

$$C=\frac{\epsilon_1(-\epsilon_1)^{1/2}}{1-\epsilon_1^2}\ ,$$
$$\Delta_\epsilon=\frac{\epsilon_2K_{sp}}{2\epsilon_1(1+\epsilon_1)}\ . \tag{4.18b}$$

The width Δ_ϵ represents the decay of polaritons due to the fact that the dielectric medium is dissipative ($\epsilon_2 \neq 0$). $\mathrm{Im}\langle M(K')\rangle$ gives the additional decay of the state with parallel wave vector K' due to the roughness; this width includes decay into other evanescent states as well as continuum states. In what follows we neglect the radiative decay in comparison with Δ_ϵ, which amounts to restricting the integration in (4.17b) to the interval $(\omega/c, \infty)$. Furthermore, if we take

$$\mathrm{Im}\langle M(K')\rangle = C^{-1}\Delta_{sp}$$

to be constant in the vicinity of the pole, and also neglect $\mathrm{Re}\langle M(K')\rangle$, we have

$$\mathrm{Im}\langle G_p(K')\rangle \approx \frac{C\Delta_{\mathrm{tot}}}{(K'-K_{sp})^2+\Delta_{\mathrm{tot}}^2} \rightarrow C\pi\delta(K'-K_{sp}) , \tag{4.19}$$

where $\Delta_{\mathrm{tot}}=\Delta_\epsilon+\Delta_{sp}$. The solution to (4.17b) is then

$$\mathrm{Im}\langle M(K_{sp})\rangle = C^{-1}\Delta_{sp} = -C^{-1}\frac{\pi\sigma^2 a^2}{2}\frac{\epsilon_1}{(1+\epsilon_1)^2}e^{-z}K_{sp}^5 L(z) , \tag{4.20}$$

where $z=K_{sp}^2 a^2/2$ and

$$L(z)=\tfrac{1}{2}I_2(z)-2I_1(z)+\tfrac{3}{2}I_0(z) . \tag{4.21}$$

With this result, the modulus squared Green function can be approximated as

$$|\langle G_p(K')\rangle|^2 \approx C\,\mathrm{Im}\langle G_p(K')\rangle/\Delta_{\mathrm{tot}} = \frac{C^2\pi}{\Delta_\epsilon+\Delta_{sp}}\delta(K'-K_{sp}) . \tag{4.22}$$

We can now solve (4.14) for $\chi^{(0)}(K_{sp})$ and $\chi^{(2)}(K_{sp})$; using (4.22) and setting $\epsilon \approx \epsilon_1$ in (4.14) (i.e., neglecting the imaginary part ϵ_2 wherever useful to simplify the expression), we find

$$\chi^{(0)}(K_{sp})=\frac{-\frac{1}{2}\epsilon_1 K_{sp}^2 e^{-z/2}}{1-\Delta_{sp}/\Delta_{\mathrm{tot}}} , \tag{4.23a}$$

$$\chi^{(2)}(K_{sp})=\frac{-\frac{1}{4}\epsilon_1 K_{sp}^2 e^{-z/2}}{1-\phi(z)\Delta_{sp}/\Delta_{\mathrm{tot}}} \tag{4.23b}$$

with $z=K_{sp}^2 a^2/2$ and

$$\phi(z)=\frac{\frac{1}{4}[I_0(z)+I_4(z)]-I_1(z)-I_3(z)+\frac{3}{2}I_2(z)}{L(z)} . \tag{4.24}$$

We now use (4.22) and (4.23) in (4.9) and (4.10) to obtain the differential reflection coefficients. The results are

$$\left[\frac{1}{|R^{(0)}|^2}\frac{dR}{d\Omega}\right]_{11} = \frac{\sigma^2 a^2}{\pi}\left[\frac{\omega}{c}\right]^4 |1+\sqrt{\epsilon}|^2 \left|\frac{(\epsilon-\sin^2\theta)^{1/2}}{\epsilon\cos\theta+(\epsilon-\sin^2\theta)^{1/2}}\right|^2 e^{-(\omega/c)^2 a^2\sin^2\theta/4} \times\cos^2\theta\left[\cos^2\phi-\frac{\pi\sigma^2 a^2 K_{sp}^5}{4}\frac{\epsilon_1}{(\epsilon_1+1)^2}e^{-z}\left[\frac{\frac{1}{2}I_2(y)+2xI_1(y)+(\frac{1}{2}+x^2)I_0(y)}{\Delta_\epsilon} + \tfrac{1}{2}\cos(2\phi)\frac{\frac{1}{2}[I_0(y)+I_4(y)]+2x[I_1(y)+I_2(y)]+2[\frac{1}{2}+x^2]I_2(y)}{\Delta_\epsilon+[1-\phi(z)]\Delta_{sp}}\right]\right] \tag{4.25}$$

and

$$\left[\frac{1}{|R^{(0)}|^2}\frac{dR}{d\Omega}\right] = \frac{\sigma^2 a^2}{\pi}\left[\frac{\omega}{c}\right]^4 |1+\sqrt{\epsilon}|^2 \left|\frac{1}{\cos\theta+(\epsilon-\sin^2\theta)^{1/2}}\right|^2 e^{-(\omega/c)^2 a^2\sin^2\theta/4}\cos^2\theta \times\left[\sin^2\phi-\frac{\pi\sigma^2 a^2 K_{sp}^5}{4}\frac{\epsilon_1}{(\epsilon_1+1)^2}e^{-z}\left[\frac{\frac{1}{2}[I_0(y)-I_2(y)]}{\Delta_\epsilon}+\tfrac{1}{2}\cos(2\phi)\frac{I_2(y)-\frac{1}{2}[I_0(y)+I_4(y)]}{\Delta_\epsilon+[1-\phi(z)]\Delta_{sp}}\right]\right] , \tag{4.26}$$

where

$$y=KK_{sp}a^2/2 , \quad x=\epsilon_1 KK_{sp}/\gamma(K)\gamma(K_{sp}) , \quad K=(\omega/c)\sin\theta , \tag{4.27}$$

and $\phi(z)$ is given by (4.24).

V. NUMERICAL CALCULATIONS FOR A SILVER SURFACE

The results of numerical calculations of polarized ($p\rightarrow p$, $s\rightarrow s$) and cross-polarized ($s\rightarrow p$, $p\rightarrow s$) differential

reflection coefficients are presented in Fig. 6, along with experimental data from Ref. 2. The substrate is a silver film that has been evaporated onto CaF_2 crystals, and the wavelength of the incident light is $\lambda=4579$ Å. The value of the dielectric constant that was used in the calculation $\epsilon=-7.5+0.24i$ was taken from Ref. 7, and the remaining parameters σ and a were adjusted by trial and error to achieve a best fit to the scattering data.

The overall magnitude of the direct scattering is fixed by the product σa, whereas the magnitude of the resonant scattering depends in addition upon the factor $\exp(K_{sp}^2 a^2/4)$. The ratio of resonant to direct scattering can be found approximately by taking the ratio of the cross-polarized reflection coefficient and the polarized reflection coefficient, since direct processes are absent from the former and are dominant in the latter. When comparing the theoretical cross-polarized reflection coefficient with the experimentally measured one of Ref. 2, it should be noted that the *angular dependence* of the scattering predicted by the theory corresponds fairly well to the data, and this dependence has not previously been accounted for except in phenomenological ways. The overall *magnitude* of the cross-polarized scattering does not compare as favorably with the data, however, and we describe the size of the discrepancy by a scale factor X that multiplies the theoretical cross-polarized reflection

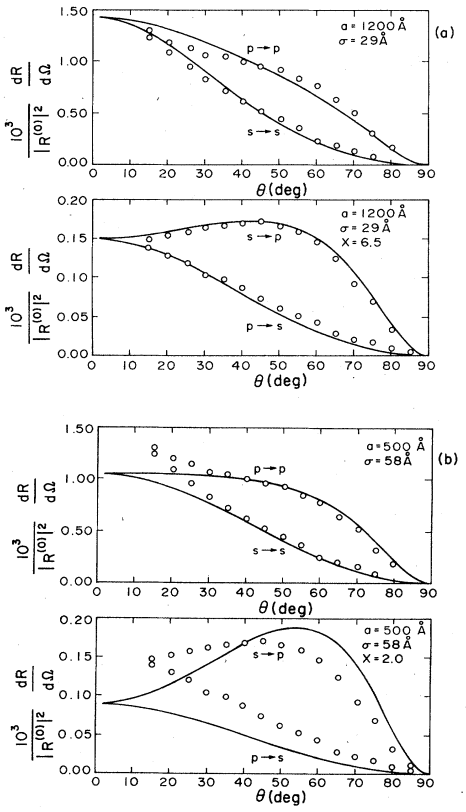

FIG. 6. Comparison of experimental data (open circles) from Ref. 2 and the results of numerical calculations for light normally incident upon a rough Ag surface. The wavelength of the light is $\lambda=4579$ Å, and the dielectric constant from Ref. 7 is $\epsilon=-7.5+0.24i$.

coefficients and brings the overall magnitude of the cross-polarized scattering into closer agreement with the experimental data. As can be seen from Fig. 6, X decreases as a decreases, although the angular distribution of cross-polarized scattering seems to favor a large value for a.

It is possible that deviations from a normally distributed surface profile could have been significant for the samples used in Ref. 2; and this could account for some of the disagreement. There is recent evidence that shows that higher-order moments of the surface profile may be larger than those implied by a normal distribution.[8] In addition, other recent studies have shown that the correlation function (2.4) may not be adequate; there may, for example, be a component of the correlation function that has its maximum displaced away from $Q=0$, so that the Gaussian form of (2.4) may not be correct.[9] We believe that it would therefore be profitable to use the techniques of Refs. 8 and 9 to characterize the roughness of samples used in optical experiments of the kind studied here. In any case, it is desirable to establish the predictions of a theory based on a simple Gaussian correlation function, whether or not there is perfect agreement with the small amount of existing data.

It should also be noted that the resonant terms in the differential reflection coefficients (4.25) and (4.26) are essentially proportional to $[\mathrm{Im}(\epsilon)]^{-1}$. By using a smaller value for $\mathrm{Im}(\epsilon)$, the calculated cross-polarized scattering would be enhanced; in fact, in a more exact calculation that includes radiative decay, it is found that resonant scattering dominates for $\mathrm{Im}(\epsilon)=0$. There does not, however, seem to be any justification for using a value for $\mathrm{Im}(\epsilon)$ smaller than the one used here.

The upturn in the polarized reflection coefficients that occurs at small angles can be explained by assuming that the roughness contains a "wavy" component, with long-range correlations on the order of 7000 Å. We omit this contribution here, since it has been previously discussed.[2] This wavy component will not affect the cross-polarized scattering, because the changes in parallel wave vector resulting from it are too small to excite surface polaritons.

In conclusion, we express the hope that, in addition to providing closed-form expressions for the differential reflection coefficient of a randomly rough surface from first principles, this work will serve as the foundation on which future studies in light scattering from rough surfaces will be made.

APPENDIX A

The diagrammatic analysis of wave propagation on rough surfaces can be established by purely algebraic methods. Two techniques are employed: one is to project out averages by the operators P and Q, defined by

$$PX=\langle X\rangle\ , \tag{A1}$$

$$QX=X-\langle X\rangle \tag{A2}$$

for any X; the other is to rewrite the typical integral equation

$$X=X_0+X_0(L_1+L_2)X \tag{A3}$$

as the two coupled equations

$$X=X_1+X_1L_2X_0\ , \tag{A4a}$$

$$X_1=X_0+X_0L_1X_1\ . \tag{A4b}$$

The result (A4) is proved most easily by first rewriting (A3) as

$$(1-X_0L_1)X=X_0+X_0L_2X\ . \tag{A5}$$

One then premultiplies by the inverse operator $(1-X_0L_1)^{-1}$ and defines $(1-X_0L_1)^{-1}X_0=X_1$.

Our first task is to derive the equation for the self-energy operator M. We start from the equation for the T matrix,

$$T=V+VG^{(0)}T\ , \tag{A6}$$

and set $G^{(0)}=G^{(0)}P+G^{(0)}Q$. We have an equation of the type (A3), where $G^{(0)}Q$ and $G^{(0)}P$ are identified with L_1 and L_2, respectively. We then find the following coupled equations, which are analogous to (A4):

$$T=M+MG^{(0)}PT\ , \tag{A7}$$

$$M=V+VG^{(0)}QM\ . \tag{A8}$$

The diagrammatic expansion for $\langle M\rangle$ is obtained by iterating (A8) and then averaging.

We can also express the exact Green function G in terms of M. G satisfies

$$G=G^{(0)}+G^{(0)}VG\ , \tag{A9}$$

and is related to T by $T=V+VGV$ and $G=G^{(0)}+G^{(0)}TG^{(0)}$. From these equations it follows that

$$\langle G\rangle=G^{(0)}+G^{(0)}\langle T\rangle G^{(0)}\ , \tag{A10}$$

$$TG^{(0)}=VG\ . \tag{A11}$$

By multiplying (A7) from the right by $G^{(0)}$ and using (A10), we find

$$TG^{(0)}=M(G^{(0)}+G^{(0)}\langle T\rangle G^{(0)})=M\langle G\rangle\ , \tag{A12}$$

which implies, using (A11),

$$VG=M\langle G\rangle\ . \tag{A13}$$

Dyson's equation

$$\langle G\rangle=G^{(0)}+G^{(0)}\langle M\rangle\langle G\rangle \tag{A14}$$

is obtained by averaging

$$G=G^{(0)}+G^{(0)}M\langle G\rangle\ , \tag{A15}$$

which is a consequence of (A9) and (A13).

We can also convert (A9) into a pair of equations such as (A4) by setting $L_1=\langle M\rangle$ and $L_2=V-\langle M\rangle$. The first equation of the pair is simply Dyson's equation (A14); the other equation,

$$G=\langle G\rangle+\langle G\rangle(V-\langle M\rangle)G=\langle G\rangle+G(V-\langle M\rangle)\langle G\rangle\ , \tag{A16}$$

is the starting point for the development of "skeleton" expansions, which contain $\langle G\rangle$ as intermediate propagators.

The skeleton equation for M can be derived from (A16) by multiplying it from the left by V and using Eq. (A13). The result is

$$M=V+M\langle G\rangle(V-\langle M\rangle)\ . \tag{A17}$$

We now turn to the evaluation of the averaged nonspecular intensity, which according to (3.4), can be expressed in terms of the modulus squared of the Green function. This quantity is a particular case of

$$G^*(\mathbf{K}_1',\mathbf{K}_0')G(\mathbf{K}_1,\mathbf{K}_0)\equiv\mathscr{G}(\mathbf{K}_1,\mathbf{K}_1';\mathbf{K}_0,\mathbf{K}_0') \tag{A18a}$$

or, in a more compact notation

$$G^*(1',0')G(1,0)=\mathscr{G}(1,1';0,0')\ . \tag{A18b}$$

An equation for $\langle\mathscr{G}(1,1';0,0')\rangle$ can be obtained by multiplying together the following equations for G and G^* [see (A16)]:

$$G(f,0)=\langle G(f,0)\rangle+\sum_{1,2}\langle G(f,2)\rangle v(2,1)G(1,0)\ , \tag{A19a}$$

$$G^*(f',0')=\langle G^*(f',0')\rangle+\sum_{1',2'}\langle G^*(f',2')\rangle v^*(2',1')G^*(1',0')\ , \tag{A19b}$$

where

$$v(\mathbf{K}_2,\mathbf{K}_1)=V(\mathbf{K}_2,\mathbf{K}_1)-\langle M(\mathbf{K}_2,\mathbf{K}_1)\rangle\ . \tag{A20}$$

From (A13) we see that $\langle vG\rangle=0$; we then find

$$\langle\mathscr{G}(f,f';0,0')\rangle=\mathscr{G}^{(0)}(f,f';0,0')+\sum_{1,1',2,2'}\mathscr{G}^{(0)}(f,f';2,2')\times\langle\mathscr{V}^{(0)}(2,2';1,1')\times\mathscr{G}(1,1';0,0')\rangle \tag{A21}$$

with

$$\mathscr{G}^{(0)}(f,f';2,2')=\langle G^*(f',2')\rangle\langle G(f,2)\rangle\ , \tag{A22a}$$

$$\mathscr{V}^{(0)}(2,2';1,1')=v^*(2',1')v(2,1)\ . \tag{A22b}$$

We note the formal correspondence between the two-polariton equation (A21) and the average of the one-polariton equation (A9). Thus, we will introduce operators τ and Γ that are the analog of T and M in the one-polariton case, and proceed to derive the Bethe-Salpeter equation, which is the analog of the Dyson equation (A14). Formally, it is convenient to regard G, $\langle\mathscr{G}\rangle$, $\mathscr{G}^{(0)}$, $\mathscr{V}^{(0)}$, τ, and Γ as matrices, according to the example

$$\langle\mathscr{G}(f,f';0,0')\rangle=\langle\mathscr{G}\rangle_{ab}\ ,$$

where the composite index $a\equiv(f,f')$ labels the rows, and $b\equiv(0,0')$ labels the columns of the matrix $\langle\mathscr{G}\rangle$.

We start by deriving an equation for τ: This is most easily accomplished by first introducing an operator t which satisfies

$$vG=t\langle G\rangle\ , \tag{A23}$$

from which it follows, using (A16) and (A20), that

$$G=\langle G\rangle+\langle G\rangle t\langle G\rangle\ , \tag{A24}$$

$$t=v+v\langle G\rangle t\ . \tag{A25}$$

From (A23) we see that $\langle t\rangle=0$. Furthermore, when (A24) and its complex conjugate are written out like (A19), and the two resulting equations are multiplied and then averaged, we find

$$\langle\mathscr{G}\rangle=\mathscr{G}^{(0)}+\mathscr{G}^{(0)}\langle\tau\rangle\mathscr{G}^{(0)}\ , \tag{A26}$$

where

$$\tau(\mathbf{K},\mathbf{K}';\mathbf{K}_0,\mathbf{K}_0')=t^*(\mathbf{K}',\mathbf{K}_0')t(\mathbf{K},\mathbf{K}_0)\ . \tag{A27}$$

Equation (A26) implies that $\langle\tau\rangle$ is the full (reducible) vertex function, as described in the main text.

From (A25) and its complex-conjugate relation, written as

$$(1-v\langle G\rangle)t=v\ , \tag{A28a}$$

$$(1-v^*\langle G\rangle^*)t^*=v^*\ , \tag{A28b}$$

we obtain

$$\tau-\mathscr{K}\tau=\mathscr{V}^{(0)}\ , \tag{A29}$$

where

$$\begin{aligned}\mathscr{K}(f,f';1,1')=&\delta(f',1')\sum_2 v(f,2)\langle G(2,1)\rangle\\&+\delta(f,1)\sum_{2'}v^*(f',2')\langle G^*(2',1')\rangle\\&-\sum_{2,2'}v(f,2)v^*(f',2')\langle G(2,1)\rangle\\&\times\langle G^*(2',1')\rangle\ .\end{aligned} \tag{A30}$$

We now define an operator $\mathscr{V}$ that is related to τ in the same way that V is related to T:

$$\tau=\mathscr{V}+\mathscr{V}\mathscr{G}^{(0)}\tau=\mathscr{V}+\tau\mathscr{G}^{(0)}\mathscr{V}\ . \tag{A31}$$

An equation for $\mathscr{V}$ can be obtained by multiplying (A29) from the right by $(1-\mathscr{G}^{(0)}\mathscr{V})$ and using (A31). We find

$$\mathscr{V}=\mathscr{V}^{(0)}+(\mathscr{K}-\mathscr{V}^{(0)}\mathscr{G}^{(0)})\mathscr{V}\ . \tag{A32}$$

The advantage of writing (A29) in the form (A31) is that we may now obtain an equation for τ in terms of $\langle\tau\rangle$, as was done for T in (A7). By using the same technique that led to (A7) and (A8), we find

$$\tau=\Gamma+\Gamma\mathscr{G}^{(0)}\langle\tau\rangle\ , \tag{A33}$$

$$\Gamma=\mathscr{V}+\mathscr{V}\mathscr{G}^{(0)}Q\Gamma\ . \tag{A34}$$

The average of (A33),

$$\langle\tau\rangle=\langle\Gamma\rangle+\langle\Gamma\rangle\mathscr{G}^{(0)}\langle\tau\rangle\ , \tag{A35}$$

shows that $\langle\Gamma\rangle$ is the irreducible vertex function, which is defined in the main text as a series of diagrams [see Fig. 5(b)]. If we multiply (A35) from the right by $\mathscr{G}^{(0)}$, multiply (A26) from the left by $\langle\Gamma\rangle$, and then subtract the resulting equations, we find that $\langle\tau\rangle\mathscr{G}^{(0)}=\langle\Gamma\rangle\langle\mathscr{G}\rangle$; Eq. (A26) then gives the Bethe-Salpeter equation

$$\langle\mathscr{G}\rangle=\mathscr{G}^{(0)}+\mathscr{G}^{(0)}\langle\Gamma\rangle\langle\mathscr{G}\rangle\ . \tag{A36}$$

Comparison with (A21) shows that

$$\langle\tau\rangle\mathscr{G}^{(0)}=\langle\Gamma\rangle\langle\mathscr{G}\rangle=\langle\mathscr{V}^{(0)}\mathscr{G}\rangle\ . \tag{A37}$$

We have thus obtained in the coupled equations (A32) and (A34) a way of generating Γ, and hence $\langle\Gamma\rangle$. These two equations may be combined into the single equation

$$\Gamma=\mathscr{V}^{(0)}+(\mathscr{K}-\mathscr{V}^{(0)}\mathscr{G}^{(0)})\Gamma+\mathscr{V}^{(0)}\mathscr{G}^{(0)}Q\Gamma\ , \tag{A38}$$

which can also be written as

$$\Gamma=\mathscr{V}^{(0)}+\mathscr{K}\Gamma-\mathscr{V}^{(0)}\mathscr{G}^{(0)}\langle\Gamma\rangle\ . \tag{A39}$$

APPENDIX B

The generalized optical theorem, Eq. (1.9) is a consequence of the Lippman-Schwinger equation for T, Eq. (1.2). By multiplying Eq. (1.2) from the left by $T^\dagger(G^{(0)})^\dagger$ and multiplying its complex conjugate from the right by GT and subtracting the two equations, we obtain

$$\begin{aligned}T^\dagger[G^{(0)}-(G^{(0)})^\dagger]T=&V^\dagger G^{(0)}T-T^\dagger(G^{(0)})^\dagger V\\&+T^\dagger(G^{(0)})^\dagger(V^\dagger-V)G^{(0)}T\ .\end{aligned} \tag{B1}$$

The first two terms on the right-hand side are rewritten

$$\begin{aligned}V^\dagger G^{(0)}T-T^\dagger(G^{(0)})^\dagger V&=(V^\dagger-V)G^{(0)}T+VG^{(0)}T-T^\dagger(G^{(0)})^\dagger(V-V^\dagger)-T^\dagger(G^{(0)})^\dagger V^\dagger\\&=(V^\dagger-V)G^{(0)}T+T-V-T^\dagger(G^{(0)})^\dagger(V-V^\dagger)-T^\dagger+V^\dagger\ ,\end{aligned} \tag{B2}$$

which, when substituted into Eq. (B1), yields Eq. (1.9).

Various versions of the Ward identity are obtained by taking suitable averages of Eq. (1.9). For our purposes it is easier to start from the equation

$$\begin{aligned}t-t^\dagger=&t^\dagger(\langle G\rangle-\langle G\rangle^\dagger)t+(1+t^\dagger\langle G\rangle^\dagger)(v-v^\dagger)\\&\times(1+\langle G\rangle t)\ ,\end{aligned} \tag{B3}$$

where, as in Appendix A, $v=V-\langle M\rangle$ and t obeys Eq. (A25), $t=v+v\langle G\rangle t$. The proof of Eq. (B3) is completely analogous to that of Eq. (1.9).

We now multiply Eq. (B3) by $\langle G\rangle^\dagger$ from the left and by $\langle G\rangle$ from the right. After using $t\langle G\rangle=vG$, $\langle G\rangle+\langle G\rangle t\langle G\rangle=G$, and their Hermitian conjugates, we obtain

$$\langle G\rangle^\dagger(t-t^\dagger)\langle G\rangle=G^\dagger v^\dagger(\langle G\rangle-\langle G\rangle^\dagger)vG+G^\dagger(v-v^\dagger)G\ . \tag{B4}$$

The average of the left-hand side of this equation vanishes because $\langle t\rangle=0$ [see Eq. (A13)]. The average of the

right-hand side then gives

$$\langle G^\dagger v^\dagger(\langle G\rangle-\langle G\rangle^\dagger)vG\rangle+\langle G^\dagger(V-V^\dagger)G\rangle$$
$$=\langle G^\dagger(\langle M\rangle-\langle M\rangle^\dagger)G\rangle\ . \quad \text{(B5)}$$

The first term on the left-hand side of Eq. (B5), which we we shall call $\langle \mathscr{Q}\rangle$, can be written in terms of the irreducible vertex function $\langle\Gamma\rangle$. Explicitly, using the notation introduced by Eq. (A18), we have

$$\langle \mathscr{Q}(1',1)\rangle=\sum_{2,2',3}\langle G^*(2',1')v^*(3',2')v(3,2)G(2,1)\rangle$$
$$\times[\langle G(3',3)\rangle-\langle G(3,3')\rangle^*]\ . \quad \text{(B6)}$$

With the definition (A22), Eq. (B6) can also be written as

$$\langle \mathscr{Q}(1',1)\rangle=\sum_{2,2',3,3'}\langle \mathscr{V}^{(0)}(3,3';2,2')\mathscr{G}(2,2',1,1')\rangle$$
$$\times[\langle G(3',3)\rangle-\langle G(3,3')\rangle^*] \quad \text{(B7)}$$

or, by using Eq. (A37) which defines $\langle\Gamma\rangle$,

$$\langle \mathscr{Q}(1',1)\rangle=\sum_{2,2',3,3'}\langle\Gamma(3,3';2,2')\rangle\langle\mathscr{G}(2,2';1,1')\rangle$$
$$\times[\langle G(3'3)\rangle-\langle G(3,3')\rangle^*]\ . \quad \text{(B8)}$$

We now substitute Eq. (B8) into Eq. (B5) and find the generalized Ward identity:

$$\sum_{2,2',3,3'}\langle\Gamma(3,3';2,2')\rangle\langle\mathscr{G}(2,2';1,1')\rangle[\langle G(3',3)\rangle-\langle G(3,3')\rangle^*]+\sum_{2,2'}\langle G(2,2';1,1')[V(2',2)-V^*(2,2')]\rangle$$
$$=\sum_{2,2'}\langle\mathscr{G}(2,2';1,1')\rangle[\langle M(2',2)\rangle-\langle M(2,2')\rangle^*]\ . \quad \text{(B9)}$$

If V is Hermitian, the second term on the left-hand side of Eq. (B9) vanishes identically. In this case we can multiply Eq. (B9) by $\langle\mathscr{G}(1,1';4,4')\rangle^{-1}$, defined by

$$\sum_{1,1'}\langle\mathscr{G}(2,2';1,1')\rangle\langle\mathscr{G}(1,1';4,4')\rangle^{-1}=\delta(2,4)\delta(2',4') \quad \text{(B10)}$$

and sum over the indices (1,1'). We find the usual Ward identity, which can be simplified further by the use of Eqs. (2.14) and (3.5):

$$\mathrm{Im}\langle M(K)\rangle=\sum_{\mathbf{K}_1}\mathrm{Im}\langle G(K_1)\rangle\langle\Gamma(\mathbf{K}_1,\mathbf{K})\rangle\ . \quad \text{(B11)}$$

APPENDIX C

We can perform the angular integrations in Eqs. (4.4)—(4.6) by making use of the well-known identity

$$e^{\alpha\cos\phi}=\sum_{m=-\infty}^{\infty}I_m(\alpha)e^{im\phi}\ , \quad \text{(C1)}$$

where $I_m(\alpha)$ is a modified Bessel function. In order to Fourier analyze Eq. (4.6), we let

$$\sum_{\mathbf{K}_2}\rightarrow\left[\frac{L}{2\pi}\right]^2\int_0^{2\pi}d\phi_{20}\int_0^\infty dK_2\,K_2\ ,$$

with the notation $\hat{\mathbf{K}}_i\cdot\hat{\mathbf{K}}_j=\cos\phi_{ij}$. If Eq. (2.4) is taken to be the form of the correlation function, Eq. (4.7a) becomes, using Eq. (C1),

$$\langle\Gamma(\mathbf{K}_1,\mathbf{K}_0)\rangle\underset{|\mathbf{K}_0|\rightarrow0}{\rightarrow}\langle\Gamma(K_1,\phi_{10})\rangle=\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\frac{\pi\sigma^2a^2}{L^2}e^{-K_1^2a^2/4}\,|\,\gamma(K_1)\gamma(0)\,|^2\cos^2\phi_{10}\ , \quad \text{(C2a)}$$

$$\langle\Gamma(\mathbf{K}_1,\mathbf{K}_2)\rangle=\langle\Gamma(K_1,K_2,\phi_{12})\rangle=\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\frac{\pi\sigma^2a^2}{L^2}e^{-(K_1^2+K_2^2)a^2/4}$$
$$\times\,|\,\gamma(K_1)\gamma(K_2)\,|^2\left|\frac{\epsilon K_1K_2}{\gamma(K_1)\gamma(K_2)}+\cos\phi_{12}\right|^2\sum_l I_l\left[\frac{K_1K_2a^2}{2}\right]e^{il\phi_{12}}\ . \quad \text{(C2b)}$$

The expansion for $\langle\tau(\mathbf{K}_1,\hat{\mathbf{K}}_0)\rangle_{11}$, written as

$$\langle\tau(\mathbf{K}_1,\hat{\mathbf{K}}_0)\rangle_{11}=\sum_m\langle\tau(K_1)\rangle_{11}^{(m)}e^{im\phi_{10}}\ , \quad \text{(C3)}$$

is then substituted into Eq. (4.6), along with Eq. (C2). The result is

$$\sum_{n'}\langle\tau(K_1)\rangle_{11}^{(n')}e^{in'\phi_{10}}=\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\frac{\pi\sigma^2a^2}{L^2}e^{-K_1^2a^2/4}\,|\gamma(K_1)|^2$$
$$\times\left[|\gamma(0)|^2\cos^2\phi_{10}+\left[\frac{L}{2\pi}\right]^2\int dK_2\,K_2\,|\langle G_p(K_2)\rangle|^2e^{-K_2^2a^2/4}\,|\gamma(K_2)|^2\right.$$
$$\times\int_0^{2\pi}d\phi_{20}\{|\eta'|^2+2\,\mathrm{Re}(\eta')\cos\phi_{12}+\tfrac{1}{2}[1+\cos(2\phi_{12})]\}$$
$$\left.\times\sum_{l,m}I_l(\alpha')\langle\tau(K_2)\rangle_{11}^{(m)}e^{il\phi_{12}}e^{im\phi_{20}}\right], \tag{C4}$$

where $\eta'=\epsilon K_1K_2/\gamma(K_1)\gamma(K_2)$ and $\alpha'=K_1K_2a^2/2$.

Since $\phi_{10}=\phi_{12}+\phi_{20}$, it is convenient to change the integration variable to ϕ_{12}. We also introduce $\chi^{(n)}(K,\hat{\mathbf{K}}_0)$, defined as

$$\langle\tau(K)\rangle_{11}^{(n)}=\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\frac{\pi\sigma^2a^2}{L^2}\,|\gamma(0)|^2\chi^{(n)}(K)\,. \tag{C5}$$

After multiplying Eq. (C4) through by $(2\pi)^{-1}e^{-in\phi_{10}}$ and integrating over ϕ_{10}, Eq. (C4) reduces to

$$\chi^{(n)}(K_1)=|\gamma(K_1)|^2e^{-K_1^2a^2/4}\left[\tfrac{1}{4}\delta_{n,\pm2}+\tfrac{1}{2}\delta_{n,0}-\frac{1}{(2\pi)^2}\left|\frac{\epsilon-1}{\epsilon^2}\right|^2\frac{\sigma^2a^2}{2}\right.$$
$$\times\sum_{l,m}\int_0^{2\pi}d\phi_{10}\int_{\phi_{10}}^{\phi_{10}-2\pi}d\phi_{12}\int dK_2\,K_2\,|\gamma(K_2)|^2e^{-K_2^2a^2/4}$$
$$\times|\langle G_p(K_2)\rangle|^2[|\eta'|^2+\tfrac{1}{2}+2\,\mathrm{Re}(\eta')\cos\phi_{12}+\tfrac{1}{2}\cos(2\phi_{12})]$$
$$\left.\times e^{-i\phi_{12}(l-m)}e^{-i\phi_{10}(n-m)}I_l(\alpha')\chi^{(m)}(K_2)\right]. \tag{C6}$$

Equation (4.14) follows after performing the angular integrations in (C6) and using the fact that $I_m(\alpha)=I_{-m}(\alpha)$. From the form of Eq. (C6) it is clear that only three Fourier components of $\chi^{(n)}(K_1)$ are nonzero, and that $\chi^{(2)}(K_1)=\chi^{(-2)}(K_1)$. With $\chi^{(m)}(K_1)$ known, Eqs. (4.4) and (4.5) can be analyzed in the same way; the result is Eqs. (4.9)—(4.12).

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