Diffraction of light from a small hole in a two-level quantum-well screen

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Quantum-mechanical linear-response theory is used to calculate the diffraction of light from a small hole in a thin flat screen. The field-induced dynamics of the charged particles (electrons) is obtained by modeling a screen without a hole as a two-level quantum well, with jellium behavior for the in-plane electron motion. Local-field corrections are calculated in a self-field approximation to a coupled-antenna theory. Particular attention is devoted to frequency resonance effects in the local field. A generalization to a screen with a hole is suggested, replicating the homogeneous jellium surface electron density by a space varying density in the vicinity of the hole. Quantum-mechanical expressions for the electric dipole moment $\mathbf{p}(\omega)$, the magnetic dipole moment $\mathbf{m}(\omega)$, and the electric quadrupole moment $\mathbf{Q}(\omega)$ of the so-called aperture current density are derived and the light scattering from these moments is studied. From the general theory results for $\mathbf{p}(\omega)$, $\mathbf{m}(\omega)$, and $\mathbf{Q}(\omega)$ in three cases are given: (i) no induced electron motion perpendicular to the plane of the screen [leading to $\mathbf{p}(\omega) = \mathbf{0}$], (ii) resonance excitation of the electron system, and (iii) a circular hole. This paper presents an extension of the quantum-mechanical diffraction theory developed in two recent papers of ours [J. Jung and O. Keller, Phys. Rev. A **90**, 043830 (2014); **92**, 012122 (2015)].

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I. INTRODUCTION

In a seminal theoretical paper Bethe studied the diffraction of electromagnetic waves by a small hole in a plane, infinitely thin and perfectly conducting screen [1]. In particular, he gave an explicit solution for a circular hole of small radius compared with the wavelength of the assumed monochromatic incident field. *Small* for Bethe meant that the electric and magnetic fields can be considered as constant over the hole. In consequence, the incident wave need not be a plane. Bethe came to the conclusion that, in the far field of the hole, the diffracted field may be considered as owing to an electric and a magnetic dipole, the first pointing in the direction of the normal to the screen and the second lying in the plane of the hole. By a careful examination, Bouwkamp revealed that the correct (under the given assumption of infinite conductivity) electric field near and in the hole differs appreciable from that following from Bethe's theory [2,3]. The result of Bethe's approach is completely different from that of Kirchhoff's method [4,5].

Although the Bethe-Bouwkamp theory may give a fair description of the diffracted field from a hole in a metal screen at long wavelengths (on the order of microwave frequencies and below), the assumption of perfect conductivity certainly is a strong idealization in general, e.g., at optical frequencies. The interaction of the incoming electromagnetic field with the charged particles (electrons, ions) of a screen with finite conductivity inevitably will give rise to frequency dispersion in the diffracted radiation. In more recent studies such material dispersion effects have almost always been accounted for by using macroscopic electrodynamics and a frequency-dependent dielectric constant (tensor) (see, e.g., Refs. [6–15] and references therein). While material dispersion effects perhaps may be accounted for by macroscopic electrodynamics for sufficiently thick screens, macroscopic approaches certainly fail for screens so thin that quantum-size phenomena play a role. The quantum description in any case requires that the unphysical assumption of vanishing screen thickness must be abandoned.

In the present theoretical work we study the diffraction of an electromagnetic field from a screen so thin and a hole so small that quantum mechanics is needed for the description of the induced electron dynamics in the screen, in particular in the vicinity of the hole. In two previous paper of ours [16,17] we established a quantum-mechanical diffraction theory for a small hole in a metallic (or semiconducting) screen dominated by diamagnetic field-matter interaction. Part of the analysis in the aforementioned papers dealt with a quantum-well screen so thin that only one bound electron level exist in relation to the electron confinement potential perpendicular to the screen. The in-plane essentially two-dimensional electron dynamics was treated in the jellium approximation. The diamagnetic interaction gives a frequency dependence of the microscopic conductivity tensor proportional to ω^{-1} [and $(\omega + i/\tau)^{-1}$ if losses are taken into account in a relaxation-time (τ) approximation].

From a conceptual point of view it is interesting to extend the quantum-mechanical diffraction theory to two-level quantum-well screens for the following (interrelated) reasons. (i) Two-level dynamics (necessarily including the paramagnetic contribution to the microscopic conductivity tensor) leads to a pronounced frequency resonance in a diffraction spectrum. (ii) In general, the resonance frequency does not coincide with the Bohr transition frequency between the two quantum levels because of local-field corrections. (iii) The self-consistent field driving the electron dynamics in

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the screen deviates from the incident field precisely because of local-field effects, and this fact is a crucial difficulty for the Bethe-Bouwkamp approach. (iv) For a two-level quantum well the local-field correction can be calculated quite accurately in a self-field approximation [18] using the so-called coupled-antenna theory [19] (Secs. II B–II E and III A). (v) In the Bethe-Bouwkamp theory and related macroscopic works, the (oscillating) induced screen current is assumed to possess no component in the normal direction to the screen, near (and at) local-field resonance, the dynamic flow of the electrons perpendicular to the screen plane certainly cannot be neglected [except in the case of (near) normal incidence of the incoming field] (see Secs. II E and III B).

Although scattering and diffraction of electromagnetic radiation often are treated as different phenomena, they have a common physical basis, namely, field-matter interaction. In many diffraction problems the role of this interaction is completely hidden or appears in a conspicuous indirect manner. For example, in all classical studies of the diffraction from large apertures (holes) in opaque, infinitely thin metal screens the interaction appears only in the form of screen surface current densities needed to satisfy idealized boundary conditions of the electromagnetic field. The close connection between scattering and diffraction occurs in a manifest manner if one compares the scattering from mesoscopic (or microscopic) objects to the diffraction from subwavelength holes. In both cases a systematic multipole description (in which most often only lowest-order multipoles are kept) is appropriate. The use of dipole moments to describe small-hole diffraction can be traced back to Rayleigh [20].

In the framework of quantum mechanics, a major part of the present work is devoted to a multipole description of the diffraction from a small hole in a two-level quantum-well screen with in-plane jellium dynamics. Notwithstanding the fact that our quantum approach conceptually is very different from the classical methods of Bethe and Bouwkamp, some similarities appear in the initial steps of the formulation. Thus, we connect the multipole expansion scheme to the dynamics in the effective optical aperture, a concept defined as the in-plane screen area in which the difference $\mathbf{\Delta} \equiv \boldsymbol{\sigma}^{\mathrm{cau}} - \boldsymbol{\sigma}^{\mathrm{cau}}_{\infty}$ between the causal microscopic conductivity tensors of identical screens with ($\boldsymbol{\sigma}^{\mathrm{cau}}$) and without a hole ($\boldsymbol{\sigma}^{\mathrm{cau}}_{\infty}$) is nonvanishing, essentially. Also in Bethe's analysis a comparison of diffraction from screens with and without a hole is central. Hence, in a zeroth-order approximation the field on a screen with a hole satisfies the standard boundary conditions everywhere on the screen but not in the hole [1].

The determination of the aperture response $\mathbf{\Delta}$ in the frequency (ω) domain is done under the justified assumption that the electromagnetic field's in-plane wave number $q_\parallel$ is (vanishing) small compared to all relevant electron wave numbers $k_\parallel$ in the two-dimensional jellium. Once an explicit expression has been obtained for $\mathbf{\Delta}$ (Sec. III B), a systematic multipole expansion scheme can be implemented. In this scheme two smallness parameters enter, viz., $q_0 d$ ($\ll 1$) and $q_0 a$ ($\ll 1$), where d is the effective width of the quantum well, a the effective hole size, and $q_0 = \omega/c$ the vacuum wave number of the field. In the Bethe-Bouwkamp theory the physically important expansion in $q_0 d$ is lost because $d = 0$ from the onset.

In previous works on small-hole diffraction going beyond the first-order electric dipole (ED) approximation, only a magnetic dipole (MD) term appears in the second order. In general, also an electric quadrupole (EQ) term is present in the second order. The EQ and MD parts are given as the symmetric and antisymmetric parts of the first-order moment of the source [19,21] (here effective aperture) current density distribution. To determine these parts, a three-dimensional analysis is required (see Appendix C).

II. INTERNAL ELECTRODYNAMICS OF A SCREEN WITHOUT A HOLE

A. Microscopic linear-response theory: General aspects and approximations

Let us assume that a screen (with or without a hole) is excited by an incident electric field, defined by $\mathbf{E}^0(\mathbf{r};\omega) \equiv \mathbf{E}^0(\mathbf{r})$ in the space-frequency ($\mathbf{r}$-ω) domain. In the framework of microscopic linear-response theory, the induced self-consistent motions of the charged particles in the screen imply that the microscopic electric field $\mathbf{E}(\mathbf{r};\omega) \equiv \mathbf{E}(\mathbf{r})$ in the arbitrary space point $\mathbf{r}$ is given by the spatially nonlocal connection [16,22]

$$\mathbf{E}(\mathbf{r}) = \int_{-\infty}^{\infty} \mathbf{\Gamma}(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}^0(\mathbf{r}') d^3r', \quad (1)$$

where $\Gamma(\mathbf{r},\mathbf{r}';\omega) \equiv \Gamma(\mathbf{r},\mathbf{r}')$ is the so-called field-field response tensor. This tensor satisfies an integral equation

$$\Gamma(\mathbf{r},\mathbf{r}') = \mathbf{U}\delta(\mathbf{r}-\mathbf{r}') + \int_{-\infty}^{\infty} \mathbf{K}(\mathbf{r},\mathbf{r}'') \cdot \Gamma(\mathbf{r}'',\mathbf{r}') d^3r'', \quad (2)$$

with a tensorial kernel $\mathbf{K}(\mathbf{r},\mathbf{r}';\omega) \equiv \mathbf{K}(\mathbf{r},\mathbf{r}')$ given by

$$\mathbf{K}(\mathbf{r},\mathbf{r}') = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r}-\mathbf{r}'') \cdot \boldsymbol{\sigma}(\mathbf{r}'',\mathbf{r}') d^3r''. \quad (3)$$

In Eq. (2), $\mathbf{U}$ is the unit tensor and δ the Dirac delta function. In Eq. (3), $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega) \equiv \boldsymbol{\sigma}(\mathbf{r},\mathbf{r}')$ is the linear microscopic conductivity tensor and $\mathbf{G}(\mathbf{R};\omega) \equiv \mathbf{G}(\mathbf{R})$ (with $\mathbf{R} = \mathbf{r} - \mathbf{r}'$) is the well-known (standard) dyadic Green's function of vacuum. Since $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}')$ is nonvanishing only when the two space points $\mathbf{r}$ and $\mathbf{r}'$ are located inside the screen (in a quantum-mechanical context, the region where the particle probability density effectively is nonvanishing), it appears from a combination of Eqs. (2) and (3) that once the loop equation for $\mathbf{\Gamma}(\mathbf{r},\mathbf{r}')$ (both points $\mathbf{r}$ and $\mathbf{r}'$ located inside the screen) has been solved, $\mathbf{\Gamma}(\mathbf{r},\mathbf{r}')$ can be determined on every pairs of points ($\mathbf{r}$ and $\mathbf{r}'$) in the entire space. For observation points $\mathbf{r}$ inside the screen $\mathbf{\Gamma}(\mathbf{r},\mathbf{r}')$ is most often called the local-field tensor in the literature [cf. Eq. (1)]. Outside the screen $\mathbf{\Gamma}(\mathbf{r},\mathbf{r}')$ relates to the scattered field $\mathbf{E}(\mathbf{r}) - \mathbf{E}^0(\mathbf{r})$. Thus,

$$\mathbf{E}(\mathbf{r}) - \mathbf{E}^0(\mathbf{r}) = \int_{\mathrm{screen}} \mathbf{K}(\mathbf{r},\mathbf{r}'') \cdot \mathbf{\Gamma}(\mathbf{r}'',\mathbf{r}') \cdot \mathbf{E}^0(\mathbf{r}') d^3r'' d^3r', \quad (4)$$

as one realizes by inserting Eq. (2) into Eq. (1). As indicated, the integrations run over coordinates located inside the screen, a circumstance which becomes obvious from an equivalent

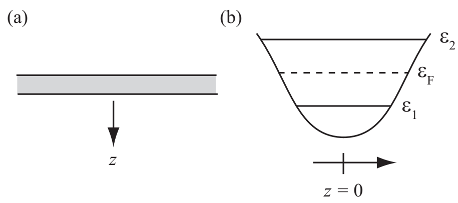

FIG. 1. (a) Planar infinitely extended screen. The z direction is placed perpendicular to the screen. (b) Two-level quantum-well potential for the electron dynamics perpendicular to the screen. The Fermi level is assumed to be in between the two quantum levels.

expression one may write for the scattered field, viz.,

$$\mathbf{E}(\mathbf{r}) - \mathbf{E}^0(\mathbf{r}) = i\mu_0\omega \int_{\text{screen}} \mathbf{G}(\mathbf{r}-\mathbf{r}'')\cdot\boldsymbol{\sigma}(\mathbf{r}'',\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')d^3r''d^3r'. \quad (5)$$

The linear-response theory analysis summarized above is quite general in the sense that it holds for screens with and without holes (apertures) and for scattering objects (media) of arbitrary forms. It is only necessary that the scattering medium in question possesses translationally invariant electrodynamic properties in time, a demand which requires that $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{r},\mathbf{r}',t-t')$ in the space-time ($\mathbf{r}$-t) domain, and that it is not necessary to take into account modifications rooted in the fact that the induced longitudinal field is not a dynamical variable [19,23]. (In theoretical studies, for instance, of spatial photon localization, photon tunneling [24], and Lamb shifts [19] carried out on the basis of photon wave mechanics or its quantum electrodynamic covering theory, it is needed to distinguish between transverse and longitudinal electrodynamics.) In the framework of the present theory, the distinction between various scattering media lies solely in the expression adopted for $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$.

Let us now consider a metallic or semiconducting planar (infinitely extended) screen without a hole and let us assume that it is so thin that it behaves like a two-level quantum well (QW) for the particle (electron) dynamics in the direction perpendicular to the screen (see Fig. 1). In the present study we may, without loss of essential generality, treat the in-plane electron dynamics in the framework of the jellium model. The translational invariance of the in-plane electrodynamic properties means that

$$\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}') = \boldsymbol{\sigma}_\infty(\mathbf{r}_\parallel - \mathbf{r}'_\parallel, z, z'), \quad (6)$$

where, in a Cartesian (x,y,z) coordinate system, the z direction is placed perpendicular to the screen, so $\mathbf{r}_\parallel = (x,y)$ [and $\mathbf{r}'_\parallel = (x',y')$]. To underline that we are dealing with a screen without a hole a subscript ∞ has been added to $\boldsymbol{\sigma}$. A two-dimensional (2D) spatial Fourier-integral transformation of $\boldsymbol{\sigma}_\infty(\mathbf{R}_\parallel, z, z')$ (with $\mathbf{R}_\parallel = \mathbf{r}_\parallel - \mathbf{r}'_\parallel$) gives the representation

$$\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}_\infty(\mathbf{R}_\parallel, z, z')e^{-i\mathbf{q}_\parallel\cdot\mathbf{R}_\parallel}d^2R_\parallel \quad (7)$$

and, as we will soon realize, the subsequent calculations can (conveniently) be carried out in the mixed 2D wave-vector–space ($\mathbf{q}_\parallel$–z) domain. In this domain the vacuum Green's tensor $\mathbf{G}(\mathbf{r}-\mathbf{r}') = \mathbf{G}(\mathbf{r}_\parallel - \mathbf{r}'_\parallel, z-z') = \mathbf{G}(\mathbf{R}_\parallel, Z)$ (with $Z = z - z'$) has a 2D Fourier amplitude $\mathbf{G}(Z;\mathbf{q}_\parallel)$ whose explicit dyadic form is well known, viz., the disk-contracted representative [22]

$$\mathbf{G}(Z;\mathbf{q}_\parallel) = -q_0^2\delta(Z)\hat{\mathbf{z}}\hat{\mathbf{z}} + \frac{i}{2\kappa_\perp q_0^2}e^{i\kappa_\perp|Z|} \times \left[q_0^2\mathbf{U} - \mathbf{q}_\parallel\mathbf{q}_\parallel - \kappa_\perp^2\hat{\mathbf{z}}\hat{\mathbf{z}} - (\mathbf{q}_\parallel\hat{\mathbf{z}} + \hat{\mathbf{z}}\mathbf{q}_\parallel)\kappa_\perp \operatorname{sgn}Z\right], \quad (8)$$

where

$$\kappa_\perp = \left(q_0^2 - q_\parallel^2\right)^{1/2}\Theta(q_0 - q_\parallel) + i\left(q_\parallel^2 - q_0^2\right)^{1/2}\Theta(q_\parallel - q_0). \quad (9)$$

In the equations above, Θ and sgn designate the unit-step and signum functions, respectively, $q_0 = \omega/c$ is the vacuum wave number of light, and $\hat{\mathbf{z}}$ is a unit vector in the z direction.

For what follows it is sufficient to calculate $\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel)$ in the long-wavelength limit ($\mathbf{q}_\parallel \to \mathbf{0}$). In consequence, all electronic intersubband transitions $(\mathbf{k}_\parallel, n) \Leftrightarrow (\mathbf{k}'_\parallel, n') = (\mathbf{k}_\parallel + \mathbf{q}_\parallel, n')$ are considered vertical. Hence, the energy momentum conservation condition for the elementary processes, i.e.,

$$\hbar\omega + \varepsilon_n - \varepsilon_{n'} + \frac{\hbar^2}{2m}k_\parallel^2 - \frac{\hbar^2}{2m}|\mathbf{k}_\parallel + \mathbf{q}_\parallel|^2 = 0, \quad (10)$$

is reduced to $\varepsilon'_n - \varepsilon_n = \hbar\omega$, giving the Bohr condition for $\varepsilon_{n'} > \varepsilon_n$. For $\varepsilon_{n'} \neq \varepsilon_n$ Eq. (10) describes the kinematics in inelastic Compton scattering.

Readers less interested in the technical details of the local-field calculation leading up to the resonance condition for excitation in the two-level QW system (Secs. II B–II E) may start reading Sec. II F.

B. Field-field response tensor

Based on the procedure used in the so-called coupled-antenna theory developed by one of the present authors (O.K.) two decades ago [25] and described in details in Refs. [19,22], we now show that it is possible to obtain an exact analytical expression for the field-field response tensor associated with a two-level QW screen without a hole. Although we will start from the long-wavelength ($\mathbf{q}_\parallel \to \mathbf{0}$) approximation for the conductivity tensor, it is possible to generalize the procedure to an arbitrary number of bound QW levels and to go beyond the $\mathbf{q}_\parallel \to \mathbf{0}$ approximation and use the general conductivity tensor $\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel,\omega)$.

A similar method has been used previously to calculate the field-field response for a two-level QW sheet, dominated by the paramagnetic part $\boldsymbol{\sigma}^{\mathrm{P}}$ of the conductivity tensor $\boldsymbol{\sigma}$ and placed on top of a substrate [18]. After the publication of Ref. [18], it was shown that also the diamagnetic part $\boldsymbol{\sigma}^{\mathrm{D}}$ of the conductivity tensor could be written as a sum of $(\mathbf{r},\mathbf{r}')$-separable tensor products [22], a circumstance which is basic to the coupled-antenna theory in its general form. The separable form of $\boldsymbol{\sigma}^{\mathrm{D}}$ was first obtained by an indirect argument, viz., the demand that the total conductivity tensor $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{P}} + \boldsymbol{\sigma}^{\mathrm{D}}$ must vanish in the static limit, i.e., $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}',\omega \to 0) = \mathbf{0}$, and then by a direct calculation [22]. Below, the long-wavelength expression for the total conductivity tensor is used in the calculation of the field-field response tensor. The quite significant progress achieved in using $\boldsymbol{\sigma}_\infty$ instead of $\boldsymbol{\sigma}^{\mathrm{P}}_\infty$ is discussed in Appendix A, where also the following expression of the long-wavelength conductivity tensor is obtained:

$$\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to 0, \omega) = a_\infty(\omega)(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z)\phi(z') + b_\infty(\omega)\hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z)\Phi(z'). \tag{11}$$

The functions ϕ and Φ are related to the orthonormalized time-independent electron wave functions $\psi_n(u)$, $n = 1, 2$, of the lower ($n = 1$) and upper ($n = 2$) energy eigenstates (both wave functions of our symmetric QW taken without loss of generality as real) as follows:

$$\phi(u) = \psi_1(u)\psi_2(u), \tag{12}$$

$$\Phi(u) = \psi_1(u)\frac{d\psi_2(u)}{du} - \psi_2(u)\frac{d\psi_1(u)}{du}. \tag{13}$$

The explicit expressions for $a_\infty(\omega)$ and $b_\infty(\omega)$ are given in Appendix A.

It appears from Eqs. (3) and (7) that the kernel for the infinitely extended jellium screen $\mathbf{K}_\infty$ is given by

$$\begin{aligned}\mathbf{K}_\infty(\mathbf{R}_\parallel, z, z') &= i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r}_\parallel - \mathbf{r}''_\parallel, z - z'') \cdot \boldsymbol{\sigma}_\infty(\mathbf{r}''_\parallel - \mathbf{r}'_\parallel, z'', z') d^2r''_\parallel dz'' \\ &= i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{R}_\parallel - \mathbf{r}''_\parallel + \mathbf{r}'_\parallel, z - z'') \cdot \boldsymbol{\sigma}_\infty(\mathbf{r}''_\parallel - \mathbf{r}'_\parallel, z'', z') d^2r''_\parallel dz''\end{aligned} \tag{14}$$

and hence represented by

$$\mathbf{K}_\infty(z, z'; \mathbf{q}_\parallel) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(z - z''; \mathbf{q}_\parallel) \cdot \boldsymbol{\sigma}_\infty(z'', z'; \mathbf{q}_\parallel) dz'' \tag{15}$$

in the mixed wave-vector and space domain. By rewriting the long-wavelength expression for $\boldsymbol{\sigma}_\infty$ [Eq. (11)] in the form

$$\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to 0) = a_\infty(\omega)\phi(z')(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}}) \cdot (\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z) + b_\infty(\omega)\Phi(z')\hat{\mathbf{z}}\hat{\mathbf{z}} \cdot \hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z), \tag{16}$$

it is realized that the tensorial kernel is an inner product of tensors of z and z', respectively. Thus,

$$\mathbf{K}_\infty(z, z'; \mathbf{q}_\parallel) = \mathbf{F}_\infty(z; \mathbf{q}_\parallel) \cdot \boldsymbol{\Theta}_\infty(z'), \tag{17}$$

where

$$\mathbf{F}_\infty(z; \mathbf{q}_\parallel) = i\mu_0\omega \int_{\mathrm{QW}} \mathbf{G}(z - z'; \mathbf{q}_\parallel) \cdot [(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})a_\infty(\omega)\phi(z') + \hat{\mathbf{z}}\hat{\mathbf{z}}b_\infty(\omega)\Phi(z')]dz' \tag{18}$$

and

$$\boldsymbol{\Theta}_\infty(z') = (\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z') + \hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z'). \tag{19}$$

In Eq. (18) we have stressed that the integration runs over the z' values inside the QW screen.

The fact that the kernel in Eq. (15) is a function of the difference $\mathbf{r}_\parallel - \mathbf{r}'_\parallel$ $(=\mathbf{R}_\parallel)$ only dictates that the same must be the case for $\boldsymbol{\Gamma}_\infty$ [cf. the structural form of Eq. (2) for $\mathbf{K} = \mathbf{K}(\mathbf{r}_\parallel - \mathbf{r}''_\parallel, z, z'')$]. In the $(\mathbf{q}_\parallel, z)$ domain, $\boldsymbol{\Gamma}_\infty(z, z', \mathbf{q}_\parallel)$ consequently satisfies the integral equation

$$\boldsymbol{\Gamma}_\infty(z, z'; \mathbf{q}_\parallel) = \mathbf{U}\delta(z - z') + \int_{-\infty}^{\infty} \mathbf{K}_\infty(z, z''; \mathbf{q}_\parallel) \cdot \boldsymbol{\Gamma}_\infty(z'', z'; \mathbf{q}_\parallel) dz''. \tag{20}$$

By inserting Eq. (17) into Eq. (20) (and letting the reference to $\mathbf{q}_\parallel$ be kept implicit) one obtains

$$\boldsymbol{\Gamma}_\infty(z, z') = \mathbf{U}\delta(z - z') + \mathbf{F}_\infty(z) \cdot \mathbf{N}_\infty(z'), \tag{21}$$

where

$$\mathbf{N}_\infty(z') = \int_{\mathrm{QW}} \boldsymbol{\Theta}_\infty(z'') \cdot \boldsymbol{\Gamma}_\infty(z'', z') dz''. \tag{22}$$

By reinserting Eq. (21) into Eq. (22) and by solving thereafter the resulting equation for $\mathbf{N}_\infty(z')$, one gets

$$\mathbf{N}_\infty(z') = \left[\mathbf{U} - \int_{\mathrm{QW}} \boldsymbol{\Theta}_\infty(z'') \cdot \mathbf{F}_\infty(z'') dz''\right]^{-1} \cdot \boldsymbol{\Theta}_\infty(z') \tag{23}$$

and finally

$$\boldsymbol{\Gamma}_\infty(z, z') = \mathbf{U}\delta(z - z') + \mathbf{F}_\infty(z) \cdot \left[\mathbf{U} - \int_{\mathrm{QW}} \boldsymbol{\Theta}_\infty(z'') \cdot \mathbf{F}_\infty(z'') dz''\right]^{-1} \cdot \boldsymbol{\Theta}_\infty(z'). \tag{24}$$

The factorization of the kernel $\mathbf{K}_\infty(z, z'; \mathbf{q}_\parallel)$ thus has enabled one to achieve an exact analytical expression for the field-field response tensor.

By now we have obtained a complete determination of the self-consistent electric field in the $(\mathbf{q}_\parallel, z)$ domain, viz.,

$$\mathbf{E}_\infty(z; \mathbf{q}_\parallel) = \mathbf{E}^0(z; \mathbf{q}_\parallel) + \mathbf{F}_\infty(z; \mathbf{q}_\parallel) \cdot \left[\mathbf{U} - \int_{\mathrm{QW}} \boldsymbol{\Theta}_\infty(z') \cdot \mathbf{F}_\infty(z'; \mathbf{q}_\parallel) dz'\right]^{-1} \cdot \int_{\mathrm{QW}} \boldsymbol{\Theta}_\infty(z') \cdot \mathbf{E}^0(z'; \mathbf{q}_\parallel) dz', \tag{25}$$

with $\mathbf{F}_\infty(z; \mathbf{q}_\parallel)$ and $\boldsymbol{\Theta}(z')$ given by Eqs. (18) and (19).

C. Causal conductivity tensor

It is well known that the microscopic Maxwell-Lorentz equations lead to the following scattering formula in the $(z; \mathbf{q}_\parallel)$ domain:

$$\mathbf{E}_\infty(z; \mathbf{q}_\parallel) = \mathbf{E}^0(z; \mathbf{q}_\parallel) + i\mu_0\omega \int_{\mathrm{QW}} \mathbf{G}(z - z'; \mathbf{q}_\parallel) \cdot \mathbf{J}_\infty(z'; \mathbf{q}_\parallel) dz'. \tag{26}$$

A comparison of this equation to Eq. (25), with Eq. (18) inserted, readily gives one an explicit expression for the current density in our two-level quantum-well screen, namely,

$$\mathbf{J}_\infty(z;\mathbf{q}_\parallel) =[(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})a_\infty(\omega)\phi(z)+\hat{\mathbf{z}}\hat{\mathbf{z}}b_\infty(\omega)\Phi(z)] \cdot\left[\mathbf{U}-\int_{\mathrm{QW}}\mathbf{\Theta}_\infty(z')\cdot\mathbf{F}_\infty(z';\mathbf{q}_\parallel)dz'\right]^{-1} \cdot\int_{\mathrm{QW}}\mathbf{\Theta}_\infty(z')\cdot\mathbf{E}^0(z';\mathbf{q}_\parallel)dz'. \quad (27)$$

In the microscopic theory of light diffraction the so-called causal conductivity tensor $\boldsymbol{\sigma}^{\mathrm{cau}}$ plays a central role [16]. In general, this tensor relates the current density in a given point in the scattering medium to the incident electric field in this and surrounding points. For a medium exhibiting two-dimensional invariance in space (perpendicular to a chosen z direction), the causal conductivity has a $(\mathbf{q}_\parallel, z)$ representation. A comparison of the general causal constitutive equation

$$\mathbf{J}_\infty(z;\mathbf{q}_\parallel)=\int_{-\infty}^{\infty}\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel)\cdot\mathbf{E}^0(z';\mathbf{q}_\parallel)dz' \quad (28)$$

and Eq. (27) gives one the following expression for $\boldsymbol{\sigma}_\infty^{\mathrm{cau}}$:

$$\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel)=[(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})a_\infty(\omega)\phi(z)+\hat{\mathbf{z}}\hat{\mathbf{z}}b_\infty(\omega)\Phi(z)] \cdot\left[\mathbf{U}-\int_{\mathrm{QW}}\mathbf{\Theta}_\infty(z')\cdot\mathbf{F}_\infty(z';\mathbf{q}_\parallel)dz'\right]^{-1} \cdot\mathbf{\Theta}_\infty(z'). \quad (29)$$

Since $\mathbf{\Theta}_\infty$ is a diagonal tensor it can be interchanged with the $[\cdots]^{-1}$ tensor, and in the view of Eq. (16), the relation between $\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel)$ and $\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel)$ is obtained,

$$\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel)=\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel\to 0)\cdot\mathbf{L}_\infty(\mathbf{q}_\parallel), \quad (30)$$

where

$$\mathbf{L}_\infty(\mathbf{q}_\parallel)=\left[\mathbf{U}-\int_{\mathrm{QW}}\mathbf{\Theta}(z)\cdot\mathbf{F}_\infty(z;\mathbf{q}_\parallel)dz\right]^{-1} \quad (31)$$

is what we call the local-field factor, a frequency-dependent $[\mathbf{L}_\infty(\mathbf{q}_\parallel)\equiv\mathbf{L}_\infty(\mathbf{q}_\parallel;\omega)]$ tensor, here for a screen without a hole.

D. Local-field corrections in the self-field approximation

It is remarkable that the local-field factor is independent of z and z'. The dependence of $\mathbf{L}_\infty(\mathbf{q}_\parallel)$ on $\mathbf{q}_\parallel$ solely appears via the vacuum Green's function $\mathbf{G}(z-z';\mathbf{q}_\parallel)$ [cf. Eq. (18)]. Since the integrations in Eqs. (18) and (31) run over z and z' coordinates inside the quantum well, one may approximate $\mathbf{G}(Z;\mathbf{q}_\parallel)$ by its self-field term and if needed add a Taylor expansion of its nonlocal part. In the self-field approximation for the Green's tensor

$$\mathbf{G}(z-z')=-q_0^{-2}\delta(z-z')\hat{\mathbf{z}}\hat{\mathbf{z}}, \quad (32)$$

even the $\mathbf{q}_\parallel$ dependence of the local-field factor disappears. By inserting Eq. (32) into Eq. (18) one obtains

$$\mathbf{F}_\infty(z)=(i\varepsilon_0\omega)^{-1}b_\infty(\omega)\Phi(z)\hat{\mathbf{z}}\hat{\mathbf{z}}. \quad (33)$$

The term proportional to $a_\infty(\omega)$ in $\mathbf{F}_\infty$ has disappeared because $\hat{\mathbf{z}}\hat{\mathbf{z}}\cdot(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})=\mathbf{0}$. With $\mathbf{F}_\infty(z)$ given by Eq. (33) we get

$$\int_{\mathrm{QW}}\mathbf{\Theta}_\infty(z)\cdot\mathbf{F}_\infty(z)dz=\frac{\hat{\mathbf{z}}\hat{\mathbf{z}}}{i\varepsilon_0\omega}b_\infty(\omega)\int_{\mathrm{QW}}\Phi^2(z)dz \quad (34)$$

and thus a local-field factor

$$\mathbf{L}_\infty^{\mathrm{SF}}=\left[\mathbf{U}-\frac{\hat{\mathbf{z}}\hat{\mathbf{z}}}{i\varepsilon_0\omega}b_\infty(\omega)\int_{\mathrm{QW}}\Phi^2(z)dz\right]^{-1}, \quad (35)$$

where the superscript SF is meant to remind the reader that the result refers to the self-field approximation. Since the tensor in the square brackets of Eq. (35) is in diagonal form, its inverse is readily determined. Hence,

$$\mathbf{L}_\infty^{\mathrm{SF}}=\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}}+\left[1-\frac{b_\infty(\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz\right]^{-1}\hat{\mathbf{z}}\hat{\mathbf{z}}. \quad (36)$$

By combining Eqs. (16), (30), and (36) one finally obtains the following expression for the causal conductivity tensor in the long-wavelength limit ($\mathbf{q}_\parallel\to 0$) and self-field approximations:

$$\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel\to\mathbf{0})=a_\infty(\omega)(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z)\phi(z') +\frac{b_\infty(\omega)}{1-\frac{b_\infty(\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz}\hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z)\Phi(z'). \quad (37)$$

In general, the causal conductivity tensor $[\boldsymbol{\sigma}^{\mathrm{cau}}(\mathbf{r},\mathbf{r}')]$ is different from the conductivity tensor itself $[\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}')]$ because of spatially nonlocal electromagnetic and electronic correlations effects (see Refs. [16,17]). In the self-field approximation only electronic correlations remain, and it appears from Eq. (37) that these in the long-wavelength limit for the conductivity tensor only make the zz components of the two diagonal conductivity tensors different. The ratio, given by

$$\frac{\sigma_{\infty,zz}^{\mathrm{cau}}(z,z';\mathbf{q}_\parallel\to\mathbf{0})}{\sigma_{\infty,zz}(z,z';\mathbf{q}_\parallel\to\mathbf{0})}=\left[1-\frac{b_\infty(\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz\right]^{-1}, \quad (38)$$

is, as we already know, independent of z and z' and may become very large at a certain frequency called the local-field resonance frequency. As we will soon realize, local-field resonances play an important role in light diffraction both from two-level quantum screens without and with a small hole.

E. The ED-ED sheet current density: Resonance condition

Let us return to the constitutive relation in Eq. (28) and recognize that a two-level QW screen in its response to light usually will behave like an electric dipole absorber and radiator [a so-called ED-ED sheet (screen)] [16]. This means that the variation of the incoming electric field across the QW is negligible, $\mathbf{E}^0(z',\mathbf{q}_\parallel)\simeq\mathbf{E}^0(0,\mathbf{q}_\parallel)[\equiv\mathbf{E}^0(\mathbf{q}_\parallel)]$, and that only the integral of the sheet current density, viz.,

$$\mathbf{J}_\infty^S(\mathbf{q}_\parallel)=\int_{\mathrm{QW}}\mathbf{J}_\infty(z;\mathbf{q}_\parallel)dz, \quad (39)$$

is needed. The quantity $\mathbf{J}_\infty^S(\mathbf{q}_\parallel)$ is called the surface (S) current density [16], here given in the 2D wave-vector ($\mathbf{q}_\parallel$)

domain. In the ED-ED approximation the constitutive relation in Eq. (28) is reduced to the algebraic form

$$\mathbf{J}^S_\infty(\mathbf{q}_\parallel) = \mathbf{S}_\infty(\mathbf{q}_\parallel)\cdot\mathbf{E}^0(\mathbf{q}_\parallel), \quad (40)$$

where

$$\mathbf{S}_\infty(\mathbf{q}_\parallel) = \int_{\mathrm{QW}} \boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z,z';\mathbf{q}_\parallel)dz'dz, \quad (41)$$

with $\mathbf{S}_\infty(\mathbf{q}_\parallel)\equiv\mathbf{S}^{\mathrm{ED\text{-}ED}}_\infty$, has been named the causal surface (or ED-ED) conductivity tensor [16]. In the long-wavelength limit ($\mathbf{q}_\parallel\to 0$) and within the self-field approximation this quantity is independent of $\mathbf{q}_\parallel$, since $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty$ is. By inserting Eq. (37) in Eq. (41) and utilizing the orthogonality of the wave functions of the two QW levels, expressed as

$$\int_{\mathrm{QW}}\phi(z)dz = 0, \quad (42)$$

one obtains

$$\mathbf{S}_\infty(\omega) = \frac{b_\infty(\omega)[\int_{\mathrm{QW}}\Phi(z)dz]^2}{1-\frac{b_\infty(\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz}\hat{\mathbf{z}}\hat{\mathbf{z}} \quad (43)$$

in the limit $\mathbf{q}_\parallel\to 0$. When $\mathbf{S}_\infty$ is independent of $\mathbf{q}_\parallel$ a 2D Fourier transform of Eq. (40) shows that the surface current density in the space-frequency ($\mathbf{r}_\parallel-\omega$) domain is given by

$$\mathbf{J}^S_\infty(\mathbf{r}_\parallel;\omega) = \hat{\mathbf{z}}\frac{b_\infty(\omega)[\int_{\mathrm{QW}}\Phi(z)dz]^2}{1-\frac{b_\infty(\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz}\hat{\mathbf{z}}\cdot\mathbf{E}^0(\mathbf{r}_\parallel;\omega). \quad (44)$$

It appears from this equation that the surface current density everywhere (for all $\mathbf{r}_\parallel$) is perpendicular to the plane of the screen and of course only driven by the z component of the incoming field $\mathbf{E}^0_z(\mathbf{r}_\parallel, z=0;\omega)$.

The local-field factor (36), and thus also the surface current density, is resonantly enhanced for frequencies $\omega^{\mathrm{res}}_\infty$, satisfying the condition

$$\frac{b_\infty(\omega^{\mathrm{res}}_\infty)}{i\varepsilon_0\omega^{\mathrm{res}}_\infty}\int_{\mathrm{QW}}\Phi^2(z)dz = 1. \quad (45)$$

In a two-level quantum well there is only one resonance frequency for the local field, and to examine the relation between the Bohr transition frequency $\omega_{\mathrm{B}} = (\varepsilon_2-\varepsilon_1)/\hbar$ and $\omega^{\mathrm{res}}_\infty$ we need the explicit expression for $b_\infty(\omega)$. Limiting ourselves to the low-temperature limit ($T\to 0$ K), we obtain (see Appendix A)

$$b_\infty(\omega) = \frac{ie^2\hbar^2\omega}{2\pi m}\left(\frac{\varepsilon_F-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right)\frac{1}{(\hbar\omega)^2-(\varepsilon_2-\varepsilon_1)^2}, \quad (46)$$

where ε_1 and ε_2 are the eigenenergies of the lower and upper QW states, respectively, and ε_F is the Fermi energy of the electrons. Above, the Fermi energy was assumed to satisfy $\varepsilon_1<\varepsilon_F<\varepsilon_2$, so only the lower level is occupied in the field unperturbed state. In the usual notation, $-e$, m, and $h=2\pi\hbar$ denote the electron charge and mass, and Planck's constant respectively. By combining Eqs. (45) and (46) it readily appears that the local-field resonance frequency is given by

$$\omega^{\mathrm{res}}_\infty = \left[\omega^2_{\mathrm{B}}+\frac{\beta_\infty}{\omega_{\mathrm{B}}}\right]^{1/2}, \quad (47)$$

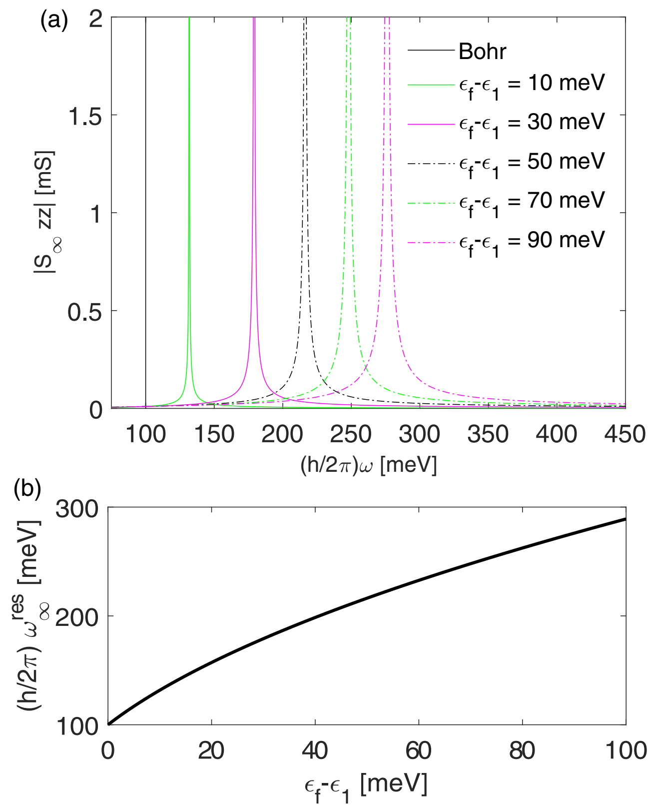

FIG. 2. (a) Frequency dependence of $|S_{\infty,zz}|$. The calculation is for a two-level GaAs quantum-well screen of thickness $d=130$ Å and it is carried out using infinite barrier wave functions. The energy distance between the lower (occupied ε_1) and upper (unoccupied ε_2) quantum state is $\hbar\omega_B=\varepsilon_2-\varepsilon_1=100$ meV. The distance of ε_1 to the Fermi level ε_F is varied from 10 to 90 meV in steps of 20 meV. If we set $\varepsilon_F-\varepsilon_1=50$ meV the resulting conduction electron density per unit area (surface electron density) is $\mathcal{N}^0_\infty = 1.39\times 10^{12}\mathrm{cm}^{-2}$ and we find the local-field resonance at $\hbar\omega^{\mathrm{res}}_\infty\approx 216$ meV. Note that $|S_{\infty,zz}|$ becomes singular at $\hbar\omega^{\mathrm{res}}_\infty$ because no damping has been introduced. The dashed line displays the Bohr energy at $\hbar\omega_B$. The resonance energy in $|S_{\infty,zz}|$ is $\hbar\omega_B$ if self-field effects are neglected. (b) Local-field resonance $\hbar\omega^{\mathrm{res}}_\infty$ for the GaAs quantum-well screen as function of $\varepsilon_F-\varepsilon_1$. Note how the resonance significantly blueshifts as ε_F rises.

with the abbreviation

$$\beta_\infty = \frac{e^2(\varepsilon_F-\varepsilon_1)}{2\pi\varepsilon_0 m\hbar}\int_{\mathrm{QW}}\Phi^2(z)dz. \quad (48)$$

In Fig. 2 we present a numerical calculation of the frequency dependence of the magnitude of the zz component of the causal surface conductivity [Eq. (43)] for a two-level GaAs quantum-well screen.

F. Overview of physical principles

A qualitative account of the key results of Secs. II A–II E is given below and illustrated in schematic form in Fig. 3. For brevity, the references to the field's wave-vector component parallel to the plane of the screen ($\mathbf{q}_\parallel$) and the angular frequency (ω) are left out of the various vector and tensor arguments.

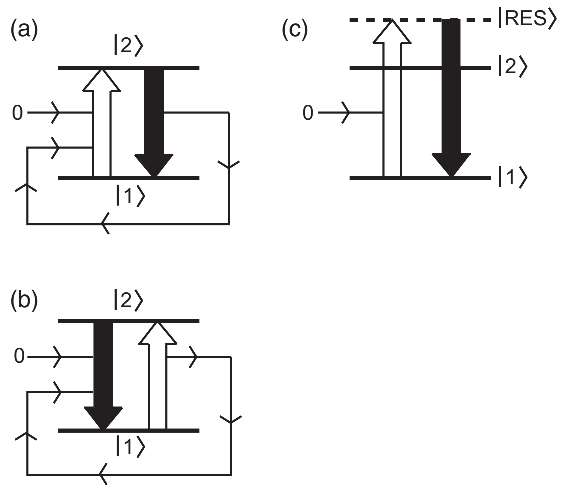

FIG. 3. Schematic diagrams showing the fundamental electron-light interactions entering the calculation of $\boldsymbol{\sigma}_\infty(z, z')$: (a) the RW loop, (b) the ARW loop, and (c) the RW loop for $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z')$. The incident field line is denoted by a zero. Upward electron transitions [$|1\rangle \to |2\rangle$ and $|1\rangle \to |\mathrm{res}\rangle$] are indicated by white arrows and downward transitions [$|2\rangle \to |1\rangle$ and $|\mathrm{res}\rangle \to |1\rangle$] by black arrows.

The field-induced current density in the two-level QW screen can be written in two forms, viz.,

$$\mathbf{J}_\infty(z) = \int_{\mathrm{QW}} \boldsymbol{\sigma}_\infty(z, z') \cdot \mathbf{E}_\infty(z') dz' \tag{49}$$

and

$$\mathbf{J}_\infty(z) = \int_{\mathrm{QW}} \boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z') \cdot \mathbf{E}^0(z') dz'. \tag{50}$$

A quantum-mechanical calculation in the random-phase approximation [19,26–29] gives an expression for the conductivity $\boldsymbol{\sigma}_\infty(z, z')$. From an experimental point of view the external field $\mathbf{E}^0$ is known, not the local field $\mathbf{E}_\infty$. Thus, in order to determine $\mathbf{J}_\infty(z)$ we seek to replace $\boldsymbol{\sigma}_\infty(z, z')$ by the causal conductivity $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z')$. The word causal refers to the fact that $\mathbf{J}_\infty(z)$ is delayed in time with respect to $\mathbf{E}^0(z)$ (in the space-time domain). The relation between $\mathbf{J}_\infty(z)$ and $\mathbf{E}_\infty(z)$ does not satisfy a strict causality criterion. To replace $\boldsymbol{\sigma}_\infty(z, z')$ by $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z')$. a determination of the field-field response tensor $\boldsymbol{\Gamma}_\infty(z, z')$ is needed [cf. Eq. (1)]; $\boldsymbol{\Gamma}_\infty(z, z')$ is calculated in Sec. II B and $\boldsymbol{\sigma}^{\mathrm{CAU}}_\infty(z, z')$ is obtained in Secs. II C–II E in various approximations.

A determination of $\boldsymbol{\sigma}_\infty(z, z')$ requires that a coherent sum of electronic loops between the lower ($|1\rangle$) and upper ($|2\rangle$) states is calculated. Two fundamental types of loops are needed to determine $\boldsymbol{\Gamma}_\infty(z, z')$ (see Fig. 3). Near resonance the so-called rotating-wave (RW) loop [30] dominates [see Fig. 3(a)]: An electron in state $|1\rangle$ is excited (stimulated absorption) to state $|2\rangle$ by the sum of the incident field (denoted by a zero in Fig. 3) and the field emitted in the downward transition ($|2\rangle \to |1\rangle$). Away from the resonance a significant contribution related to the so-called counterrotating-wave (CRW) [30] loop is present [see Fig. 3(b)]: an electron is deexcited from state $|2\rangle$ to $|1\rangle$ by stimulated emission. The field inducing this transition is the sum of the incoming field and the field emitted in the upward ($|1\rangle \to |2\rangle$) transition. In a self-consistent theory both loops are present [30].

In the calculation of $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z')$, only the incident field drives the two loops. The loops now are between the ground state $|1\rangle$ and the so-called resonant state $|\mathrm{res}\rangle$. Here $|\mathrm{res}\rangle$ represents a blueshift of the excited state $|2\rangle$. The blueshift originates in the local-field correction. Figure 3(c) shows the RW loop. We urge the reader to draw the CRW loop for $\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(z, z')$.

III. INTERNAL ELECTRODYNAMICS OF A SCREEN WITH A SMALL HOLE

A. Causal surface conductivity: Partially heuristic approach

An *ab initio* calculation of the causal conductivity tensor $[\boldsymbol{\sigma}^{\mathrm{cau}}_\infty(\mathbf{r}_\parallel, \mathbf{r}'; \omega) \equiv \boldsymbol{\sigma}^{\mathrm{cau}}_\infty(\mathbf{r}_\parallel, \mathbf{r}'_\parallel, z, z'; \omega)]$ for a jellium quantum-well screen with a hole is a formidable (if not impossible) task taking us far beyond the scope of this paper. Let us therefore, in a partially heuristic manner, try to generalize the result given in Eq. (37) for a screen without a hole. This result was achieved by retaining only the self-field part of the vacuum Green's tensor and by using the long-wavelength ($\mathbf{q}_\parallel \to \mathbf{0}$) expression for the conductivity tensor.

A hint of how to make the generalization is obtained by a certain rewriting of the low-temperature ($T \to 0$) expressions for $a_\infty(\omega)$ [Eq. (A28)] and $b_\infty(\omega)$ [Eq. (A11)]. In the $T \to 0$ limit the electron density of a jellium screen with an arbitrary number of bound QW levels is given by

$$n^0_\infty(z; T \to 0) = \frac{m}{\pi\hbar^2} \sum_n (\varepsilon_F - \varepsilon_n)|\psi_n(z)|^2, \quad \varepsilon_n < \varepsilon_F, \tag{51}$$

where $\psi_n(z)$ is the normalized wave function of energy eigenstate number n. As indicated, the summation only runs over occupied stats ($\varepsilon_n < \varepsilon_F$). For our two-level system (with $\varepsilon_1 < \varepsilon_F < \varepsilon_2$) we get

$$n^0_\infty(z; T \to 0) = \frac{m}{\pi\hbar^2}(\varepsilon_F - \varepsilon_1)|\psi_1(z)|^2 \tag{52}$$

and hence a related surface electron density

$$\mathcal{N}^0_\infty = \int_{\mathrm{QW}} n^0_\infty(z; T \to 0) dz = \frac{m}{\pi\hbar^2}(\varepsilon_F - \varepsilon_1). \tag{53}$$

The result in Eq. (53) allows one to rewrite the expressions for $a_\infty(\omega)$ [Eq. (A28)] and $b_\infty(\omega)$ [Eq. (A11)] as follows:

$$a_\infty(\omega) = \pi i\omega \left(\frac{e\hbar^2}{m}\right)^2 \frac{1}{(\hbar\omega)^2 - (\varepsilon_2 - \varepsilon_1)^2} \frac{\left(\mathcal{N}^0_\infty\right)^2}{\varepsilon_2 - \varepsilon_1} \tag{54}$$

and

$$b_\infty(\omega) = \frac{i\omega}{2} \left(\frac{e\hbar^2}{m}\right)^2 \frac{1}{(\hbar\omega)^2 - (\varepsilon_2 - \varepsilon_1)^2} \frac{\mathcal{N}^0_\infty}{\varepsilon_2 - \varepsilon_1}. \tag{55}$$

Our alternative formula for $b_\infty(\omega)$ and $a_\infty(\omega)$ contain the position ($\mathbf{r}_\parallel$) -independent surface electron density (and its square) as factors.

For a screen with a hole we heuristically replace $\mathcal{N}^0_\infty$ by the corresponding position-dependent surface electron density $\mathcal{N}^0(\mathbf{r}_\parallel)$. This quantity, which depends on $\mathbf{r}_\parallel$ in the vicinity of the hole, was studied (calculated) on the basis of a two-dimensional microscopic extinction-theorem approach in Ref. [17]. Our generalized expressions for $a(\mathbf{r}_\parallel;\omega)$ and $b(\mathbf{r}_\parallel;\omega)$ thus are given by

$$a(\mathbf{r}_\parallel;\omega) = \pi i\omega\left(\frac{e\hbar^2}{m}\right)^2 \frac{1}{(\hbar\omega)^2-(\varepsilon_2-\varepsilon_1)^2}\frac{[\mathcal{N}^0(\mathbf{r}_\parallel)]^2}{\varepsilon_2-\varepsilon_1} \quad (56)$$

and

$$b(\mathbf{r}_\parallel;\omega) = \frac{i\omega}{2}\left(\frac{e\hbar^2}{m}\right)^2 \frac{1}{(\hbar\omega)^2-(\varepsilon_2-\varepsilon_1)^2}\frac{\mathcal{N}^0(\mathbf{r}_\parallel)}{\varepsilon_2-\varepsilon_1}. \quad (57)$$

Hence, for a two-level QW screen with a hole we suggest to apply the expression for the causal conductivity tensor

$$\boldsymbol{\sigma}^{\text{cau}}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel,z,z';\omega) = \delta(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)\tilde{\boldsymbol{\sigma}}^{\text{cau}}(\mathbf{r}_\parallel,z,z';\omega), \quad (58)$$

where

$$\tilde{\boldsymbol{\sigma}}^{\text{cau}}(\mathbf{r}_\parallel,z,z';\omega) = a(\mathbf{r}_\parallel;\omega)(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z)\phi(z') + \frac{b(\mathbf{r}_\parallel;\omega)}{1-\frac{b(\mathbf{r}_\parallel;\omega)}{i\varepsilon_0\omega}\int_{\text{QW}}\Phi^2(z)dz}\hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z)\Phi(z'). \quad (59)$$

B. Effective aperture current density

In the framework of linear microscopic theory the screen current density is given by

$$\mathbf{J}(\mathbf{r}_\parallel,z;\omega) = \int_{\text{QW}}\int_{-\infty}^{\infty}\boldsymbol{\sigma}^{\text{cau}}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel,z,z';\omega) \cdot\mathbf{E}^0(\mathbf{r}'_\parallel,z';\omega)d^2r'_\parallel dz' \quad (60)$$

in the most general situation. However, in our heuristic approach the connection between $\mathbf{J}$ and $\mathbf{E}^0$ is spatially local in the coordinate parallel to the plane of the screen [see Eq. (58)]. The screen thus appears as an inhomogeneous medium in these coordinates with a constitutive equation of the form

$$\mathbf{J}(\mathbf{r}_\parallel,z;\omega) = \int_{\text{QW}}\tilde{\boldsymbol{\sigma}}^{\text{cau}}(\mathbf{r}_\parallel,z,z';\omega)\cdot\mathbf{E}^0(\mathbf{r}_\parallel,z';\omega)dz'. \quad (61)$$

The causal conductivity tensor $\boldsymbol{\sigma}^{\text{cau}}(\mathbf{r},\mathbf{r}';\omega)$ consists of para- and diamagnetic parts. The diamagnetic part is spatially local in the $\mathbf{r}_\parallel$ ($\mathbf{r}'_\parallel$) coordinates and a function of the surface electron density $\mathcal{N}^0(\mathbf{r}_\parallel)$ [cf. Eqs. (56), (57), and (59)]. The paramagnetic part always is spatially nonlocal in form and in the heuristic approach it is this part which we treat in an approximate sense. In frequency regions where the diamagnetic response is the dominating one we expect the expression given for $\tilde{\boldsymbol{\sigma}}^{\text{cau}}(\mathbf{r}_\parallel,z,z';\omega)$ in Eq. (59) to be quite accurate. The local structure of the diamagnetic response in the z (z') coordinate is broken due to the fact that only two energy levels are taken into account in the z dynamics of the electrons.

Based on general considerations [16], it turns out to be useful to introduce the so-called effective aperture $\mathcal{A}$ current density

$$\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\parallel,z;\omega) \equiv \mathbf{J}(\mathbf{r}_\parallel,z;\omega) - \mathbf{J}_\infty(\mathbf{r}_\parallel,z;\omega), \quad (62)$$

defined as the difference between the current densities of identical screens with and without a hole. By identical we mean that, apart for the electronic disturbance caused by the hole, the optical properties of the screens are exactly alike. It is further assumed that the incident electromagnetic field giving rise to the current densities is the same in the two cases.

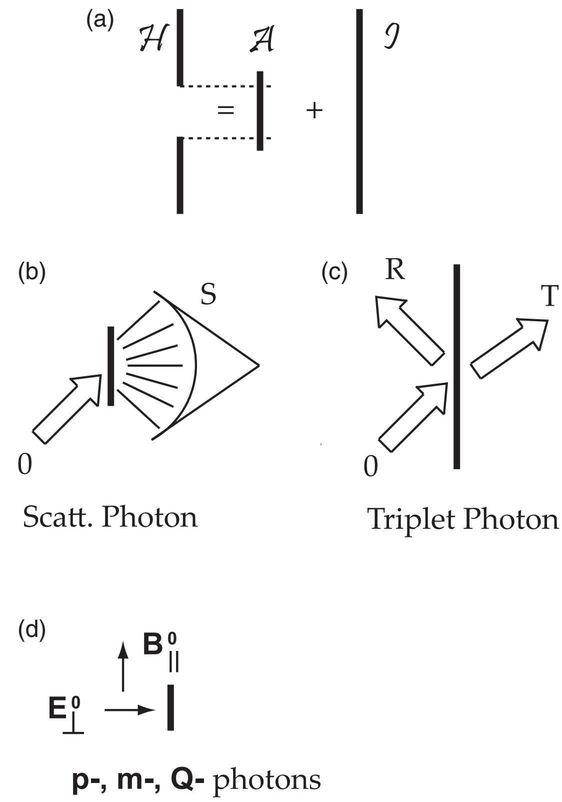

FIG. 4. Schematic illustrations of (a) the division of the current density of a screen with a hole ($\mathcal{H}$) into infinite screen ($\mathcal{I}$) and effective aperture ($\mathcal{A}$) parts, (b) the multipole aperture scattering, and (c) the triplet photon scattering. (d) It is indicated that the $\mathbf{p}(\mathbf{E}^0_\perp)$, $\mathbf{m}(\mathbf{E}^0_\perp,\mathbf{B}^0_\parallel)$, and $\mathbf{Q}(\mathbf{E}^0_\perp,\mathbf{B}^0_\parallel)$ moments are induced by the components of the incoming electric field perpendicular to the two-level QW ($\mathbf{E}^0_\perp$) and the magnetic field parallel to the screen ($\mathbf{B}^0_\parallel$).

It is obvious that the constitutive equation relating $\mathbf{J}^{\mathcal{A}}$ to $\mathbf{E}^0$ is given by

$$\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\parallel,z;\omega) = \int_{\text{QW}}\boldsymbol{\Delta}(\mathbf{r}_\parallel,z,z';\omega)\cdot\mathbf{E}^0(\mathbf{r}_\parallel,z';\omega)dz', \quad (63)$$

where

$$\boldsymbol{\Delta}(\mathbf{r}_\parallel,z,z';\omega) = [a(\mathbf{r}_\parallel;\omega)-a_\infty(\omega)](\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\phi(z)\phi(z') + [\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]\hat{\mathbf{z}}\hat{\mathbf{z}}\Phi(z)\Phi(z'), \quad (64)$$

with the abbreviation

$$\tilde{b}(\mathbf{r}_\parallel;\omega) = \frac{b(\mathbf{r}_\parallel;\omega)}{1-\frac{b(\mathbf{r}_\parallel;\omega)}{i\varepsilon_0\omega}\int_{\text{QW}}\Phi^2(z)dz} \quad (65)$$

and an analogous one for $\tilde{b}_\infty(\omega)$, obtained by the replacement $b(\mathbf{r}_\parallel;\omega)\Rightarrow b_\infty(\omega)$ in Eq. (65).

The qualitative idea behind the calculations (Secs. III A and III B) of the current density $\mathbf{J}(z)$ inside a two-level QW with a hole $\mathcal{H}$ is presented in schematic form in Fig. 4. The field-unperturbed surface electron density $\mathcal{N}^0(\mathbf{r}_\parallel)$ varies in the vicinity of the hole, and this fact makes a direct calculation of the diffraction pattern difficult. The $\mathcal{H}$ current density is divided into a sum of contributions from a screen without a hole $\mathcal{I}$ and a so-called effective aperture $\mathcal{A}$. The $\mathcal{I}$ surface electron density $\mathcal{N}_\infty^0$ is constant across the screen, whereas the $\mathcal{A}$ surface electron density various across $\mathcal{A}$. As indicated in Fig. 4(a), the $\mathcal{A}$ area is larger than the geometrical size of the hole in general. This fact is associated with two physical effects: (i) the finite penetration depth of the field in matter and (ii) a quantum electronic density variation near a vacuum-matter interface. In a photon formulation the amplitude scattering from $\mathcal{I}$ [incident (0), reflected (R), and transmitted (T) field] may be described as consisting of triplet photons [31] [Figs. 4(b) and 4(c)]. If the hole is sufficiently small, it is useful to expand the incident field induced $\mathcal{A}$ current density in a multipole series. The first three terms relate to electric dipole (**p**), magnetic dipole (**m**), and electric quadropole (**Q**) moments of the $\mathcal{A}$ current density; **p**, **m**, and **Q** and the scattered fields from these moments are calculated in Secs. III C–III E, and IV A–IV C. The key results, relating **p**, **m**, and **Q** to the components of the incoming electric and magnetic fields, are discussed in Sec. V. Readers not interested in the detailed calculations may skip Secs. III C–III E and IV A–IV C (in a first reading of the paper).

C. Multipole expansion of aperture electrodynamics

Since the characteristic wavelength of the incident electromagnetic fields, which are of interest in this work, always are assumed to be much larger that the thickness of the QW screen, it is possible to treat the internal screen (aperture) electrodynamics on the basis of a multipole expansion scheme. Below we will concentrate on the two lowest-order terms in the scheme.

Let us start by dividing the aperture current density into its components parallel ($\|$) and perpendicular ($\perp$) to the plane of the screen, i.e.,

$$\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) = \mathbf{J}_\|^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) + \mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) \tag{66}$$

in the space-frequency domain. From Eqs. (63) and (64) we readily get the explicit expressions

$$\mathbf{J}_\|^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) = [a(\mathbf{r}_\|;\omega) - a_\infty(\omega)]\phi(z) \times \int_{\mathrm{QW}} \phi(z')\mathbf{E}_\|^0(\mathbf{r}_\|, z';\omega)dz' \tag{67}$$

and

$$\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) = [\tilde{b}(\mathbf{r}_\|;\omega) - \tilde{b}_\infty(\omega)]\Phi(z) \times \int_{\mathrm{QW}} \Phi(z')\mathbf{E}_\perp^0(\mathbf{r}_\|, z';\omega)dz', \tag{68}$$

where $\mathbf{E}_\|^0 = (\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\cdot\mathbf{E}^0$ and $\mathbf{E}_\perp^0 = \hat{\mathbf{z}}\hat{\mathbf{z}}\cdot\mathbf{E}^0$.

Next we employ a moment expansion of the aperture current density in the z coordinate, i.e.,

$$\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\|, z;\omega) = \delta(z)\int_{\mathrm{QW}} \mathbf{J}^{\mathcal{A}}(\mathbf{r}_\|, z;\omega)dz - \frac{d\delta(z)}{dz}\int_{\mathrm{QW}} z\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\|, z;\omega)dz + \cdots, \tag{69}$$

and a Taylor series expansion (in z) of the incident electric field, viz.,

$$\mathbf{E}^0(\mathbf{r}_\|, z;\omega) = \mathbf{E}^0(\mathbf{r}_\|, 0;\omega) + z\frac{\partial\mathbf{E}^0}{\partial z}(\mathbf{r}_\|, 0;\omega) + \cdots. \tag{70}$$

By inserting Eqs. (69) and (70) into Eqs. (67) and (68) and making use of the orthogonality of the two QW states [Eq. (42)]

$$\int_{\mathrm{QW}} \phi(z)dz = 0 \tag{71}$$

and their opposite parity

$$\int_{\mathrm{QW}} z\Phi(z)dz = 0, \tag{72}$$

one obtains the following result correct to second order:

$$\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r}_\|, z;\omega|\mathrm{ED}) = \delta(z)[\tilde{b}(\mathbf{r}_\|;\omega) - \tilde{b}_\infty(\mathbf{r}_\|;\omega)] \times \left[\int_{\mathrm{QW}} \Phi(z)dz\right]^2 \mathbf{E}_\perp^0(\mathbf{r}_\|, 0;\omega) \tag{73}$$

and

$$\mathbf{J}_\|^{\mathcal{A}}(\mathbf{r}_\|, z;\omega|\mathrm{EQ\text{-}MD}) = -\frac{d\delta(z)}{dz}[a(\mathbf{r}_\|;\omega) - a_\infty(\mathbf{r}_\|;\omega)] \times \left[\int_{\mathrm{QW}} z\phi(z)dz\right]^2 \frac{\partial\mathbf{E}_\|^0}{\partial z}(\mathbf{r}_\|, 0;\omega). \tag{74}$$

The expression given in Eq. (73) reflects the fact that the component of the aperture current density perpendicular to the plane of the QW screen ($\mathbf{J}_\perp^{\mathcal{A}}$) relates to an approximation where the effective aperture is both an ED absorber and radiator [16]. In $\mathbf{J}_\perp^{\mathcal{A}}$ there is no term where the aperture behaves like an EQ plus MD in both absorption and radiation. Furthermore, mixed terms corresponding to an ED (absorption) and an EQ plus MD (radiation), or an EQ plus MD (absorption) and ED (radiation) do not exist. As the readers may prove to themselves, such terms vanish because of the orthogonality [Eq. (71)] and opposite parity [Eq. (72)] of the two neighboring QW levels. Mixed terms also are absent in the aperture current density's component along the plane of the screen ($\mathbf{J}_\|^{\mathcal{A}}$). The lowest-order terms in $\mathbf{J}_\|^{\mathcal{A}}$ is of the EQ plus MD type [Eq. (74)]. We have thus reached the conclusion that the effective aperture current density to second order in a multipole expansion consists of an ED current density perpendicular to the plane of the screen plus an EQ-MD current density parallel to this plane. As required, $\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r}_\|, z;\omega|\mathrm{ED})$ and $\mathbf{J}_\|^{\mathcal{A}}(\mathbf{r}_\|, z;\omega|\mathrm{EQ\text{-}MD})$ are proportional to $\mathbf{E}_\perp^0(\mathbf{r}_\|, 0;\omega)$ and $\mathbf{E}_\|^0(\mathbf{r}_\|, 0;\omega)$, respectively.

It follows from the analysis in Appendix B that the integrals appearing in Eqs. (73) and (74) satisfy the relation

$$\int_{\mathrm{QW}} \Phi(z)dz = \frac{2m}{\hbar^2}(\varepsilon_1 - \varepsilon_2)\int_{\mathrm{QW}} z\phi(z)dz. \tag{75}$$

We already know that the electrodynamics related to the electron motion perpendicular to the plane of the screen is subjected to a local-field correction. Within the framework of the self-field approximation, where the zz component of the space-dependent local-field factor for a screen with a hole is given by

$$L_{zz}^{\mathrm{SF}}(\mathbf{r}_\parallel;\omega)=\left[1-\frac{b(\mathbf{r}_\parallel;\omega)}{i\varepsilon_0\omega}\int_{\mathrm{QW}}\Phi^2(z)dz\right]^{-1} \quad (76)$$

and the right-hand side of Eq. (36) equals the zz component of the space-independent local-field factor for a screen without a hole $[L_{\infty,zz}^{\mathrm{SF}}(\omega)]$, it is readily shown that

$$\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)=L_{\infty,zz}^{\mathrm{SF}}(\omega)L_{zz}^{\mathrm{SF}}(\mathbf{r}_\parallel,\omega)[b(\mathbf{r}_\parallel;\omega)-b_\infty(\omega)]. \quad (77)$$

The role of the local-field correction appears in explicit form in Eq. (77).

In the general multipole formalism the second-rank tensor $\int_{-\infty}^{\infty}\mathbf{J}(\mathbf{r})\mathbf{r}\,d^3r$ relates to the sum of electric quadrupole and magnetic dipole dynamics, and the symmetric $[\frac{1}{2}\int_{-\infty}^{\infty}(\mathbf{Jr}+\mathbf{rJ})d^3r]$ and antisymmetric $[\frac{1}{2}\int_{-\infty}^{\infty}(\mathbf{Jr}-\mathbf{rJ})d^3r]$ parts relate to the EQ and MD dynamics, respectively. Hence, it is reasonable to characterize the QW dynamics proportional to $\int_{\mathrm{QW}}z\mathbf{J}^{\mathcal{A}}(\mathbf{r}_\parallel,z;\omega)dz$ [Eq. (69)], as EQ-MD dynamics (the z dynamics is described via the terms in the third column of $\mathbf{Jr}$ integrated over z).

Since

$$b(\mathbf{r}_\parallel;\omega)-b_\infty(\omega)\propto\mathcal{N}^0(\mathbf{r}_\parallel)-\mathcal{N}^0_\infty, \quad (78)$$

it is the difference between the electron surface density for screens with and without a hole which in the present (approximate) approach determines the size of the effective aperture for the dynamics perpendicular to the plane of the screen. Because

$$\begin{aligned}a(\mathbf{r}_\parallel;\omega)-a_\infty(\omega)&\propto[\mathcal{N}^0(\mathbf{r}_\parallel)]^2-\left(\mathcal{N}^0_\infty\right)^2\\&=\left[\mathcal{N}^0(\mathbf{r}_\parallel)-\mathcal{N}^0_\infty\right]\left[\mathcal{N}^0(\mathbf{r}_\parallel)+\mathcal{N}^0_\infty\right],\end{aligned} \quad (79)$$

the effective aperture related to the in-plane dynamics essentially is the same. This result, which need not hold in general, is a consequence of our heuristic replacement $\mathcal{N}^0_\infty\to\mathcal{N}^0(\mathbf{r}_\parallel)$.

D. Magnetic dipole moment

Although we have classified part of the scattering from the effective optical aperture as magnetic dipole scattering, we have not yet given an explicit expression for the magnetic dipole moment of the hole. In order to calculate this moment we use the fact that the antisymmetric second-rank tensor $\mathbf{J}^{\mathcal{A}}_{\mathrm{MD}}(\omega)$, given in Eq. (C3), can be written in the dyadic cross-product form [19]

$$\mathbf{J}^{\mathcal{A}}_{\mathrm{MD}}(\omega)=\mathbf{U}\times\mathbf{m}(\omega), \quad (80)$$

where

$$\mathbf{m}(\omega)=\frac{1}{2}\int_{-\infty}^{\infty}\mathbf{r}\times\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)d^3r \quad (81)$$

is the sought-for magnetic dipole moment of the optical aperture. From the rewriting

$$\begin{aligned}\mathbf{m}(\omega)&=\frac{1}{2}\int_{-\infty}^{\infty}\mathbf{r}\times[\mathbf{J}^{\mathcal{A}}_\parallel(\mathbf{r};\omega)+\mathbf{J}^{\mathcal{A}}_\perp(\mathbf{r};\omega)]d^3r\\&=\frac{1}{2}\int_{-\infty}^{\infty}(x\hat{\mathbf{x}}+y\hat{\mathbf{y}}+z\hat{\mathbf{z}})\times\left(J^{\mathcal{A}}_{\parallel,x}\hat{\mathbf{x}}+J^{\mathcal{A}}_{\parallel,y}\hat{\mathbf{y}}+J^{\mathcal{A}}_{\perp,z}\hat{\mathbf{z}}\right)d^3r,\end{aligned} \quad (82)$$

use of Eqs. (67), (68), (71), and (72) leads to the expression

$$\mathbf{m}(\omega)=\frac{1}{2}\int_{-\infty}^{\infty}\left[z\left(J^{\mathcal{A}}_{\parallel,x}\hat{\mathbf{y}}-J^{\mathcal{A}}_{\parallel,y}\hat{\mathbf{x}}\right)+J^{\mathcal{A}}_\perp(y\hat{\mathbf{x}}-x\hat{\mathbf{y}})\right]d^3r \quad (83)$$

or in compact form

$$\mathbf{m}(\omega)=\frac{1}{2}\int_{-\infty}^{\infty}\hat{\mathbf{z}}\times[z\mathbf{J}^{\mathcal{A}}_\parallel(\mathbf{r};\omega)-\mathbf{r}_\parallel J^{\mathcal{A}}_\perp(\mathbf{r};\omega)]d^3r. \quad (84)$$

It appears from Eq. (84) that the magnetic dipole moment of the aperture lies in the plane of the screen.

In the small-hole limit, where Eqs. (67) and (68), via a Taylor expansion of $\mathbf{E}^0(\mathbf{r}_\parallel,z;\omega)$ in z, give

$$\begin{aligned}\mathbf{J}^{\mathcal{A}}_\parallel(\mathbf{r};\omega)&=[a(\mathbf{r}_\parallel;\omega)-a_\infty(\omega)]\phi(z)\\&\quad\times\left[\int_{\mathrm{QW}}z\phi(z)dz\right]\frac{\partial\mathbf{E}^0_\parallel}{\partial z}(\mathbf{0};\omega)\end{aligned} \quad (85)$$

and

$$\begin{aligned}\mathbf{J}^{\mathcal{A}}_\perp(\mathbf{r};\omega)&=[\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]\Phi(z)\\&\quad\times\left[\int_{\mathrm{QW}}\Phi(z)dz\right]\mathbf{E}^0_\perp(\mathbf{0};\omega),\end{aligned} \quad (86)$$

the magnetic dipole moment takes the explicit form

$$\begin{aligned}\mathbf{m}(\omega)&=\frac{1}{2}\left[\int_{\mathrm{QW}}z\phi(z)dz\right]^2\int_{-\infty}^{\infty}[a(\mathbf{r}_\parallel;\omega)-a_\infty(\omega)]d^2r_\parallel\hat{\mathbf{z}}\\&\quad\times\frac{\partial\mathbf{E}^0_\parallel}{\partial z}(\mathbf{0};\omega)+\frac{1}{2}\left[\int_{\mathrm{QW}}\Phi(z)dz\right]^2\\&\quad\times\int_{-\infty}^{\infty}[\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]\mathbf{r}_\parallel d^2r_\parallel\times\mathbf{E}^0_\perp(\mathbf{0};\omega).\end{aligned} \quad (87)$$

In the small-hole limit, where $\partial\mathbf{E}^0_\parallel/\partial x=\partial\mathbf{E}^0_\parallel/\partial y=\mathbf{0}$ across the effective aperture, it follows from the Maxwell equation $\nabla\times\mathbf{E}^0=i\omega\mathbf{B}^0$ that the incoming magnetic field in the hole is parallel to the plane of the screen and given by

$$\mathbf{B}^0(\mathbf{0};\omega)[=\mathbf{B}^0_\parallel(\mathbf{0};\omega)]=\frac{1}{i\omega}\hat{\mathbf{z}}\times\frac{\partial\mathbf{E}^0_\parallel}{\partial z}(\mathbf{0};\omega). \quad (88)$$

Using this relation, Eq. (87) may be written in the elegant form

$$\mathbf{m}(\omega)=\boldsymbol{\beta}_{\mathbf{B}}(\omega)\cdot\mathbf{B}^0(\mathbf{0};\omega)+\boldsymbol{\beta}_{\mathbf{E}}(\omega)\cdot\mathbf{E}^0(\mathbf{0};\omega), \quad (89)$$

where

$$\begin{aligned}\boldsymbol{\beta}_{\mathbf{B}}(\omega)&=\frac{i\omega}{2}\left[\int_{\mathrm{QW}}z\phi(z)dz\right]^2\\&\quad\times\int_{\mathcal{A}}[a(\mathbf{r}_\parallel;\omega)-a_\infty(\omega)]d^2r_\parallel(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\end{aligned} \quad (90)$$

and

$$\begin{aligned}\boldsymbol{\beta}_{\mathbf{E}}(\omega)&=\frac{1}{2}\left[\int_{\mathrm{QW}}\Phi(z)dz\right]^2\\&\quad\times\int_{\mathcal{A}}[\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]\mathbf{r}_\parallel d^2r_\parallel\times\hat{\mathbf{z}}\hat{\mathbf{z}}.\end{aligned} \quad (91)$$

It appears from Eq. (89) that the induced magnetic dipole moment of the effective aperture in the small-hole limit in general must be characterized by two frequency-dependent

MD-polarizability tensors, viz., $\boldsymbol{\beta}_{\mathbf{B}}(\omega)$ and $\boldsymbol{\beta}_{\mathbf{E}}(\omega)$. The tensorial forms of these quantities reflect the fact that only the components of the incoming magnetic and electric fields, respectively parallel ($\mathbf{B}_{\parallel}^{0}$) and perpendicular ($\mathbf{E}_{\perp}^{0}$) to the plane of the screen, enter the formula for $\mathbf{m}(\omega)$.

Local-field resonance enhancement may appear in $\boldsymbol{\beta}_{\mathbf{E}}(\omega)$ and this can be discussed along the same lines as the corresponding tensors in the ED polarizability, which will be discussed in Sec. IV B. For certain geometrical aperture forms it may happen that only one of the two MD-polarizability tensors is nonvanishing. For a circular hole, for instance, where $a(\mathbf{r}_{\parallel};\omega)=a(|\mathbf{r}_{\parallel}|;\omega)$ and $b(\mathbf{r}_{\parallel};\omega)=b(|\mathbf{r}_{\parallel}|;\omega)$ [and thus also $\tilde{b}(\mathbf{r}_{\parallel};\omega)=\tilde{b}(|\mathbf{r}_{\parallel}|;\omega)$], it is clear that $\boldsymbol{\beta}_{\mathbf{E}}(\omega)=\mathbf{0}$ (the integral over $\mathcal{A}$ is zero since the integrand is uneven in x and y). In this particular case no local-field resonance effects can appear.

Finally, it should be noted that if the component of the electronic current density perpendicular to the plane of the screen is neglected [$\mathbf{J}_{\perp}^{\mathcal{A}}(\mathbf{r};\omega)=\mathbf{0}$], as it has been in many previous macroscopic studies, the induced magnetic dipole moment is proportional to $\mathbf{B}^{0}$ alone, i.e.,

$$\mathbf{m}(\omega)=\boldsymbol{\beta}_{B}(\omega)\cdot\mathbf{B}^{0}(\mathbf{0};\omega). \tag{92}$$

In such macroscopic models the diffraction from a small hole can be considered as caused by the combined effect of an electric dipole and a magnetic dipole. The reader may wonder why no electric quadrupole radiation is present in these models. However, a comparison of Eqs. (C16) and (C17) shows that $\mathbf{E}_{\mathrm{EQ}}^{\mathcal{A}}(\mathbf{r};\omega)=\mathbf{E}_{\mathrm{MD}}^{\mathcal{A}}(\mathbf{r};\omega)$ if one sets $\mathbf{J}_{\perp}^{\mathcal{A}}(\mathbf{r};\omega)=\mathbf{0}$. Therefore, one may take $\mathbf{E}_{\mathrm{EQ}}^{\mathcal{A}}+\mathbf{E}_{\mathrm{MD}}^{\mathcal{A}}=2\mathbf{E}_{\mathrm{MD}}^{\mathcal{A}}$ and hence consider the combined EQ-MD radiators alone as a magnetic dipole radiator.

E. Electric quadrupole moment

It is known that the first-order tensorial moment $\mathbf{J}^{\mathcal{A}}(t|\text{EQ-MD})=\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}(\mathbf{r},t)\mathbf{r}\,d^{3}r$ of the aperture current density distribution $\mathbf{J}^{\mathcal{A}}(\mathbf{r},t)$, when divided into symmetric and antisymmetric parts, may be written as [19]

$$\mathbf{J}^{\mathcal{A}}(t|\text{EQ-MD})=\frac{d}{dt}\mathbf{Q}(t)+\mathbf{U}\times\mathbf{m}(t), \tag{93}$$

where $\mathbf{Q}(t)$ is the symmetric quadrupole moment tensor, given in the frequency domain by

$$\mathbf{Q}(\omega)\equiv\frac{i}{\omega}\mathbf{J}_{EQ}^{\mathcal{A}}(\omega)=\frac{i}{2\omega}\int_{-\infty}^{\infty}[\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}+\mathbf{r}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)]d^{3}r. \tag{94}$$

The tensor $\mathbf{J}_{EQ}^{\mathcal{A}}(\omega)$ is calculated in Appendix C. When the general result [Eq. (C8)] is taken in the small-hole limit and Eq. (88) is used to eliminate $\partial\mathbf{E}_{\parallel}^{0}(\mathbf{0};\omega)/dz$ in favor of $\mathbf{B}_{\parallel}^{0}$ ($\partial\mathbf{E}_{\parallel}^{0}/\partial z=-i\omega\hat{\mathbf{z}}\times\mathbf{B}_{\parallel}^{0}$), one obtains the dyadic expression for the quadrupole moment tensor

$$\mathbf{Q}(\omega)=\boldsymbol{\mu}(\omega)\mathbf{E}_{\perp}^{0}(\mathbf{0};\omega)+\eta(\omega)\hat{\mathbf{z}}\hat{\mathbf{z}}\times\mathbf{B}_{\parallel}^{0}(\mathbf{0};\omega)+\mathbf{T}, \tag{95}$$

where $\mathbf{T}$ is the transpose of the sum of the first two terms. The scalar

$$\eta(\omega)=\frac{1}{2}\left[\int_{\mathrm{QW}}z\phi(z)dz\right]^{2}\int_{\mathcal{A}}[a(\mathbf{r}_{\parallel};\omega)-a_{\infty}(\omega)]d^{2}r_{\parallel} \tag{96}$$

and the vector

$$\boldsymbol{\mu}(\omega)=\frac{i}{2\omega}\left[\int_{\mathrm{QW}}\Phi(z)dz\right]^{2}\int_{\mathcal{A}}[\tilde{b}(\mathbf{r}_{\parallel};\omega)-\tilde{b}_{\infty}(\omega)]\mathbf{r}_{\parallel}d^{2}r_{\parallel} \tag{97}$$

relate to the light-induced electron dynamics of the effective aperture parallel and perpendicular to the plane of the screen, respectively. A comparison of Eqs. (96) and (97) to Eqs. (89)–(91) shows that the magnetic moment may be written in the alternative form

$$\mathbf{m}(\omega)=i\omega[\eta(\omega)\mathbf{B}_{\parallel}^{0}(\mathbf{0};\omega)-\boldsymbol{\mu}(\omega)\times\mathbf{E}_{\perp}^{0}(\mathbf{0};\omega)]. \tag{98}$$

In Sec. V we discuss the results obtained in Eqs. (95) and (98).

IV. SCATTERING FROM A SMALL HOLE

A. Aperture field: ED and EQ-MD contributions

The effective optical aperture field

$$\mathbf{E}^{\mathcal{A}}(\mathbf{r};\omega)\equiv\mathbf{E}(\mathbf{r},\omega)-\mathbf{E}_{\infty}(\mathbf{r};\omega), \tag{99}$$

which is associated with the difference between the electric fields scattered from identical screens with and without a hole by the same incident field, may be conceived as a field radiated by the effective aperture current density. Hence

$$\mathbf{E}^{\mathcal{A}}(\mathbf{r};\omega)=i\mu_{0}\omega\int_{\mathcal{A}}\mathbf{G}(\mathbf{r}-\mathbf{r}';\omega)\cdot\mathbf{J}^{\mathcal{A}}(\mathbf{r}';\omega)d^{3}r', \tag{100}$$

in general. On the basis of the second-order approximations given in Eqs. (73) and (74) for the two parts of $\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)$ [Eq. (66)], we have

$$\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)=\delta(z)\mathbf{I}_{\perp}^{\mathcal{A}}(\mathbf{r}_{\parallel};\omega)-\frac{d\delta(z)}{dz}\mathbf{I}_{\parallel}^{\mathcal{A}}(\mathbf{r}_{\parallel};\omega), \tag{101}$$

where

$$\mathbf{I}_{\perp}^{\mathcal{A}}(\mathbf{r}_{\parallel};\omega)=[\tilde{b}(\mathbf{r}_{\parallel};\omega)-\tilde{b}_{\infty}(\mathbf{r}_{\parallel};\omega)]\times\left[\int_{\mathrm{QW}}\Phi(z)dz\right]^{2}\mathbf{E}_{\perp}^{0}(\mathbf{r}_{\parallel},z=0;\omega) \tag{102}$$

and

$$\mathbf{I}_{\parallel}^{\mathcal{A}}(\mathbf{r}_{\parallel};\omega)=[a(\mathbf{r}_{\parallel};\omega)-a_{\infty}(\mathbf{r}_{\parallel};\omega)]\left[\int_{\mathrm{QW}}z\phi(z)dz\right]^{2}\times\frac{\partial\mathbf{E}_{\parallel}^{0}}{\partial z}(\mathbf{r}_{\parallel},z=0;\omega). \tag{103}$$

The effective aperture field stemming from the current density distribution in Eq. (100) thus is the sum of two parts, i.e.,

$$\mathbf{E}^{\mathcal{A}}(\mathbf{r};\omega)=\mathbf{E}_{\mathrm{ED}}^{\mathcal{A}}(\mathbf{r};\omega)+\mathbf{E}_{\text{EQ-MD}}^{\mathcal{A}}(\mathbf{r};\omega). \tag{104}$$

The first, so-called ED part is given by

$$\mathbf{E}_{\mathrm{ED}}^{\mathcal{A}}(\mathbf{r};\omega)=i\mu_{0}\omega\int_{\mathcal{A}}\mathbf{G}(\mathbf{r}_{\parallel}-\mathbf{r}_{\parallel}',z;\omega)\cdot\mathbf{I}_{\perp}^{\mathcal{A}}(\mathbf{r}_{\parallel}';\omega)d^{2}r_{\parallel}',\quad z\neq0. \tag{105}$$

The second, named the EQ-MD part,

$$\mathbf{E}_{\text{EQ-MD}}^{\mathcal{A}}(\mathbf{r};\omega)=i\mu_{0}\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r}_{\parallel}-\mathbf{r}_{\parallel}',z-z';\omega)\left(-\frac{d\delta(z')}{dz'}\right)\cdot\mathbf{I}_{\parallel}^{\mathcal{A}}(\mathbf{r}_{\parallel}';\omega)dz'd^{2}r_{\parallel}',\quad z\neq0, \tag{106}$$

can be rewritten in a simplified form by carrying out first a partial integration (in z') and then making use of the fact that

$$\frac{\partial}{\partial z'}\mathbf{G}(\mathbf{r}-\mathbf{r}';\omega) = -\frac{\partial}{\partial z}\mathbf{G}(\mathbf{r}-\mathbf{r}';\omega). \tag{107}$$

Hence, one obtains

$$\mathbf{E}^{\mathcal{A}}_{\text{EQ-MD}}(\mathbf{r};\omega) = -i\mu_0\omega\int_{\mathcal{A}}\frac{\partial}{\partial z}\mathbf{G}(\mathbf{r}_\parallel-\mathbf{r}'_\parallel, z;\omega)\cdot\mathbf{I}^{\mathcal{A}}_\parallel(\mathbf{r}'_\parallel;\omega)d^2r'_\parallel,\quad z\neq 0. \tag{108}$$

B. Electric dipole hole

If the size (linear extension) of the effective optical aperture is sufficiently small, the variations of the Green's tensor and the incident electric field across $\mathcal{A}$ may be neglected and the effective aperture then behaves as an electric dipole absorber and radiator source with respect to the coordinates parallel to the plane of the screen. For such a sheet source it is physically meaningful only to consider the field outside the sheet (the field diverges everywhere in the $z = 0$ plane), as indicated on the right-hand sides of Eqs. (105) and (108).

In the small-hole limit, where, as mentioned,

$$\mathbf{G}(\mathbf{r}_\parallel-\mathbf{r}'_\parallel, z;\omega) = \mathbf{G}(\mathbf{r}_\parallel, z;\omega) \tag{109}$$

[$=\mathbf{G}(\mathbf{r};\omega)$] and

$$\mathbf{E}(\mathbf{r}_\parallel, 0;\omega) = \mathbf{E}(\mathbf{0}, 0;\omega) \tag{110}$$

[$=\mathbf{E}(\mathbf{0};\omega)$] for a point inside $\mathcal{A}$, the ED part of the aperture field [Eq. (105)] is simplified to

$$\mathbf{E}^{\mathcal{A}}_{\text{ED}}(\mathbf{r};\omega) = i\mu_0\omega\left[\int_{\text{QW}}\Phi(z)dz\right]^2 \times\left[\int_{\mathcal{A}}[\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]d^2r_\parallel\right] \times\mathbf{G}(\mathbf{r};\omega)\cdot\mathbf{E}^0_\perp(\mathbf{0};\omega). \tag{111}$$

Due to the fact that we have made the electric dipole approximation in the coordinates both perpendicular and parallel to the plane of the screen, it is not surprising to find that the effective optical aperture behaves like an electric point dipole radiator for the sheet currents perpendicular to the aperture plane,

$$\mathbf{E}^{\mathcal{A}}_{\text{ED}}(\mathbf{r};\omega) = \mu_0\omega^2\mathbf{G}(\mathbf{r};\omega)\cdot\mathbf{p}(\omega), \tag{112}$$

where

$$\mathbf{p}(\omega) = \boldsymbol{\alpha}(\omega)\cdot\mathbf{E}^0(\mathbf{0};\omega) \tag{113}$$

is the electric dipole moment induced by the incident electric field. A comparison of Eqs. (111)–(113) shows that the (generally anisotropic) ED-polarizability tensor of the optical aperture is given by

$$\boldsymbol{\alpha}(\omega) = \frac{i}{\omega}\left[\int_{\text{QW}}\Phi(z)dz\right]^2\int_{\mathcal{A}}[\tilde{b}(\mathbf{r}_\parallel;\omega)-\tilde{b}_\infty(\omega)]d^2r_\parallel\hat{\mathbf{z}}\hat{\mathbf{z}} = \frac{i}{\omega}L^{\text{SF}}_{\infty,zz}\left[\int_{\text{QW}}\Phi(z)dz\right]^2 \times\int_{\mathcal{A}}L^{\text{SF}}_{zz}(\mathbf{r}_\parallel;\omega)[b(\mathbf{r}_\parallel;\omega)-b_\infty(\omega)]d^2r_\parallel\hat{\mathbf{z}}\hat{\mathbf{z}}. \tag{114}$$

It appears from the second term of Eq. (114) that the space-dependent local-field factor $L^{\text{SF}}_{zz}(\mathbf{r}_\parallel;\omega)$ only enters the formalism via a weighted integral [weighting factor $b(\mathbf{r}_\parallel;\omega)-b_\infty(\omega)$] over $\mathcal{A}$. This circumstance softens the possible spatially local resonance enhancements associated with $L^{\text{SF}}_{zz}(\mathbf{r}_\parallel;\omega)$ itself. In the small-hole limit one may expect therefore that the most pronounced frequency resonance in $\boldsymbol{\alpha}(\omega)$ is associated with the resonance condition for the screen without a hole [$L^{\text{SF}}_{\infty,zz}$ appears in Eq. (114)].

In the framework of our heuristic approach, $\boldsymbol{\alpha}(\omega)$ only has a nonvanishing zz component. In consequence, the induced electric dipole is oriented perpendicular to the plane of the screen. Although the same conclusion is reached in the classical Bethe-Bouwkamp theory for a circular hole [1–3], this does not mean that the microscopic theory (here for a two-level QW jellium screen) justifies a classical approach (cf. the general analysis in Ref. [16]). In the Bethe-Bouwkamp theory the ED polarizability has no frequency dependence. This fact is obvious from the fact that the screen in the Bethe-Bouwkamp theory is taken as infinitely thin and has infinite conductivity. The frequency dependence of $\boldsymbol{\alpha}(\omega)$, given in Eq. (114), reflects the microscopic electrodynamics of our two-level QW jellium screen.

Our calculation of the internal electrodynamics of the screen has resulted in a quite complicated result for the frequency dependence of $\boldsymbol{\alpha}(\omega)$. Since the complications originates in the local-field factors $L^{\text{SF}}_{zz}(\mathbf{r}_\parallel;\omega)$ and $L^{\text{SF}}_{\infty,zz}(\omega)$, it may be useful to give a few remarks on the expression obtained for the induced polarizability when local-field corrections are neglected [$L^{\text{SF}}_{zz}(\mathbf{r}_\parallel;\omega) = L^{\text{SF}}_{\infty,zz}(\omega) = 1$]. From Eqs. (55), (57), and (114) one immediately gets

$$\boldsymbol{\alpha}(\omega) = \frac{KN_{\text{eff}}\hat{\mathbf{z}}\hat{\mathbf{z}}}{\omega^2-\omega_B^2}, \tag{115}$$

where

$$K = \frac{1}{2}\left(\frac{e\hbar}{m}\right)^2\frac{1}{\varepsilon_2-\varepsilon_1}\left[\int_{\text{QW}}\Phi(z)dz\right]^2 \tag{116}$$

is a frequency-independent quantity and

$$N_{\text{eff}} = \int_{\mathcal{A}}[\mathcal{N}^0_\infty-\mathcal{N}^0(\mathbf{r}_\parallel)]d^2r_\parallel \tag{117}$$

is the total number of mobil electrons in the effective optical aperture. In the absence of the local-field effects these electrons move independently of each other in the external field, thus making $\boldsymbol{\alpha}(\omega)$ proportional to N_{eff} (>0). Furthermore, the resonance frequency of $\boldsymbol{\alpha}(\omega)$ is at the Bohr transition frequency (in the absence of irreversible damping mechanisms).

The independent field-induced motion of the electrons in the optical aperture in the absence of local-field corrections means that the formula given in Eq. (115) for the polarizability must be identical to the standard result obtained in the electric dipole approximation on the basis of one-electron theory. As shown in Appendix B, the expression for K can be written as

$$K = \frac{2\omega_B}{\hbar}d_z^{1\to2}d_z^{2\to1}, \tag{118}$$

where $d_z^{1\to2}$ ($d_z^{2\to1}$) is the z component of the matrix element of the dipole moment operator $\mathbf{d} = -e\hat{\mathbf{r}}$ ($e > 0$) belonging to the transition $1 \to 2$ ($2 \to 1$). Thus,

$$d_z^{1\to 2} = \hat{\mathbf{z}} \cdot \langle \psi_2 | -e\hat{\mathbf{r}} | \psi_1 \rangle = d_z^{2\to 1}. \tag{119}$$

In the last equality of Eq. (119) we have made use of the fact that lower- and upper-state wave functions are (taken as) real. In general, $d_z^{1\to 2} = (d_z^{2\to 1})^*$. With K given by Eq. (118), $\alpha_{zz}(\omega)$ takes the standard (textbook) form [32]

$$\alpha_{zz}(\omega) = \frac{2\omega_B}{\hbar} \frac{N_{\text{eff}}}{\omega^2 - \omega_B^2} d_z^{1\to 2} d_z^{2\to 1}. \tag{120}$$

In the literature one will see the denominator $\omega^2 - \omega_B^2$ replaced by $\omega_B^2 - \omega^2$, corresponding to the replacement $N_{\text{eff}}/(\omega^2 - \omega_B^2) \Rightarrow -N_{\text{eff}}/(\omega_B^2 - \omega^2)$. The negative sign in front of N_{eff} relates to the fact that in our analysis we subtract $\mathbf{J}_\infty^S(\mathbf{r}_\parallel;\omega)$ from $\mathbf{J}^S(\mathbf{r}_\parallel;\omega)$ to obtain what we define as the aperture current density $\mathbf{J}_S^{\mathcal{A}}(\mathbf{r}_\parallel;\omega)$ [see Eqs. (39) and (62)]. To comply with this one might have used the new definition $N_{\text{eff}}^{\text{new}} = -N_{\text{eff}} < 0$ [cf. Eq. (117)].

C. Electric quadrupole–magnetic dipole hole

Let us return to Eq. (108) and make the small-hole approximation for the Green's tensor [Eq. (109)] and the incident electric field [Eq. (110)] across $\mathcal{A}$. With these approximations the EQ-MD aperture field becomes

$$\mathbf{E}_{\text{EQ-MD}}^{\mathcal{A}}(\mathbf{r};\omega) = -i\mu_0\omega\left[\int_{\text{QW}} z\phi(z)dz\right]^2 \times \left[\int_{\mathcal{A}} [a(\mathbf{r}_\parallel;\omega) - a_\infty(\omega)]d^2r_\parallel\right] \times \frac{\partial \mathbf{G}(\mathbf{r};\omega)}{\partial z} \cdot \frac{\partial \mathbf{E}_\parallel^0(\mathbf{0};\omega)}{\partial z}. \tag{121}$$

At this stage the reader may note the structural similarity between the ED [Eq. (111)] and EQ-MD [Eq. (121)] parts of the aperture field.

V. DISCUSSION OF KEY RESULTS

In the now classical Bethe-Bouwkamp theory of diffraction from a small circular hole (of radius a) it was concluded that the diffracted far field of the hole is equivalent to the coherent superposition of the radiations from induced electric and magnetic dipoles of moments (in SI units)

$$\mathbf{p}(\omega) = \frac{4\varepsilon_0}{3}a^3\mathbf{E}_\perp^\infty(\mathbf{0}^-;\omega), \quad \mathbf{m}(\omega) = -\frac{8}{3\mu_0}a^3\mathbf{B}_\parallel^\infty(\mathbf{0}^-;\omega), \tag{122}$$

where $\mathbf{E}_\perp^\infty(\mathbf{0}^-;\omega)$ and $\mathbf{B}_\parallel^\infty(\mathbf{0}^-;\omega)$ are the fields which would be present on the $z = 0^-$ side of the screen in the absence of the hole. In the Bethe-Bouwkamp approach it was assumed that the screen is infinitely thin and an ideal ($\sigma \to \infty$) conductor. In the half space $z > 0$ the electromagnetic fields hence vanish identically if there is no hole. It appears from the expressions above that the electric ($4\varepsilon_0 a^3/3$) and magnetic ($-8a^3/3\mu$) polarizabilities are dispersion-free (frequency independent) and equal to those obtained from static (stationary) calculations (see Ref. [21], Secs. 3.13, 5.13, and 9.5).

To make the bridge from our analysis to the Bethe-Bouwkamp theory, we note that $\tilde{\mathbf{b}}(\mathbf{r}_\parallel;\omega) = \tilde{\mathbf{b}}(|\mathbf{r}_\parallel|;\omega)$ for a circular hole. In consequence, $\boldsymbol{\mu}(\omega) = \mathbf{0}$, since the integral over $\mathcal{A}$ in Eq. (97) now has an integrand which is uneven in x (and y). The reduced dipole moments become

$$\mathbf{p}(\omega) = \alpha_\perp(\omega)\mathbf{E}_\perp^0(\mathbf{0};\omega), \quad \mathbf{m}(\omega) = i\omega\eta(\omega)\mathbf{B}_\parallel^0(\mathbf{0};\omega). \tag{123}$$

It follows from Eqs. (96), (114), and (123) that the polarizabilities are frequency dependent and determined by the electron dynamics perpendicular [$\boldsymbol{\alpha}(\omega) = \alpha_\perp(\omega)\hat{\mathbf{z}}\hat{\mathbf{z}}$] and parallel [$\eta(\omega)$] to the plane of the screen in the present theory. Instead of the assumed known fields ($\mathbf{E}_\perp^\infty$ and $\mathbf{B}_\parallel^\infty$) in the Bethe-Bouwkamp theory, the prescribed incident fields ($\mathbf{E}_\perp^0$ and $\mathbf{B}_\parallel^0$) appear in our theory. The consequence of the replacement $\mathbf{E}_\perp^\infty$ ($\mathbf{B}_\parallel^\infty$) $\Rightarrow$ $\mathbf{E}_\perp^0$ ($\mathbf{B}_\parallel^0$) is that it is necessary to solve a quite complicated local-field problem [$b_\infty(\omega) \Rightarrow \tilde{b}_\infty(\omega)$], for the screen without a hole, and suggest a partly heuristic generalization [$b(\mathbf{r}_\parallel;\omega) \Rightarrow \tilde{b}(\mathbf{r}_\parallel;\omega)$]. For a circular hole [$\boldsymbol{\mu}(\omega) = \mathbf{0}$] the quadrupole moment tensor is given by

$$\mathbf{Q}(\omega) = \eta(\omega)[\hat{\mathbf{z}}\mathbf{B}_\parallel^0(\mathbf{0};\omega) \times \hat{\mathbf{z}} + \mathbf{B}_\parallel^0(\mathbf{0};\omega) \times \hat{\mathbf{z}}\hat{\mathbf{z}}]. \tag{124}$$

It appears from our analysis that the local-field effects solely are associated with the self-consistent electron motion perpendicular to the plane of the screen. Hence, these effects always are present in the electric dipole moment [see Eqs. (113) and (114)] and they may show up in both the magnetic dipole moment [Eq. (89)] and the electric quadrupole moment [Eq. (95)]. In the expressions for $\mathbf{m}(\omega)$ and $\mathbf{Q}(\omega)$ the local-field phenomenon is contained in the terms containing $\boldsymbol{\mu}(\omega)$ [cf. Eq. (97)]. In all cases the phenomenon stems from a correction of the incident electric field component $\mathbf{E}_\perp^0$. Pronounced local-field resonances may occur in the two-level electron dynamics in a certain frequency range. At (or near) resonance it may be reasonable to keep only terms involving $\mathbf{E}_\perp^0$. In this case

$$\mathbf{m}(\omega) \simeq -i\omega\boldsymbol{\mu}(\omega) \times \mathbf{E}_\perp^0(\mathbf{0};\omega) \tag{125}$$

and

$$\mathbf{Q}(\omega) \simeq \boldsymbol{\mu}(\omega)\mathbf{E}_\perp^0(\mathbf{0};\omega) + \mathbf{E}_\perp^0(\mathbf{0};\omega)\boldsymbol{\mu}(\omega). \tag{126}$$

However, the reader should note that local-field effects do not occur in $\mathbf{m}(\omega)$ and $\mathbf{Q}(\omega)$ for a circular hole [cf. Eqs. (123) and (124)].

If one writes the unit tensor in the dyadic (sum) form

$$\mathbf{U} = \hat{\mathbf{B}}_\parallel^0\hat{\mathbf{B}}_\parallel^0 + \hat{\mathbf{B}}_{\parallel,T}^0\hat{\mathbf{B}}_{\parallel,T}^0 + \hat{\mathbf{z}}\hat{\mathbf{z}}, \tag{127}$$

where $\hat{\mathbf{B}}_{\parallel,T}^0 \equiv \hat{\mathbf{z}} \times \hat{\mathbf{B}}_\parallel^0$ is a vector transverse (subscript T) to $\mathbf{B}_\parallel^0$ in the plane of the screen, one obtains [via Eq. (98)]

$$\mathbf{U} \times \mathbf{m}(\omega) = i\omega\{\eta(\omega)[\hat{\mathbf{z}}\hat{\mathbf{z}} \times \mathbf{B}_\parallel^0(\mathbf{0};\omega) - \hat{\mathbf{z}} \times \mathbf{B}_\parallel^0(\mathbf{0};\omega)\hat{\mathbf{z}}] + \boldsymbol{\mu}(\omega)\mathbf{E}_\perp^0(\mathbf{0};\omega) - \mathbf{E}_\perp^0(\mathbf{0};\omega)\boldsymbol{\mu}(\omega)\}. \tag{128}$$

With $\mathbf{Q}(\omega)$ taken from Eq. (95), it appears that the first-order moment of the aperture current density distribution distribution is given by the tensor

$$\mathbf{J}^{\mathcal{A}}(\omega|\text{EQ-MD}) = \mathbf{U} \times \mathbf{m}(\omega) - i\omega\mathbf{Q}(\omega) = 2[i\omega\eta(\omega)\mathbf{B}_\parallel^0(\mathbf{0};\omega) \times \hat{\mathbf{z}}\hat{\mathbf{z}} - \mathbf{E}_\perp^0(\mathbf{0};\omega)\boldsymbol{\mu}(\omega)]. \tag{129}$$

The key results for a small hole are shown as follows: In general,

$$\mathbf{p} = \alpha_\perp \mathbf{E}_\perp^0,$$
$$\mathbf{m} = i\omega[\eta \mathbf{B}_\parallel^0 - \boldsymbol{\mu} \times \mathbf{E}_\perp^0],$$
$$\mathbf{Q} = \eta \hat{\mathbf{z}}\hat{\mathbf{z}} \times \mathbf{B}_\parallel^0 + \boldsymbol{\mu}\mathbf{E}_\perp^0 + \mathbf{T};$$

for $\mathbf{J}_\perp^{\mathcal{A}} = \mathbf{0}$,

$$\mathbf{p} = \mathbf{0},$$
$$\mathbf{m} = i\omega\eta \mathbf{B}_\parallel^0,$$
$$\mathbf{Q} = \eta \hat{\mathbf{z}}\hat{\mathbf{z}} \times \mathbf{B}_\parallel^0 + \mathbf{T};$$

near resonance,

$$\mathbf{p} \simeq \alpha_\perp \mathbf{E}_\perp^0,$$
$$\mathbf{m} \simeq -i\omega\boldsymbol{\mu} \times \mathbf{E}_\perp^0,$$
$$\mathbf{Q} \simeq \boldsymbol{\mu}\mathbf{E}_\perp^0 + \mathbf{T};$$

and for a circular (c) hole,

$$\mathbf{p} = \alpha_\perp^c \mathbf{E}_\perp^0,$$
$$\mathbf{m} = i\omega\eta^c \mathbf{B}_\parallel^0,$$
$$\mathbf{Q} = \eta^c \hat{\mathbf{z}}\hat{\mathbf{z}} \times \mathbf{B}_\parallel^0 + \mathbf{T}$$

for ED ($\mathbf{p}$), MD ($\mathbf{m}$), and EQ ($\mathbf{Q}$) moments of a small hole. The frequency-dependent coefficients $\alpha_\perp(\omega)$, $\eta(\omega)$, and $\boldsymbol{\mu}(\omega)$ ($\perp\hat{\mathbf{z}}$) are determined by quantum-mechanical response theory. If the electron motion perpendicular to the plane of the hole is neglected ($\mathbf{J}_\perp^{\mathcal{A}} = \mathbf{0}$), only terms with β are present and thus $\mathbf{p} = \mathbf{0}$. Near frequency resonance terms with $\alpha_\perp$ and $\boldsymbol{\mu}$ dominate. For a circular hole (of radius a), the Bethe theory is recovered if (i) $\mathbf{Q} = \mathbf{0}$ (unjustified), (ii) frequency dispersion is neglected, $\alpha_\perp^c = 4\varepsilon_0 a^3/3$, and $i\omega\eta^c = -8a^3/3\mu_0$, and (iii) the prescribed incident field ($\mathbf{E}_\perp^0, \mathbf{B}_\parallel^0$) is replaced by the assumed known fields for a screen without a hole ($\mathbf{E}_\perp^\infty, \mathbf{B}_\parallel^\infty$).

APPENDIX A: LONG-WAVELENGTH CONDUCTIVITY TENSOR $\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to \mathbf{0}, \omega)$

1. Calculation of $b_\infty(\omega)$

For a closed system with spin degeneracy the linear one-electron conductivity tensor is in usual notation given by [19,26–28]

$$\boldsymbol{\sigma}_\infty(\mathbf{r}, \mathbf{r}'; \omega) = \frac{2\hbar}{i} \sum_{i,j(i\neq j)} \frac{f_j - f_i}{E_j - E_i} \frac{1}{\hbar\omega + E_j - E_i} \times \mathbf{J}_{i\to j}(\mathbf{r})\mathbf{J}_{j\to i}(\mathbf{r}') \tag{A1}$$

for an infinitely extended screen. In the jellium approximation, where $\boldsymbol{\sigma}_\infty(\mathbf{r}, \mathbf{r}'; \omega) = \boldsymbol{\sigma}_\infty(\mathbf{r}_\parallel - \mathbf{r}'_\parallel, z, z'; \omega)$, the eigenstates belonging to the motion in the plane of the screen may be taken as plane-wave states $(2\pi)^{-1}\exp(i\mathbf{k}_\parallel \cdot \mathbf{r})$, and the wave vectors (double set of quantum numbers) $\mathbf{k}_\parallel$ form a continuum. The 2D Fourier transform of $\boldsymbol{\sigma}_\infty$ we denote by $\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel, \omega)$, as in Sec. II A. In the long-wavelength limit ($\mathbf{q}_\parallel \to \mathbf{0}$) all in-plane quantum transitions entering $\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to \mathbf{0}, \omega)$ are vertical [see Eq. (10)]. If we denote pairs of the discrete quantum numbers for the eigenstates perpendicular to the plane of the screen by n, n' and the related wave functions and energies by $\psi_n(z)$, $\psi'_n(z)$ and ε_n, ε'_n, respectively, one obtains [19,27–29]

$$\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to \mathbf{0}, \omega) = \frac{2\hbar}{i} \int_{-\infty}^{\infty} \sum_{n,n'} \frac{f\left(\varepsilon_n + \frac{\hbar^2}{2m}k_\parallel^2\right) - f\left(\varepsilon'_n + \frac{\hbar^2}{2m}k_\parallel^2\right)}{(\varepsilon_n - \varepsilon'_n)(\hbar\omega + \varepsilon_n - \varepsilon'_n)} \times \mathbf{J}_{n\to n'}(z; \mathbf{k}_\parallel)\mathbf{J}_{n'\to n}(z'; \mathbf{k}_\parallel)\frac{d^2k_\parallel}{(2\pi)^2}, \tag{A2}$$

where f is the Fermi-Dirac distribution function (in thermal equilibrium). The transition current densities entering Eq. (A2) are given by

$$\mathbf{J}_{n\to n'}(z; \mathbf{k}_\parallel) = -\frac{e\hbar}{2im}\left\{2i\mathbf{k}_\parallel \psi_n(z)\psi_{n'}^*(z) + \hat{\mathbf{z}}\left[\psi_{n'}(z)\frac{d\psi_n(z)}{dz} - \psi_n(z)\frac{d\psi_{n'}(z)}{dz}\right]\right\}, \tag{A3}$$

with an analogous expression for $\mathbf{J}_{n'\to n}(z'; \mathbf{k}_\parallel)$ [making the replacements $n \Rightarrow n'$, $n' \Rightarrow n$, and $z \Rightarrow z'$ in Eq. (A3)].

For a two-level system [$(n, n') = (1, 2)$ or (2,1)] we have

$$\mathbf{J}_{1\to 2}(z; \mathbf{k}_\parallel) = -\frac{e\hbar}{2im}[2i\mathbf{k}_\parallel \phi(z) - \hat{\mathbf{z}}\Phi(z)] \tag{A4}$$

and

$$\mathbf{J}_{2\to 1}(z'; \mathbf{k}_\parallel) = -\frac{e\hbar}{2im}[2i\mathbf{k}_\parallel \phi(z') + \hat{\mathbf{z}}\Phi(z')], \tag{A5}$$

where $\phi(u)$ and $\Phi(u)$ (with $u = z, z'$) are the functions given in Eqs. (12) and (13). If we decompose $\mathbf{k}_\parallel$ into Cartesian components

$$\mathbf{k}_\parallel = k_{\parallel,x}\hat{\mathbf{x}} + k_{\parallel,y}\hat{\mathbf{y}}, \tag{A6}$$

a moment of reflection shows that $\boldsymbol{\sigma}_\infty(z, z'; \mathbf{q}_\parallel \to \mathbf{0}, \omega)$ for a two-level QW system must have the dyadic form given in Eq. (11). This reason originates in the fact that all integrals uneven in $k_{\parallel,x}$ or $k_{\parallel,y}$ will vanish upon integration over the $\mathbf{k}_\parallel$ coordinates.

Since the quantity

$$\hat{\mathbf{z}} \cdot \mathbf{J}_{1\to 2}(z; \mathbf{k}_\parallel)\mathbf{J}_{2\to 1}(z'; \mathbf{k}_\parallel) \cdot \hat{\mathbf{z}} = \hat{\mathbf{z}} \cdot \mathbf{J}_{2\to 1}(z; \mathbf{k}_\parallel)\mathbf{J}_{1\to 2}(z'; \mathbf{k}_\parallel) \cdot \hat{\mathbf{z}} = -\left(-\frac{e\hbar}{2im}\right)^2 \Phi(z)\Phi(z') \tag{A7}$$

is independent of $\mathbf{k}_\parallel$, it appears from Eq. (A2), applied to a two-level QW screen, that the zz component of the conductivity tensor in a first step is given by

$$\sigma_{\infty,zz}(z,z';\mathbf{q}_\parallel\to\mathbf{0},\omega)=\frac{2\hbar}{i}\left(-\frac{e\hbar}{2im}\right)^2(-1)\Phi(z)\Phi(z')\frac{1}{\varepsilon_1-\varepsilon_2}\left(\frac{1}{\hbar\omega+\varepsilon_1-\varepsilon_2}+\frac{1}{\hbar\omega+\varepsilon_2-\varepsilon_1}\right)\times\int_{-\infty}^{\infty}\left[f\left(\varepsilon_1+\frac{\hbar^2k_\parallel^2}{2m}\right)-f\left(\varepsilon_2+\frac{\hbar^2k_\parallel^2}{2m}\right)\right]\frac{d^2k_\parallel}{(2\pi)^2}. \tag{A8}$$

In the low-temperature limit and with $\varepsilon_1<\varepsilon_F<\varepsilon_2$, $f(\varepsilon_2+\hbar^2k_\parallel^2/2m)=0$. The integral over the $k_\parallel$ plane in Eq. (A8) therefore becomes

$$\int_{-\infty}^{\infty}f\left(\varepsilon_1+\frac{\hbar^2k_\parallel^2}{2m}\right)\frac{d^2k_\parallel}{(2\pi)^2}=\int_0^{\infty}f\left(\varepsilon_1+\frac{\hbar^2k_\parallel^2}{2m}\right)\frac{d(k_\parallel^2)}{4\pi}=\frac{m}{2\pi\hbar^2}\int_0^\infty f(\varepsilon_1+x)dx=\frac{m}{2\pi\hbar^2}(\varepsilon_F-\varepsilon_1). \tag{A9}$$

After a little algebra one reaches the result

$$\sigma_{\infty,zz}(z,z';\mathbf{q}_\parallel\to\mathbf{0},\omega)=b_\infty(\omega)\Phi(z)\Phi(z'), \tag{A10}$$

where

$$b_\infty(\omega)=\frac{ie^2\hbar^2\omega}{2\pi m}\left(\frac{\varepsilon_F-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right)\frac{1}{(\hbar\omega)^2-(\varepsilon_2-\varepsilon_1)^2}, \tag{A11}$$

as cited in Eq. (46).

2. Diamagnetic contribution $b_\infty^{\mathrm{D}}(\omega)$

It is known [19] that the diamagnetic part $\boldsymbol{\sigma}_\infty^{\mathrm{D}}(\mathbf{r},\mathbf{r}';\omega)$ of the conductivity tensor $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$ is given by

$$\boldsymbol{\sigma}_\infty^{\mathrm{D}}(\mathbf{r},\mathbf{r}';\omega)=\frac{2}{i\omega}\sum_{i,j\,(i\neq j)}\frac{f_j-f_i}{E_j-E_i}\mathbf{J}_{i\to j}(\mathbf{r})\mathbf{J}_{j\to i}(\mathbf{r}'). \tag{A12}$$

This result was used in our extinction-theorem approach to the quantum-mechanical diffraction theory of light from a small hole [17]. Note in Eq. (5) of Ref. [17] that a factor of 2 (typographical error) is missing (but present in subsequent equations).

Having gone through the various steps in the calculation of $\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel\to0,\omega)$ it is pretty clear that

$$\sigma_{\infty,zz}^{\mathrm{D}}(z,z';\mathbf{q}_\parallel\to0,\omega)=\frac{2}{i\omega}\left(-\frac{e\hbar}{2im}\right)^2(-1)\Phi(z)\Phi(z')\frac{2}{\varepsilon_1-\varepsilon_2}\times\int_{-\infty}^{\infty}\left[f\left(\varepsilon_1+\frac{\hbar^2k_\parallel^2}{2m}\right)-f\left(\varepsilon_2+\frac{\hbar^2k_\parallel^2}{2m}\right)\right]\frac{d^2k_\parallel}{(2\pi)^2} \tag{A13}$$

and hence in the low-temperature limit

$$\sigma_{\infty,zz}^{\mathrm{D}}(z,z';\mathbf{q}_\parallel\to0,\omega)=b_\infty^{\mathrm{D}}(\omega)\Phi(z)\Phi(z'), \tag{A14}$$

where

$$b_\infty^{\mathrm{D}}(\omega)=\frac{ie^2}{2\pi m\omega}\frac{\varepsilon_F-\varepsilon_1}{\varepsilon_2-\varepsilon_1}. \tag{A15}$$

A brief glance at Eqs. (A14) and (A15) seems to indicate that we have reached an unusual (and unsatisfactory) result because the universal diamagnetic effect basically is structure independent [19] and local and thus only depends on the particle number density (and the frequency ω). In a three-dimensional scenario

$$\sigma_{\infty,zz}^{\mathrm{D}}(\mathbf{r},\mathbf{r}';\omega)=\frac{ie^2}{m\omega}n^0(\mathbf{r}), \tag{A16}$$

where $n^0(\mathbf{r})$ is the field-unperturbed charge particle (electron density) [19]. The result in Eqs. (A14) and (A15) which is structure dependent (via ε_1, ε_2, ε_F, and Φ) originates in the fact that we have reduced the general diamagnetic formalism by taking into account only two levels in the z dynamics. This becomes apparent if one uses Eq. (53) to eliminate $\varepsilon_F-\varepsilon_1$ in favor of the surface electron density $\mathcal{N}_\infty^0$ in Eq. (A15). For $\sigma_{\infty,zz}^{\mathrm{D}}$ we then get

$$\sigma_{\infty,zz}^{\mathrm{D}}(z,z';\mathbf{q}_\parallel\to0,\omega)=\frac{ie^2}{m\omega}\mathcal{N}_\infty^0\frac{\hbar^2}{2m(\varepsilon_2-\varepsilon_1)}\Phi(z)\Phi(z'). \tag{A17}$$

The factor $ie^2\mathcal{N}_\infty^0/m\omega$ obviously is the two-dimensional version of Eq. (A16) for a homogenous density distribution.

3. Paramagnetic contribution $b_\infty^{\mathrm{P}}(\omega)$

From the paramagnetic part $\boldsymbol{\sigma}_\infty^{\mathrm{P}}(\mathbf{r},\mathbf{r}';\omega)$ of the conductivity tensor $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$, viz.,

$$\boldsymbol{\sigma}_\infty^{\mathrm{P}}(\mathbf{r},\mathbf{r}';\omega)=\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)-\boldsymbol{\sigma}_\infty^{\mathrm{D}}(\mathbf{r},\mathbf{r}';\omega), \tag{A18}$$

one immediately obtains by subtracting Eq. (A14) from Eq. (A10) the result

$$\sigma_{\infty,zz}^{\mathrm{P}}(z,z';\mathbf{q}_\parallel\to0,\omega)=b_\infty^{\mathrm{P}}(\omega)\Phi(z)\Phi(z'), \tag{A19}$$

where

$$b_\infty^{\mathrm{P}}(\omega)=b_\infty(\omega)-b_\infty^{\mathrm{D}}(\omega)=\frac{ie^2}{2\pi m\omega}\frac{(\varepsilon_2-\varepsilon_1)(\varepsilon_F-\varepsilon_1)}{(\hbar\omega)^2-(\varepsilon_2-\varepsilon_1)^2}. \tag{A20}$$

The ratio between the zz components of the paramagnetic and the total conductivities is particularly simple:

$$\frac{\sigma_{\infty,zz}^{\mathrm{P}}(z,z';\mathbf{q}_\parallel\to0,\omega)}{\sigma_{\infty,zz}(z,z';\mathbf{q}_\parallel\to0,\omega)}=\frac{b_\infty^{\mathrm{P}}(\omega)}{b_\infty(\omega)}=\left(\frac{\varepsilon_2-\varepsilon_1}{\hbar\omega}\right)^2. \tag{A21}$$

Both $b_\infty^{\mathrm{P}}(\omega)$ and $b_\infty^{\mathrm{D}}(\omega)$ diverge in the low-frequency limit ($\omega\to0$), whereas $b_\infty(\omega\to0)=0$. This underlines the importance of keeping the often neglected [32] gauge-invariant diamagnetic part of the conductivity tensor in linear electrodynamics analyses.

4. Calculation of $a_\infty(\omega)$

It appears from Eq. (11) that the quantity $a_\infty(\omega)$ relates to the components of the conductivity tensor $\boldsymbol{\sigma}_\infty(z,z';\mathbf{q}_\parallel,\omega)$

which lie in the plane of the screen. To determine the explicit expression for $a_\infty(\omega)$, we follow the procedure used above to calculate $b_\infty(\omega)$. We already know that the conductivity tensor in the long-wavelength limit has the diagonal form

$$\boldsymbol{\sigma}_\infty = \begin{pmatrix} \sigma_\infty^\parallel & 0 & 0 \\ 0 & \sigma_\infty^\parallel & 0 \\ 0 & 0 & \sigma_\infty^\perp \end{pmatrix} \tag{A22}$$

in the chosen Cartesian coordinate system ($\sigma_\infty^\perp = \sigma_{\infty,zz}, \sigma_\infty^\parallel = \sigma_{\infty,xx} = \sigma_{\infty,yy}$). From Eqs. (A2), (A4), and (A5) one sees that the important combination of transition current densities for a calculation of $\sigma_\infty^\parallel$ is

$$\begin{aligned}(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}}) &\cdot \mathbf{J}_{1\to 2}(z; \mathbf{k}_\parallel)\mathbf{J}_{2\to 1}(z'; \mathbf{k}_\parallel) \cdot (\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}}) \\ &= \left(-\frac{e\hbar}{2im}\right)^2 (2i)^2 \phi(z)\phi(z')[k_{\parallel,x}^2 \hat{\mathbf{x}}\hat{\mathbf{x}} + k_{\parallel,y}^2 \hat{\mathbf{y}}\hat{\mathbf{y}} \\ &\quad + k_{\parallel,x}k_{\parallel,y}(\hat{\mathbf{x}}\hat{\mathbf{y}} + \hat{\mathbf{y}}\hat{\mathbf{x}})].\end{aligned} \tag{A23}$$

Since the off-diagonal components disappear upon integration over the $k_\parallel$ plane, it readily appears that the only integral necessary to calculate is

$$\begin{aligned}\int_{-\infty}^{\infty} f\left(\varepsilon_1 + \frac{\hbar^2 k_\parallel^2}{2m}\right) k_{\parallel,x}^2 \frac{d^2 k_\parallel}{(2\pi)^2} &= \int_{-\infty}^{\infty} f\left(\varepsilon_1 + \frac{\hbar^2 k_\parallel^2}{2m}\right) k_{\parallel,y}^2 \frac{d^2 k_\parallel}{(2\pi)^2} \\ &= \frac{1}{2}\int_{-\infty}^{\infty} f\left(\varepsilon_1 + \frac{\hbar^2 k_\parallel^2}{2m}\right) k_\parallel^2 \frac{d^2 k_\parallel}{(2\pi)^2},\end{aligned} \tag{A24}$$

recalling that $f(\varepsilon_2 + \hbar^2 k_\parallel^2/2m) = 0$ in the low-temperature limit. As the readers may show to themselves, one obtains in the $T \to 0$ K limit

$$\frac{1}{2}\int_{-\infty}^{\infty} f\left(\varepsilon_1 + \frac{\hbar^2 k_\parallel^2}{2m}\right) k_\parallel^2 \frac{d^2 k_\parallel}{(2\pi)^2} = \frac{m^2}{2\pi\hbar^4}(\varepsilon_F - \varepsilon_1)^2. \tag{A25}$$

Gathering now the various factors [as in Eq. (A8)], one gets

$$\boldsymbol{\sigma}_\infty^\parallel(z, z'; \mathbf{q}_\parallel \to 0, \omega) \equiv \sigma_\infty^\parallel(z, z'; \mathbf{q}_\parallel \to 0, \omega)(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}}), \tag{A26}$$

where

$$\sigma_\infty^\parallel(z, z'; \mathbf{q}_\parallel \to 0, \omega) = a_\infty(\omega)\phi(z)\phi(z'), \tag{A27}$$

with the following explicit expression for $a_\infty(\omega)$:

$$a_\infty(\omega) = \frac{ie^2\omega}{\pi}\frac{(\varepsilon_F - \varepsilon_1)^2}{\varepsilon_2 - \varepsilon_1}\frac{1}{(\hbar\omega)^2 - (\varepsilon_2 - \varepsilon_1)^2}. \tag{A28}$$

The paramagnetic part of $a_\infty(\omega)$, denoted by $a_\infty^{\mathrm{P}}(\omega)$, is given in Refs. [18,26] and the expression for the diamagnetic part of the $a_\infty(\omega)$ coefficient $a_\infty^{\mathrm{D}}(\omega)$ is easily obtained from $a_\infty^{\mathrm{D}}(\omega) = a_\infty(\omega) - a_\infty^{\mathrm{P}}(\omega)$. The reader may note that

$$\frac{a_\infty^{\mathrm{P}}(\omega)}{a_\infty(\omega)} = \left(\frac{\varepsilon_2 - \varepsilon_1}{\hbar\omega}\right)^2. \tag{A29}$$

This ratio is the same as for $b_\infty^{\mathrm{P}}(\omega)/b_\infty(\omega)$ [see Eq. (A21)].

APPENDIX B: SMALL-HOLE POLARIZABILITY WRITTEN IN STANDARD FORM

In the small-hole (ED-ED) limit the aperture field $\mathbf{E}^{\mathcal{A}}(\mathbf{r}; \omega)$ becomes identical to that of an electric dipole oriented perpendicular to the plane of the screen. Due to the presence of local-field effects the dipolar polarizability $\boldsymbol{\alpha}(\omega) = \alpha_{zz}(\omega)\hat{\mathbf{z}}\hat{\mathbf{z}}$ exhibits a quite complicated frequency dependence [see Eq. (114)]. If local-field corrections can be neglected, the frequency dependence of $\alpha_{zz}(\omega)$ takes the simple form $(\omega^2 - \omega_B^2)^{-1}$ [see Eq. (115)]. In the standard quantum theory for the electric dipole polarizability of an atomic point dipole local-field corrections are neglected and the polarizability tensor also exhibits the frequency dependence $(\omega^2 - \omega_{B,ij}^2)^{-1}$ in the part related to the $i \to j$ transition: $\omega_{B,ij} = |\varepsilon_i - \varepsilon_j|/\hbar$. Although the expression derived for the hole (optical aperture) polarizability in this paper was obtained on the basis of the fundamental interaction (I) Hamiltonian

$$\hat{H}_I = \frac{e}{2m}[\hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{r}, t) + \mathbf{A}(\mathbf{r}, t) \cdot \hat{\mathbf{p}}] + \frac{e^2}{2m}\mathbf{A}(\mathbf{r}, t) \cdot \mathbf{A}(\mathbf{r}, t), \tag{B1}$$

$\hat{\mathbf{p}} = (\hbar/i)\nabla$ being the electron momentum operator (in the $\mathbf{r}$ representation), it is well known [19] that $\hat{H}_I$ is equivalent to the electric dipole interaction Hamiltonian

$$\hat{H}_I = e\hat{\mathbf{r}} \cdot \mathbf{E}(\mathbf{r}, t) \tag{B2}$$

in the long-wavelength (ED) limit where the vector potential $\mathbf{A}(\mathbf{r}, t)$ does not vary in space across the given object (atom, small hole, etc.), i.e., $\mathbf{A}(\mathbf{r}, t) \simeq \mathbf{A}(\mathbf{0}, t)$ (with the object centered at the origin of our coordinate system). In the $\mathbf{r}$ representation the electron position operator is $\hat{\mathbf{r}} = \mathbf{r}$. The considerations above indicate that it should be possible to rewrite the small-hole expression given in Eq. (115) for $\alpha_{zz}(\omega)$ of a two-level QW screen in a form formally identical to that of $\alpha_{zz}(\omega)$ for a two-level pointlike atom.

To achieve the aforementioned goal let us consider the integral $\int_{\mathrm{QW}} \Phi(z)dz$ appearing in the expression for K [Eq. (116)]. A partial integration of either the first or the second term in $\Phi(z)$ [Eq. (13)] gives [$\psi_1(z)$ and $\psi_2(z)$ vanish asymptotically]

$$\begin{aligned}\frac{\hbar}{i}\int_{\mathrm{QW}} \Phi(z)dz &= 2\int_{\mathrm{QW}} \psi_1(z)\frac{\hbar}{i}\frac{d\psi_2(z)}{dz}dz \\ &= -2\int_{\mathrm{QW}} \psi_2(z)\frac{\hbar}{i}\frac{d\psi_1(z)}{dz}dz.\end{aligned} \tag{B3}$$

Hence, recalling that $\psi_1(z)$ and $\psi_2(z)$ are real, one has

$$\frac{\hbar}{i}\int_{\mathrm{QW}} \Phi(z)dz = 2p_z^{2\to 1} = -2p_z^{1\to 2}, \tag{B4}$$

where

$$p_z^{i\to j} = \langle\psi_j|\hat{p}_z|\psi_i\rangle, \quad (i, j) = (1, 2) \text{ or } (2, 1), \tag{B5}$$

is the matrix element of the momentum operator relating to the transition from i to j. From Eq. (B4) we obtain

$$\left[\int_{\mathrm{QW}} \Phi(z)dz\right]^2 = \frac{4}{\hbar^2}p_z^{2\to 1}p_z^{1\to 2}. \tag{B6}$$

If we denote the (assumed local [17]) QW potential by $V_\perp(z)$, the (well-known) commutator relation

$$[\hat{z}, \hat{H}_0] = \left[\hat{z}, \frac{\hat{p}_z^2}{2m} + V_\perp(z)\right] = \frac{i\hbar}{m}\hat{p}_z \tag{B7}$$

allows one to rewrite the matrix element in Eq. (B5) as

$$\begin{aligned}\langle\psi_j|\hat{p}_z|\psi_i\rangle &= \frac{m}{i\hbar}\langle\psi_j|[\hat{z}, \hat{H}_0|\psi_i\rangle \\ &= \frac{m}{i\hbar}(\varepsilon_i - \varepsilon_j)\langle\psi_j|\hat{z}|\psi_i\rangle,\end{aligned} \tag{B8}$$

where ε_i and ε_j are the eigenenergies belonging to the stationary QW states i and j. Since

$$d_z^{i\to j} = \langle\psi_j| - e\hat{z}|\psi_i\rangle, \quad e > 0, \tag{B9}$$

is just the z component of the transition ($i \to j$) matrix element of the electric dipole moment operator $\hat{\mathbf{d}} = -e\hat{\mathbf{r}}$, we have

$$p_z^{i\to j} = \frac{m}{i\hbar e}(\varepsilon_j - \varepsilon_i)d_z^{i\to j}. \tag{B10}$$

By combining Eqs. (116), (B6), and (B10) one obtains the result cited for K in Eq. (118). With this expression one is led to the standard formula [32] for $\alpha_{zz}(\omega)$ [Eq. (120)]. Q.E.D.

APPENDIX C: ELECTRIC QUADRUPOLE AND MAGNETIC DIPOLE DIFFRACTION

In Sec. IV we discussed the scattering from a small hole on the basis of a one-dimensional moment expansion of the aperture current density in the direction perpendicular to the plane of the screen [Sec. III, Eq. (69)]. Although this expansion may dure the essential part of the physics related to the diffraction from a two-level QW screen, not least near the electronic ($\hbar\omega \approx \varepsilon_2 - \varepsilon_1$) and local-field resonances [see Eqs. (65), (73), and (74), with the a's and b's given by Eqs. (54)–(57)], a division of the second-order aperture current density $\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r}_\parallel, z; \omega|\text{EQ-MD})$ into its electric quadrupole and magnetic dipole parts requires a three-dimensional moment expansion.

1. Symmetric and antisymmetric tensorial moments of the aperture current density: Scattered EQ and MD fields

The electric field radiated from a prevailing aperture current density $\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)$ is given by Eq. (100). The combined electric quadrupole and magnetic dipole contribution to the aperture field is obtained from Eq. (100) by replacing $\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)$ by the first [superscript (1)] -moment expression [19]

$$\mathbf{J}_{(1)}^{\mathcal{A}}(\mathbf{r};\omega) = -\left[\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}d^3r\right]\cdot\nabla\delta(\mathbf{r}). \tag{C1}$$

This equation is the 3D generalization of the second term on the right-hand side of Eq. (69). The symmetric and antisymmetric parts of the second-rank tensor integral in front of $\nabla\delta(\mathbf{r})$, viz.,

$$\mathbf{J}_{\text{EQ}}^{\mathcal{A}}(\omega) = \frac{1}{2}\int_{-\infty}^{\infty}[\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r} + \mathbf{r}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)]d^3r \tag{C2}$$

and

$$\mathbf{J}_{\text{MD}}^{\mathcal{A}}(\omega) = \frac{1}{2}\int_{-\infty}^{\infty}[\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r} - \mathbf{r}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)]d^3r, \tag{C3}$$

relate to the source of the electric quadrupole and magnetic dipole radiation, as indicated by the subscripts. In Eqs. (C1)–(C3) dyadic notation has been used.

In order to determine $\mathbf{J}_{\text{EQ}}^{\mathcal{A}}(\omega)\mathbf{J}_{\text{MD}}^{\mathcal{A}}(\omega)$ we start from the tensor

$$\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}\,d^3r = \int_{-\infty}^{\infty}[\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega) + \mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega)]\mathbf{r}\,d^3r, \tag{C4}$$

where the explicit formulas for $\mathbf{J}_\parallel^{\mathcal{A}}$ and $\mathbf{J}_\perp^{\mathcal{A}}$ are given in Eqs. (67) and (68) in our two-level QW approximation. The tensor (integral) associated with the aperture current density's component perpendicular to the plane of the screen takes the dyadic form

$$\begin{aligned}\int_{-\infty}^{\infty}\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}\,d^3r &= \int_{-\infty}^{\infty}J_\perp^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{z}}\mathbf{r}\,d^3r \\ &= \int_{-\infty}^{\infty}J_\perp^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{z}}(x\hat{\mathbf{x}} + y\hat{\mathbf{y}})d^3r.\end{aligned} \tag{C5}$$

The last term of Eq. (C5) is obtained from the fact that the integral of $J_\perp^{\mathcal{A}}(\mathbf{r};\omega)z\hat{z}$ over z vanishes because of the parity condition in Eq. (72). The tensor (integral) related to the in-plane component of $\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)$ becomes

$$\begin{aligned}&\int_{-\infty}^{\infty}\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}\,d^3r \\ &= \int_{-\infty}^{\infty}\left[J_{\parallel,x}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{x}} + J_{\parallel,y}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{y}}\right](x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}})d^3r \\ &= \int_{-\infty}^{\infty}z\left[J_{\parallel,x}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{x}}\hat{\mathbf{z}} + J_{\parallel,y}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{y}}\hat{\mathbf{z}}\right]d^3r,\end{aligned} \tag{C6}$$

where the last term follows by use of the wave-function orthogonality [Eq. (71)]. The symmetric and antisymmetric parts of

$$\begin{aligned}\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}\,d^3r = \int_{-\infty}^{\infty}&\left[zJ_{\parallel,x}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{x}} + \hat{\mathbf{z}} + zJ_{\parallel,y}^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{y}}\hat{\mathbf{z}}\right. \\ &\left.+ xJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{z}}\hat{\mathbf{x}} + yJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\hat{\mathbf{z}}\hat{\mathbf{y}}\right]d^3r\end{aligned} \tag{C7}$$

hence are given by

$$\begin{aligned}\mathbf{J}_{\text{EQ}}^{\mathcal{A}}(\omega) &= \frac{1}{2}\int_{-\infty}^{\infty}\left\{\left[zJ_{\parallel,x}^{\mathcal{A}}(\mathbf{r};\omega) + xJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\right](\hat{\mathbf{x}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{x}})\right. \\ &\quad\left.+\left[zJ_{\parallel,y}^{\mathcal{A}}(\mathbf{r};\omega) + yJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\right](\hat{\mathbf{y}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{y}})\right\}d^3r \\ &= \frac{1}{2}\int_{-\infty}^{\infty}[\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{z} + \mathbf{z}\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega) \\ &\quad+ \mathbf{r}_\parallel\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega) + \mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}_\parallel]d^3r\end{aligned} \tag{C8}$$

and

$$\begin{aligned}\mathbf{J}_{\text{MD}}^{\mathcal{A}}(\omega) &= \frac{1}{2}\int_{-\infty}^{\infty}\left\{\left[zJ_{\parallel,x}^{\mathcal{A}}(\mathbf{r};\omega) - xJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\right](\hat{\mathbf{x}}\hat{\mathbf{z}} - \hat{\mathbf{z}}\hat{\mathbf{x}})\right. \\ &\quad\left.+\left[zJ_{\parallel,y}^{\mathcal{A}}(\mathbf{r};\omega) - yJ_\perp^{\mathcal{A}}(\mathbf{r};\omega)\right](\hat{\mathbf{y}}\hat{\mathbf{z}} - \hat{\mathbf{z}}\hat{\mathbf{y}})\right\}d^3r \\ &= \frac{1}{2}\int_{-\infty}^{\infty}[\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{z} - \mathbf{z}\mathbf{J}_\parallel^{\mathcal{A}}(\mathbf{r};\omega) \\ &\quad+ \mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega)\mathbf{r}_\parallel - \mathbf{r}_\parallel\mathbf{J}_\perp^{\mathcal{A}}(\mathbf{r};\omega)]d^3r.\end{aligned} \tag{C9}$$

In the general 3D analysis the diffracted electric quadrupole field from the effective aperture therefore is given by

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{EQ}}(\mathbf{r};\omega) = -i\mu_0\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r}-\mathbf{r}';\omega)\cdot\mathbf{J}^{\mathcal{A}}_{\mathrm{EQ}}(\omega)\cdot\nabla'\delta(\mathbf{r}')d^3r' \quad \text{(C10)}$$

and the magnetic dipole field by

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{MD}}(\mathbf{r};\omega) = -i\mu_0\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r}-\mathbf{r}';\omega)\cdot\mathbf{J}^{\mathcal{A}}_{\mathrm{MD}}(\omega)\cdot\nabla'\delta(\mathbf{r}')d^3r'. \quad \text{(C11)}$$

At this point we note that the zeroth [subscript (0)] moment of the aperture current density, namely,

$$\mathbf{J}^{\mathcal{A}}_{(0)}(\mathbf{r};\omega) = \delta(\mathbf{r})\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega)d^3r = \delta(\mathbf{r})\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)d^3r, \quad \text{(C12)}$$

readily leads to the result obtained for the electric dipole hole in Sec. IV B. The last term in Eq. (C12) follows from the fact that the integral of $\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)$ [Eq. (67)] vanishes due to the wave-function orthogonality [Eq. (71)]. Thus, with $\mathbf{J}^{\mathcal{A}}(\mathbf{r};\omega) = \mathbf{J}^{\mathcal{A}}_{(0)}(\mathbf{r};\omega)$ one has

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{ED}}(\mathbf{r};\omega) = i\mu_0\omega\mathbf{G}(\mathbf{r};\omega)\cdot\left[\int_{-\infty}^{\infty}\mathbf{J}^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)d^3r\right], \quad \text{(C13)}$$

and thereafter, by means of the explicit expression for $\mathbf{J}^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)$ [Eq. (68)] and the small-hole approximation for the incoming field [Eq. (110)], one regains the result in Eq. (111).

2. Aperture fields in the one-dimensional moment expansion

In order to make a connection with the analysis in Sec. III C we neglect the δ-function derivatives in the plane of the screen. Thus, with

$$\nabla\delta(\mathbf{r}) \approx \hat{\mathbf{z}}\frac{\partial\delta(\mathbf{r})}{\partial z} = \hat{\mathbf{z}}\delta(\mathbf{r}_\parallel)\frac{d\delta(z)}{dz}, \quad \text{(C14)}$$

Eq. (C10) is reduced to

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{EQ}}(\mathbf{r};\omega) = -i\mu_0\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r}_\parallel, z-z';\omega)\cdot\mathbf{J}^{\mathcal{A}}_{\mathrm{EQ}}(\omega)\cdot\hat{\mathbf{z}}\frac{\partial\delta(z')}{\partial z'}dz' = -i\mu_0\omega\frac{\partial\mathbf{G}(\mathbf{r};\omega)}{\partial z}\cdot\mathbf{J}^{\mathcal{A}}_{\mathrm{EQ}}(\omega)\cdot\hat{\mathbf{z}}. \quad \text{(C15)}$$

The last term of Eq. (C15) is obtained upon a partial integration and use of Eq. (107). By means of the explicit expression for $\mathbf{J}^{\mathcal{A}}_{\mathrm{EQ}}(\omega)$ [Eq. (C8)] one obtains

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{EQ}}(\mathbf{r};\omega) = -\frac{i\mu_0\omega}{2}\frac{\partial\mathbf{G}(\mathbf{r};\omega)}{\partial z}\cdot\left[\int_{-\infty}^{\infty}[z\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)+\mathbf{r}_\parallel J^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)]d^3r\right]. \quad \text{(C16)}$$

An analogous calculation leads to the following formula for the magnetic dipole field:

$$\mathbf{E}^{\mathcal{A}}_{\mathrm{MD}}(\mathbf{r};\omega) = -\frac{i\mu_0\omega}{2}\frac{\partial\mathbf{G}(\mathbf{r};\omega)}{\partial z}\cdot\left[\int_{-\infty}^{\infty}[z\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)-\mathbf{r}_\parallel J^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)]d^3r\right]. \quad \text{(C17)}$$

If one adds the EQ and MD aperture fields one obtains a result which only depends on the integral of $z\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)$, i.e.,

$$\mathbf{E}^{\mathcal{A}}_{\text{EQ-MD}}(\mathbf{r};\omega) = \mathbf{E}^{\mathcal{A}}_{\mathrm{EQ}}(\mathbf{r};\omega) + \mathbf{E}^{\mathcal{A}}_{\mathrm{MD}}(\mathbf{r};\omega) = -i\mu_0\omega\frac{\partial\mathbf{G}(\mathbf{r};\omega)}{\partial z}\cdot\left[\int_{-\infty}^{\infty}z\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)d^3r\right]. \quad \text{(C18)}$$

For the one-dimensional model we can conclude that, although the combined EQ-MD aperture field $\mathbf{E}^{\mathcal{A}}_{\mathrm{EQ/MD}}(\mathbf{r};\omega)$ depends solely on the current density parallel to the plane of the screen [$\mathbf{J}^{\mathcal{A}}_{\parallel}(\mathbf{r};\omega)$], the current density perpendicular to the screen [$\mathbf{J}^{\mathcal{A}}_{\perp}(\mathbf{r};\omega)$] is needed in order to divide the aperture field into its electric quadrupole [$\mathbf{E}^{\mathcal{A}}_{\mathrm{EQ}}(\mathbf{r};\omega)$] and magnetic dipole [$\mathbf{E}^{\mathcal{A}}_{\mathrm{MD}}(\mathbf{r};\omega)$] components.

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