Quantum-mechanical diffraction theory of light from a small hole: Extinction-theorem approach

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In a recent paper [Phys. Rev. A **90**, 043830 (2014)] it was shown that the so-called aperture response tensor is the central concept in the microscopic quantum theory of light diffraction from a small hole in a flat screen. It was further shown that the quantum mechanical theory of diffraction only requires a preknowledge of the incident field plus the electronic properties of identical screens with and without a hole. Starting from the quantum mechanical expression for the linear conductivity tensor, we study the related causal conductivity tensor paying particular attention to diamagnetic electron dynamics. Using a nonlocal-potential separation assumption, we present a calculation of the diamagnetic causal surface conductivity for a jellium quantum-well screen using a two-dimensional Hartree-Fock model. In the diamagnetic case the difference between the light-unperturbed electron densities for screens with (n^0) and without (n^0_∞) holes are the primary quantities for the diffraction theory. In a central part (Sec. IV) of this article we determine n^0 via a quantum-mechanical two-dimensional extinction-theorem approach related to elastic electron scattering from a hole with an electronic selvedge. For heuristic purposes we illustrate aspects of the extinction-theorem theory by applying the approach for an infinitely high potential barrier to the vacuum hole. Finally, we calculate and discuss the aperture response tensor in the small hole limit and in the zeroth-order Born approximation. Our final result for the aperture response tensor establishes the bridge to the anisotropic electric dipole polarizability tensor of the hole. It turns out that the effective optical aperture (hole) size relates closely to the extension of the relevant electronic wave functions scattered from the hole.

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I. INTRODUCTION

According to Huygens' scalar construction, every point of a given optical wave front may be considered as a center of emission of secondary noninterfering spherical wavelets, and the wave front at any later instant may be regarded as the envelope of these wavelets [1,2]. By supplementing Huygens' construction with the postulate that the secondary wavelets interfere mutually, Fresnel was able to account for a number of important observations [3]. The Huygens-Fresnel scalar theory was put on a sounder mathematical basis by Kirchhoff [4,5] using a procedure already known from Helmholtz's studies in acoustics [6]. The resulting Helmholtz-Kirchhoff integral theorem [7,8], possibly with a vectorial generalization included, has since been the starting point for many electromagnetic diffraction studies. In the Huygens-Fresnel-Kirchhoff approach there exists in a certain sense sources for emission of electromagnetic fields, e.g., light, in every point in vacuum. In a given diffraction scenario these sources are active at the centers of the various wavelets. Although it appears from the Maxwell equations that the sources or sinks of electromagnetic fields are seated in electrically charged matter (massive) particles, the Huygens-Fresnel-Kirchhoff idea has its place in modern notation, where the field propagation even in the photon approach may be described in terms of the transverse electromagnetic propagator in so-called spherical contraction [9,10].

Once it is realized that electromagnetic diffraction has its roots in field-matter interaction, and as such is a scattering phenomenon, one is faced with (i) a boundary value problem at the matter-vacuum (air) interface(s) and (ii) a dynamical problem for the space-time evolution of the particle motion induced by the given incoming electromagnetic field, a motion subsequently responsible for the emission of the diffracted (scattered) field. In diffraction from an aperture (a hole) in a solid screen, it is intuitively plausible that the field-matter interaction in the vicinity (edge) of the aperture plays the major role in understanding the diffraction characteristics. The importance of the edge was already known to Young, who regarded the diffraction pattern as arising from the interference of the incident wave and a reflected "boundary wave" from the edge [11]. It was left to Sommerfeld to put the idea of Young on a firm theoretical basis. He did this via his mathematically rigorous solution for the diffraction of plane waves by a plane semi-infinite perfectly reflecting screen [8,12].

In the so-called rigorous diffraction theories [8,13–17] point (i) above is in focus, and point (ii) in a sense completely neglected assuming that the given screen, usually taken as infinitely thin, is black or a perfect reflector. The enormous amount of literature (see, e.g., Refs. [15] and [18] and references therein), not least on perfectly conducting metal screens, has shown that the "rigorous diffraction theory" leads to quantitatively good prediction in many cases, not least at long wavelengths. However, it is not completely correct to claim that a perfect conductor (reflector) screen is dynamically inactive. The screen must carry a finite current density to satisfy the necessary (macroscopic) boundary conditions on the various electromagnetic-field quantities. Mathematically, the product of an infinite conductivity ($\sigma \to \infty$) and an internal electric field which goes to zero ($\mathbf{E} \to \mathbf{0}$) must equal the relevant finite screen current density $\mathbf{J} = \sigma\mathbf{E}$.

Recent optical studies, not least in near-field optics and of diffraction from micro (nano)-sized holes (see, e.g., the experimental studies in Refs. [19–23]), have made it necessary to put more emphasis on point (ii). Following a long tradition

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in physical optics, the field-matter interaction is almost always treated on the basis of a macroscopic refractive index (n) [or equivalently a complex dielectric constant (ε)] concept (see, e.g., Refs. [24–31]). In such an approach, the variable light-induced matter dynamics is hidden in the frequency dependence of the dielectric constant (tensor), $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\omega)$.

To obtain a deeper (better) understanding of the diffraction of light from mesocopic holes, it is, in general, necessary to include the concept of spatial nonlocality when dealing with the field-matter interaction. Some studies of nonlocality have appeared in recent years within the field of nanoplasmonics [32–37]. However, most of these studies are performed within the hydrodynamical approximation. A full incorporation of nonlocality in most situations means that one has to abandon macroscopic electrodynamics and instead base the calculations on the microscopic Maxwell-Lorentz equations. In these the fields are generated by the microscopic charge and current densities, and to obtain these the field-coupled (many-body) Schrödinger equation must be combined with the microscopic Maxwell-Lorentz equations in a self-consistent manner [9].

The quantum regime of plasmon resonances in subnanometer gaps between metallic nanodimers has for some years been studied using time-dependent density functional theory and the phenomenological quantum-correction model [38–45]. In the present work, we present a quantum-mechanical theory of diffraction of light from a small hole based on a different approach. We take as a starting point a microscopic theory of diffraction recently established by the present authors [46]. On the basis of linear microscopic response theory, we showed how the diffraction characteristics can be expressed solely in terms of a preknowledge of the incident field and the optical electronic properties of the given screen. Indirectly, quantum physics entered our previous paper via the nonlocal microscopic conductivity tensor $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$, an object in the space $(\mathbf{r},\mathbf{r}')$-frequency (ω) domain. By comparing (subtracting) the fields scattered by the *same incident field* from screens with and without a hole, the diffraction stemming from the field-matter interaction in the vicinity of the hole is brought in focus. In the heart of our diffraction theory [46] stands the so-called *effective causal aperture response tensor*, $\boldsymbol{\Delta}(\mathbf{r},\mathbf{r}';\omega)$, which is the central quantity that needs to be calculated in order to apply the microscopic theory of diffraction [46]. In this work we show how the effective causal aperture response tensor may be calculated quantum mechanically for a plane quantum-well jellium screen in the case where the diamagnetic coupling dominates the field-matter interaction.

In Sec. II and Appendix A we present some general aspects of the quantum-mechanical diffraction theory. In Appendix A a few remarks on classical diffraction theory and its limitations are given (Sec. 1 of Appendix A), whereafter we proceed with a brief summary of the microscopic formalism [46] leading to a general expression of the effective causal aperture response tensor (Sec. 2 of Appendix A). In Sec. II the quantum-mechanical structure of the microscopic conductivity tensor (Sec. II A), the theory of diamagnetic electron dynamics (Sec. II B), and the framework for our study of jellium quantum-well screens (Sec. II C) are presented. From Sec. II B, and in the subsequent part of our work, we limit ourselves to the diamagnetic response. The locality of $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ simplifies the integral equation for the local-field tensor somewhat and leads to a spatially local relation between the causal (cau) diamagnetic conductivity tensor, $\boldsymbol{\sigma}^{\mathrm{cau}}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$, and the local field tensor.

When the plane screen is sufficiently thin it behaves like an electric dipole (ED) absorber and ED radiator sheet (ED-ED sheet) [46] and the electron motion in the direction perpendicular to the screen becomes bound-state dynamics in a quantum-well (QW) potential. For such QW screens the central concept of the microscopic quantum theory of diffraction is the ED-ED approximation of $\boldsymbol{\Delta}(\mathbf{r},\mathbf{r}';\omega)$, i.e., the ED-ED causal effective aperture response tensor $\boldsymbol{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ [46]. In this article, we focus on diamagnetic QW screens and we pursue a calculation of $\boldsymbol{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$. We start in Sec. II C by *assuming* that the screen potential can be separated in such a manner that the time-independent Schrödinger equation decouples into parts associated with the stationary-state problems along and perpendicular to the plane of the screen. The electron dynamics in the plane of the QW screen we treat on the basis of the well-known jellium model. As described in Appendix B, a two-dimensional (2D) Hartree-Fock calculation gives us for a screen without a hole the eigenenergies associated with a complete set of 2D plane waves.

From our previous work [46] we know that the ED-ED aperture response tensor is given by the difference between the causal surface conductivity tensors for identical screens with $[\mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)]$ and without $[\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)]$ a hole: $\boldsymbol{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) - \mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$. In Sec. III, we determine the diamagnetic causal surface conductivity tensor for a screen without a hole $\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$, retaining only the self-field part of the electromagnetic Green's function. In the self-field approximation the integral equation for the local-field tensor, $\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}';\omega)$, is replaced with an algebraic equation, and this allows one to obtain an "exact" solution for $\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}';\omega)$. In general, a Born series approximation is needed to determine $\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}';\omega)$ from the underlying integral equation. In the self-field approximation electromagnetic retardation effects across the QW screen are neglected [47,48]. Apart from a few cases related to paramagnetic QW resonance excitation [48], the neglect of retardation is justified. The one-electron density needed for an explicit calculation of $\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ is calculated in Sec. III B.

Having obtained the surface conductivity tensor $\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ we turn our attention towards a calculation of $\mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ in Sec. IV. In the diamagnetic case, and within the framework of the self-field approximation for the electromagnetic Green's function, the central problem is a determination of the electron density, $n^0(\mathbf{r})$. To obtain $n^0(\mathbf{r})$, one must calculate the relevant electronic energy eigenstates and the associated Fermi-Dirac factors for a screen with a hole. In the plane of the screen the relevant energy eigenstate wave functions are determined comprehending the hole as a 2D scatterer of incident plane waves. The potential scattering from the hole is attacked using a 2D microscopic extinction-theorem approach for the electrons. Readers interested in the basics of potential scattering, the 3D extinction theorem, and its use in physical optics may consult Refs. [49–51]. The theorem was established first by Ewald [52,53] and Oseen [54] (in the framework of molecular optics) and later extended to nonrelativistic quantum-mechanical potential scattering

by Pattanayak and Wolf [55]. The extinction approach is particularly convenient because it allows one to treat a hole surrounded by an electronic selvedge. The selvedge area (in 2D) is the region in which the electron density changes from its bulk value to zero (in the vacuum hole). In Sec. IV A, we start from a 2D electron version of the famous optical (acoustic) integral theorem of Helmholtz and Kirchhoff [4–6]. The associated outgoing 2D scalar propagator is the Hankel function of zeroth order and first kind. In Sec. IV B, the relevant extinction theorems for the hole, selvedge, and bulk areas are established, and it is shown how one from these may obtain integral equations, basically form identical to those used in conventional potential scattering theory [49,50]. The Fermi-Dirac factors entering the calculation of $n^0(\mathbf{r})$ and $n^0_\infty(\mathbf{r})$ must be identical because the potential scattering from the hole selvedge area is elastic. We prove this assertion by an explicit calculation. In Sec. IV C, we discuss the simplified case in which it is assumed that the potential barrier to vacuum is infinitely high.

In Sec. V, we finish our paper with a calculation of the ED-ED aperture response tensor $\boldsymbol{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) - \mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$, paying particular attention to its integrated form, $\boldsymbol{\Delta}(\omega)$, which is the primary quantity in the small-hole limit. The tensorial form of $\boldsymbol{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ [identical to that of $\boldsymbol{\Delta}(\omega)$] is discussed and compared to the form obtained for $\boldsymbol{\Delta}(\omega)$ in our previous article [46] for a 2D screen-plus-hole system exhibiting infinitesimal rotational symmetry and reflection symmetry.

II. QUANTUM THEORY OF DIFFRACTION: DIAMAGNETIC COUPLING IN A JELLIUM QUANTUM-WELL SCREEN

As indicated in the Introduction, the present authors recently established a quantum theory of diffraction of light from a small hole based on the solution of the microscopic Maxwell-Lorentz equations [46]. In Sec. 2 of Appendix A, we present a short summary of our quantum theory of diffraction. From a knowledge of the difference between the microscopic conductivity tensors for screens with $[\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)]$ and without $[\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)]$ a hole, one can obtain the causal effective aperture (hole) response tensor, $\boldsymbol{\Delta}(\mathbf{r},\mathbf{r}';\omega)$. A comprehensive literature exists for the calculation of $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$ in various approximations (see, e.g., Refs. [9], [56], and [48] and references therein). Here we base our analysis on a single-particle random-phase-approximation (RPA) expression for $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$ and its form-identical version for $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$. Apart from the electromagnetic angular frequency (ω), only light-unperturbed electronic properties and statistics enter the formula for $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$ [and $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$].

A. Quantum theory of the microscopic conductivity tensor

We start by turning our attention towards the quantum-mechanical structure of the conductivity tensor $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$ [or $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$, as they are form identical]. The quantum-mechanical calculation of $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$ can be found, e.g., in Ref. [9]. Readers interested in a deeper understanding of linear nonlocal quantum-mechanical theory as such may also consult Ref. [57], where also a comprehensive list of relevant literature is given. Although a many-body calculation of $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$ can be carried out, it is for the present purpose sufficient to base our considerations on the single-particle (one-electron) expression for $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$. For a *closed system* with spin degeneracy one has [9]

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

where $\mathbf{J}_{i\to j}(\mathbf{r})$ and $\mathbf{J}_{j\to i}(\mathbf{r}')$ are the transition current densities from state i to state j, and from j to i, respectively. As indicated, these current densities are evaluated at the space points $\mathbf{r}$ and $\mathbf{r}'$. The states (i,j) are stationary states with energies (E_i,E_j) and time-independent wave functions: $[\Psi^i(\mathbf{r}),\Psi^j(\mathbf{r})]$. The expressions for the transition current densities are given by

$$\mathbf{J}_{i\to j}(\mathbf{r}) = -\frac{e\hbar}{2mi}[\Psi^{j*}(\mathbf{r})\nabla\Psi^i(\mathbf{r}) - \Psi^i(\mathbf{r})\nabla\Psi^{j*}(\mathbf{r})] \tag{2}$$

and

$$\mathbf{J}_{j\to i}(\mathbf{r}) = [\mathbf{J}_{i\to j}(\mathbf{r})]^*, \tag{3}$$

$-e$ being the electron charge and m the electron mass. In Eq. (2) f_i (f_j) is the occupation factor for state i (j). In thermal equilibrium f_i equals the Fermi-Dirac distribution function, viz.,

$$f_i = (\exp\{[E_i - \mu(T)]/(kT)\} + 1)^{-1}, \tag{4}$$

where $\mu(T)$ is the chemical potential at the absolute temperature T, and k is Boltzmann's constant. The factor 2 in front of the summation sign in Eq. (1) originates in the summation over (assumed) degenerate spin states, and f_i, therefore, with the help of $\mu(T)$, is normalized to half the number of electrons in the given system.

A generalization of Eq. (1) to *open systems* is a difficult task in most cases, if not impossible. However, using a simple relaxation-time approximation for open systems, Eq. (1) holds with the replacement $\omega \to \omega + i/\tau$, τ being the relevant (overall) energy relaxation time [9,58].

B. Diamagnetic electron dynamics

In the mid- and far-infrared regions the microscopic conductivity of metals and semiconductors usually is well described retaining only the diamagnetic contribution to $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$, and in a BCS superconductor the conductivity is purely diamagnetic for frequencies below the superconducting gap frequency. The diamagnetic (dia) contribution to the conductivity, $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$, originates in the local gauge invariance demand on quantum electrodynamics [9] and is thus always present. It can be shown by a rather elaborate calculation that [9,57]

$$\boldsymbol{\sigma}_{\rm dia}(\mathbf{r},\mathbf{r}';\omega) = \frac{1}{i\omega}\sum_{i\neq j}\frac{f_j - f_i}{E_j - E_i}\mathbf{J}_{i\to j}(\mathbf{r})\mathbf{J}_{j\to i}(\mathbf{r}'). \tag{5}$$

For $\omega \to 0$, $\boldsymbol{\sigma}_{\rm dia}(\mathbf{r},\mathbf{r}';\omega) \to \infty$, a result in agreement with the fact that the dc conductivity of a superconductor is infinite. Although the individual (i,j) contributions to $\boldsymbol{\sigma}_{\rm dia}(\mathbf{r},\mathbf{r}';\omega)$

are spatially nonlocal, it turns out that the sum of these contributions become local and isotropic. Thus [9,57],

$$\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega) = \Sigma(\mathbf{r};\omega)\delta(\mathbf{r}-\mathbf{r}')\mathbf{U}, \tag{6}$$

where, with the inclusion of a phenomenological relaxation time,

$$\Sigma(\mathbf{r};\omega) = \frac{ie^2}{m(\omega+i/\tau)}n^0(\mathbf{r}). \tag{7}$$

The quantity $n^0(\mathbf{r})$ is the local field-unperturbed electron density given by

$$n^0(\mathbf{r}) = 2\sum_i f_i|\Psi^i(\mathbf{r})|^2. \tag{8}$$

Written in the form of Eqs. (6) and (7), $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ resembles the well-known phenomenological Drude formula for the conductivity of a free-electron metal, and in a certain sense $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ *does* represent a *generalized* quantum mechanical version of the Drude model.

Apart from the fact that $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ may give one the dominating contribution to the screen conductivity in a number of cases, the local structure of $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ makes the calculation of the causal effective aperture response tensor, $\boldsymbol{\Delta}(\mathbf{r},\mathbf{r};\omega)$, somewhat easier. Furthermore, the local form underlines in an illuminating manner the difference between $\boldsymbol{\sigma}^{\mathrm{cau}}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ and $\boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$, as we realize now. By combining Eqs. (A5) and (6) one obtains

$$\boldsymbol{\sigma}^{\mathrm{cau}}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega) = \Sigma(\mathbf{r};\omega)\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega). \tag{9}$$

The nonlocality and anisotropy of the causal diamagnetic conductivity hence are solely associated with the field-field response tensor relating the local electric field at $\mathbf{r}$, $\mathbf{E}(\mathbf{r};\omega)$, to the incident field, $\mathbf{E}^0(\mathbf{r}';\omega)$, in surrounding points, $\mathbf{r}'$.

In the diamagnetic case the integral equation for the field-field response tensor [Eq. (A6)] is simplified to

$$\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega) = \mathbf{U}\delta(\mathbf{r}-\mathbf{r}') + i\mu_0\omega\int_{-\infty}^{\infty}\Sigma(\mathbf{r}'';\omega)\mathbf{G}(\mathbf{r},\mathbf{r}'';\omega) \cdot \boldsymbol{\Gamma}(\mathbf{r}'',\mathbf{r}';\omega)d^3r''. \tag{10}$$

In cases where the local-field correction is small one may rely on an iterative solution of Eq. (10), that is,

$$\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega) = \mathbf{U}\delta(\mathbf{r}-\mathbf{r}') + i\mu_0\omega\mathbf{G}(\mathbf{r},\mathbf{r}';\omega)\Sigma(\mathbf{r}';\omega) + (i\mu_0\omega)^2\int_{-\infty}^{\infty}\Sigma(\mathbf{r}'';\omega)\mathbf{G}(\mathbf{r},\mathbf{r}'';\omega) \cdot \mathbf{G}(\mathbf{r}'',\mathbf{r}';\omega)\Sigma(\mathbf{r}';\omega)d^3r'' + \cdots. \tag{11}$$

In the iterative approach the local-field tensor is composed as a sum of scattering terms of increasing order, as shown schematically in Fig. 1. In general, the multiple scattering correlating the incident and local fields in the space points $\mathbf{r}'$ and $\mathbf{r}$, is mediated by both electronic and electromagnetic couplings; cf. the form of the kernel $\mathbf{K}(\mathbf{r},\mathbf{r}';\omega)$ in Eq. (A7), and the schematic illustration in Fig. 2. In the *first Born approximation* (1B), where only the first two terms on the right side of Eq. (11) are kept, the causal diamagnetic conductivity

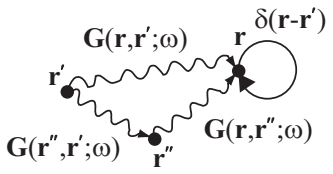

FIG. 1. Zero-, first-, and second-order contributions to the local-field tensor in the diamagnetic case.

is given by

$$\boldsymbol{\sigma}^{\mathrm{cau}}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega) = \boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega) + i\mu_0\omega\Sigma(\mathbf{r};\omega) \times \mathbf{G}(\mathbf{r},\mathbf{r}';\omega)\Sigma(\mathbf{r}';\omega),\ (1\mathrm{B}), \tag{12}$$

and the spatial nonlocality in $\boldsymbol{\sigma}^{\mathrm{cau}}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ alone is related to *direct* electromagnetic-field propagation between $\mathbf{r}'$ and $\mathbf{r}$.

C. Jellium quantum-well screen

As already indicated, the diffraction of light from high-density electron-gas screens will be in focus in this paper. We shall base our considerations on an *effective* one-electron picture, and assume that the positive charge (ion) "background" is fixed and uniform. An electron gas with a uniformly smeared-out fixed ion background is called a *jellium* and is a dream matter for theorists. Although the single-particle approximation often is a crude one, it appears difficult to go beyond this approach considering the fact that an understanding of the electron dynamics in the vicinity of the hole is decisive for a description of the diffraction process. The expression for the conductivity tensor, $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$, in Eq. (1) hence is obtained within the framework of what historically has been called the dynamical RPA (or the *self-consistent field* method) [58,59].

A reduction of the jellium formalism from a many-body to an effective one-body description in general requires an introduction of a *spatially nonlocal scalar potential*, $V(\mathbf{r},\mathbf{r}')$. In the framework of the Hartree-Fock theory [58,59] this potential nonlocality is associated with the exchange term in the electron-electron interaction.

Starting from the effective one-electron time-independent Schrödinger equation with a static nonlocal potential, viz.,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + \int V(\mathbf{r},\mathbf{r}')\Psi(\mathbf{r}')d^3r' = E\Psi(\mathbf{r}), \tag{13}$$

where $\Psi(\mathbf{r})$ is a stationary-state wave function and E its associated energy, we *assume* that the potential can be separated as

$$V(\mathbf{r},\mathbf{r}') = V_{\parallel}(\mathbf{r}_{\parallel},\mathbf{r}'_{\parallel})\delta(z-z') + V_{\perp}(z,z')\delta(\mathbf{r}_{\parallel}-\mathbf{r}'_{\parallel}), \tag{14}$$

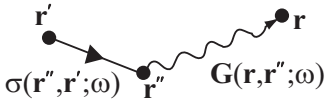

FIG. 2. Schematic illustration of the electronic and electromagnetic couplings in the kernel $\mathbf{K}(\mathbf{r},\mathbf{r}';\omega)$ entering the integral equation for the local-field tensor $\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega)$.

where $\mathbf{r}_\parallel(\mathbf{r}'_\parallel) = (x(x'), y(y'))$ and $z(z')$ are the Cartesian coordinates parallel ($\parallel$) and perpendicular ($\perp$) to the plan of our flat screen. Although the assumption certainly not is correct in general, it appears to be a fair approximation when the screen is so thin it behaves like a QW for the electron dynamics perpendicular the plane of the screen. Under the assumption in Eq. (14), the time-independent Schrödinger equation is reduced to the form

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + \int V_\parallel(\mathbf{r}_\parallel,\mathbf{r}'_\parallel)\Psi(\mathbf{r}'_\parallel,z)d^2r'_\parallel + \int V_\perp(z,z')\Psi(\mathbf{r}_\parallel,z')dz' = E\Psi(\mathbf{r}), \quad (15)$$

and the product ansatz

$$\Psi(\mathbf{r}_\parallel,z) = \psi(\mathbf{r}_\parallel)\phi(z), \quad (16)$$

in turn, decouples the Schrödinger equation into parts associated with stationary-state problems along and perpendicular to the screen. Hence,

$$-\frac{\hbar^2}{2m}\nabla^2_\parallel\psi(\mathbf{r}_\parallel) + \int V_\parallel(\mathbf{r}_\parallel,\mathbf{r}'_\parallel)\psi(\mathbf{r}'_\parallel)d^2r'_\parallel = E_\parallel\psi(\mathbf{r}_\parallel), \quad (17)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\phi(z) + \int_{\mathrm{QW}} V_\perp(z,z')\phi(z')dz' = E_\perp\phi(z), \quad (18)$$

with total energy

$$E = E_\parallel + E_\perp, \quad (19)$$

and $\nabla^2_\parallel = \partial^2/\partial x^2 + \partial^2/\partial y^2$. In Eq. (18) it has been emphasized that the screen potential in the z direction is that of a QW and that the electrons are bound in the well potential. In a QW system it is often a good approximation to consider the potential as local, i.e., $V_\perp(z,z') = V_\perp(z)\delta(z-z')$.

In the present work we assume that the screen is so thin that there is only one bound QW state. In this case the electron dynamics is confined to the plane of the screen, essentially, and a 2D analysis starting from Eq. (17) is sufficient. In a forthcoming article [60] we shall extend our theory to two-level QW screens. In the context of the study in Ref. [46], resonance excitation between the two levels makes it important to keep the field-induced QW current density perpendicular to the plane of the screen in the theoretical calculation. In Appendix B we briefly discuss a 2D version of the Hartree-Fock theory for a screen without a hole. The theory shows that the eigenfunctions of the time-independent Schrödinger equation may be taken as plane waves and that the eigenenergies are modified (lowered) in comparison to those in the Hartree (free-electron) case.

III. DIAMAGNETIC CAUSAL SURFACE (ED-ED) CONDUCTIVITY OF A SCREEN WITHOUT A HOLE

A. Local field tensor in self-field approximation

When a QW is sufficiently thin it is usually a good approximation to neglect electromagnetic retardation effects across the well. Remembering that the relevant Green's function for QW screens must be described in disk contraction [61–63], the nonretarded (self-field) part of the dyadic $\mathbf{G}$ is in the mixed representation [9] given by [63]

$$\mathbf{G}(z-z') = -\left(\frac{c}{\omega}\right)^2\delta(z-z')\hat{\mathbf{z}}\hat{\mathbf{z}}, \quad (20)$$

where $\hat{\mathbf{z}}$ is a unit vector in the z direction. The result in Eq. (20) and Ref. [63] deviate by a factor of -1 because of different sign conventions for the Green's function in Ref. [63] and here (a factor of (-1) is missing on the self-field term in Eq. (65) of Ref. [46]). As indicated, the self-field part of $\mathbf{G}(z-z';\omega) \equiv \mathbf{G}(z-z')$ is independent of the wave vector ($\mathbf{q}_\parallel$) along the QW plane. By 2D Fourier integral transformation one then obtains in the space-frequency domain

$$\mathbf{G}(\mathbf{r}-\mathbf{r}') = \int_{-\infty}^{\infty}\mathbf{G}(z-z')e^{i\mathbf{q}_\parallel\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}\frac{d^2q_\parallel}{(2\pi)^2} = -\left(\frac{c}{\omega}\right)^2\delta(\mathbf{r}-\mathbf{r}')\hat{\mathbf{z}}\hat{\mathbf{z}}, \quad (21)$$

a well-known result in view of the fact that the so-called self-field dyadic ($\mathbf{L}$) [9] is $\mathbf{L} = \hat{\mathbf{z}}\hat{\mathbf{z}}$ in disk contraction [64]. Note that the neglect of retardation across the QW leads to a suppression of retardation effects along the plane of the well.

In the self-field approximation, the integral equation for the local field tensor $\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}';\omega) \equiv \boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}')$ [Eq. (10)] is reduced to the algebraic form

$$\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}') = \mathbf{U}\delta(\mathbf{r}-\mathbf{r}') + \frac{1}{i\varepsilon_0\omega}\Sigma_\infty(\mathbf{r})\hat{\mathbf{z}}\hat{\mathbf{z}}\cdot\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}'), \quad (22)$$

where the subscript ∞ is added to remind the reader that we are studying a QW screen without a hole. To determine $\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}')$, we multiply Eq. (22) by the dyads $\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}}$ and $\hat{\mathbf{z}}\hat{\mathbf{z}}$, respectively. This gives

$$(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\cdot\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}') = (\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\delta(\mathbf{r}-\mathbf{r}'), \quad (23)$$

$$\hat{\mathbf{z}}\hat{\mathbf{z}}\cdot\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\hat{\mathbf{z}}\hat{\mathbf{z}} + \frac{\Sigma_\infty(\mathbf{r})}{i\varepsilon_0\omega}\hat{\mathbf{z}}\hat{\mathbf{z}}\cdot\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}'). \quad (24)$$

From Eq. (24) now we find

$$\hat{\mathbf{z}}\hat{\mathbf{z}}\cdot\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}') = \frac{\delta(\mathbf{r}-\mathbf{r}')\hat{\mathbf{z}}\hat{\mathbf{z}}}{1-(i\varepsilon_0\omega)^{-1}\Sigma_\infty(\mathbf{r})}. \quad (25)$$

Note that the $\hat{\mathbf{z}}\hat{\mathbf{z}}$ part of $\boldsymbol{\Gamma}_\infty$ in the collisionless limit ($\omega\tau\to\infty$) has a resonance at the local plasma frequency, $\omega_p^\infty(\mathbf{r}) = [n_\infty^0(\mathbf{r})e^2/(m\varepsilon_0)]^{1/2}$. By adding Eqs. (23) and (25), we have the solution for the local-field factor, namely,

$$\boldsymbol{\Gamma}_\infty(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\left[\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}} + \frac{\hat{\mathbf{z}}\hat{\mathbf{z}}}{1-(i\varepsilon_0\omega)^{-1}\Sigma_\infty(\mathbf{r})}\right]. \quad (26)$$

We know from our previous work [46] that the so-called causal surface conductivity tensor in the limit where the QW screen behaves like an ED radiator and absorber sheet (ED-ED sheet) is given by

$$\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel) = \int_{\mathrm{QW}}\boldsymbol{\sigma}_\infty^{\mathrm{cau}}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel,z,z')dz'dz. \quad (27)$$

By combining Eqs. (9), (26), and (27), we obtain the following integral expression for the diamagnetic causal surface

conductivity of a screen without a hole:

$$\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \delta(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\Big[(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\int_{\mathrm{QW}} \Sigma_\infty(\mathbf{r};\omega)dz + \hat{\mathbf{z}}\hat{\mathbf{z}}\int_{QW} \frac{\Sigma_\infty(\mathbf{r};\omega)dz}{1-(i\varepsilon_0\omega)^{-1}\Sigma_\infty(\mathbf{r};\omega)}\Big]. \quad (28)$$

In deriving Eq. (28) the integral over z' was carried out utilizing that $\delta(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\delta(z-z')$.

Before continuing the general line of development let us return to Eq. (26). In the 1B, where $[1-(i\varepsilon_0\omega)^{-1}\Sigma_\infty]^{-1} \approx 1 + (i\varepsilon_0\omega)^{-1}\Sigma_\infty$, the local-field tensor becomes

$$\mathbf{\Gamma}^{\mathrm{1B}}_\infty(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')[\mathbf{U} + \hat{\mathbf{z}}\hat{\mathbf{z}}(i\varepsilon_0\omega)^{-1}\Sigma_\infty(\mathbf{r})], \quad (29)$$

in agreement with the expression in Eq. (11), with $\mathbf{G}$ given by Eq. (21). In the self-field limit we do not need to rely on an iterative solution (approximation) for the local-field tensor; we have an "exact" solution [Eq. (26)].

B. Quantum-well single-electron density

A comparison of Eqs. (7) and (28) tells us that we only need to determine the one-electron density $n^0_\infty(\mathbf{r})$ in order to be able to calculate the diamagnetic surface conductivity tensor in the self-field approximation (at a given frequency). When the potential is separable [Eq. (14)], the energy eigenstates have product form with $i = (m,n)$, i.e.,

$$\Psi^i(\mathbf{r}) \equiv \Psi^{m,n}(\mathbf{r}_\parallel,z) = \psi^m(\mathbf{r}_\parallel)\phi^n(z), \quad (30)$$

where m and n are the quantum numbers characterizing the various eigenstates. With $i = (m,n)$, it appears from Eq. (8) that the electron density is given by

$$n^0_\infty(\mathbf{r}) = 2\sum_{m,n} f_{m,n}|\psi^m(\mathbf{r}_\parallel)|^2|\phi^n(z)|^2. \quad (31)$$

In the Hartree-Fock theory the wave function $\psi^m(\mathbf{r}_\parallel)$ may, as shown in Appendix B, be taken as plane-wave states, and in the continuum limit ($m \to \mathbf{k}_\parallel$) where (with Dirac normalization)

$$\psi^m(\mathbf{r}_\parallel) \to \frac{1}{2\pi}e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}, \quad (32)$$

the electron density takes the form

$$n^0_\infty(z) = 2\sum_n |\phi^n(z)|^2\int_{-\infty}^{\infty} f_n(E(k_\parallel))\frac{d^2k_\parallel}{(2\pi)^2} = 2\sum_n |\phi^n(z)|^2\int_0^\infty f_n(E(k_\parallel))\frac{k_\parallel dk_\parallel}{2\pi}. \quad (33)$$

The last member of Eq. (33) follows from the fact that the Fermi factor $f_n(E(k_\parallel))$ only depends on the magnitude of the wave vector $\mathbf{k}_\parallel$ [via the eigenenergy $E(k_\parallel)$ associated with the state $\exp(i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel)$]. In the 2D Hartree-Fock approach $E(k_\parallel)$ is given by Eq. (B9). In the low-temperature limit [$T \to 0$ K, $\mu(T\to 0) \equiv E_F$] the states below the Fermi energy (E_F) are occupied, and those above are empty. If the eigenenergy belonging to $\phi^n(z)$ is denoted ε_n, one has

$$f_n(E(k_\parallel);T\to 0) = \Theta(\mu(T\to 0) - \varepsilon_n - E(k_\parallel)), \quad (34)$$

where Θ is the Heaviside unit step function. The equation

$$\mu(T\to 0) - \varepsilon_n - E(k^n_\parallel) = 0 \quad (35)$$

determines for a given n the upper limit $k^n_\parallel$ for the magnitude of the wave vector $\mathbf{k}_\parallel$ of the occupied states at $T = 0$. In the low-temperature limit the electron density hence is given by

$$n^0_\infty(z;T\to 0) = \frac{1}{\pi}\sum_n |\phi^n(z)|^2\int_0^{k^n_\parallel} k_\parallel dk_\parallel = \frac{1}{2\pi}\sum_n (k^n_\parallel)^2|\phi^n(z)|^2. \quad (36)$$

In the Hartree approximation, where $(k^n_\parallel)^2 = 2m(E_F - \varepsilon_n)/\hbar^2$ one obtains the well-known result

$$n^0_\infty(z;T\to 0) = \frac{m}{\pi\hbar^2}\sum_n (E_F - \varepsilon_n)|\phi^n(z)|^2, \quad \varepsilon_n < E_F. \quad (37)$$

It is known [9,48] that the paramagnetic part of the conductivity tensor, viz., $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega) - \boldsymbol{\sigma}_{\mathrm{dia}}(\mathbf{r},\mathbf{r}';\omega)$ can give rise to strong light-induced microscopic density flows perpendicular to the QW plane when resonance excitations occur between a pair of n levels. However, in a single-level QW such resonances are absent. The isotropic form of the diamagnetic conductivity tensor implies that a weak field-induced current density flow always will be present in the z direction, even in a single-level QW screen.

By inserting Eqs. (7) and (33) into Eq. (28) the reader may write down the final result for the diamagnetic causal surface conductivity tensor of a QW screen without a hole, $\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$. Because $\Sigma_\infty(\mathbf{r};\omega) = \Sigma_\infty(z;\omega)$, the terms in the square bracket in Eq. (28) are independent of $\mathbf{r}_\parallel$. Since

$$\int_{\mathrm{QW}} |\phi^n(z)|^2 dz = 1, \forall\, n, \quad (38)$$

it furthermore appears that the first term in Eq. (28) is independent of the form of the QW potential [given the relevant $\phi^n(z)$'s].

In the 1B Eq. (28) is reduced to

$$\mathbf{S}^{\mathrm{1B}}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \delta(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\Big\{(\mathbf{U} - \hat{\mathbf{z}}\hat{\mathbf{z}})\int_{\mathrm{QW}}\Sigma_\infty(z;\omega)dz + \hat{\mathbf{z}}\hat{\mathbf{z}}\int_{QW}\Sigma_\infty(z;\omega)[1 + (i\varepsilon_0\omega)^{-1}\Sigma_\infty(z;\omega)]dz\Big\}, \quad (39)$$

and then

$$\mathbf{S}^{\mathrm{1B}}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \delta(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\Big\{\mathbf{U}\frac{ie^2}{m(\omega + i/\tau)}\int_{\mathrm{QW}} n^0_\infty(z)dz - \hat{\mathbf{z}}\hat{\mathbf{z}}(i\varepsilon_0\omega)^{-1}\Big[\frac{e^2}{m(\omega+i/\tau)}\Big]^2\int_{\mathrm{QW}}\big[n^0_\infty(z)\big]^2 dz\Big\}. \quad (40)$$

In Eq. (40) the quantity

$$\mathcal{N}^0_\infty = \int_{\mathrm{QW}} n^0_\infty(z)dz, \quad (41)$$

is the number of electrons per unit area of the screen, also called the surface electron density. In view of Eq. (38) we have the obvious result

$$\mathcal{N}_\infty^0 = 2\sum_n \int_0^\infty f_n(E(k_\parallel))\frac{k_\parallel dk_\parallel}{2\pi}. \tag{42}$$

In the Hartree approximation the surface electron density takes the simple form

$$\mathcal{N}_\infty^0(T\to 0) = \frac{m}{\pi\hbar^2}\sum_n (E_F-\varepsilon_n)\Theta(E_F-\varepsilon_n) \tag{43}$$

in the low-temperature limit.

IV. DIAMAGNETIC CAUSAL SURFACE (ED-ED) CONDUCTIVITY OF A SCREEN WITH A HOLE: 2D EXTINCTION-THEOREM APPROACH

It appears from the calculation leading to the result for the diamagnetic causal surface conductivity given in Eq. (28) that a form-identical expression holds for a screen with a hole. Thus, one "just" needs to make the replacement $\Sigma_\infty(\mathbf{r};\omega)\to\Sigma(\mathbf{r};\omega)$. The central problem in a calculation of $\mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ hence is a determination of the electron density $n^0(\mathbf{r})$ [Eq. (8)], assuming that the phenomenological relaxation time (τ) is the same as before. To obtain $n^0(\mathbf{r})$, we must calculate the relevant energy eigenstates [$\Psi^i(\mathbf{r})$] for a screen with a hole [and the associated Fermi-Dirac factors (f_i)]; see Eq. (8). Below, we base this calculation on potential scattering theory formulated in terms of a set of microscopic extinction theorems for the one-electron states.

A. Two-dimensional propagator approach for a hole with a selvedge

In Sec. III, we studied the diamagnetic causal surface conductivity, $\mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$, in the limit where the QW screen is so thin that it behaves electrodynamically as an ED-ED sheet. In the same limit the potential scattering from the hole region becomes a 2D problem. In Fig. 3 we show a top view of the hole and its surrounding selvedge, together with a qualitative schematic illustration of the potential profile. The selvedge is the surface region surrounding the hole in which the electron density changes from its bulk value (here for jellium) to zero in the (vacuum) hole.

In the bulk region we assume that the electron dynamics is well described by the Hartree (possibly Hartree-Fock) description for a screen without a hole. Such an assumption certainly will be good in the case of mesoscopic holes in a macroscopic screen. The incident electronic wave functions being scattered from the hole + selvedge area we take as plane waves, $(2\pi)^{-1}\exp(i\mathbf{k}^i_\parallel\cdot\mathbf{r}_\parallel)$, with free-electron energies (Hartree approximation) or energies modified by exchange in the calculation of the Fermi-Dirac factors. Without loss of essential generality for the present problem, we may set the bulk potential to zero; cf. Fig. 3(b).

Hence, the starting point for our stationary potential scattering analysis is the time-independent 2D Schrödinger

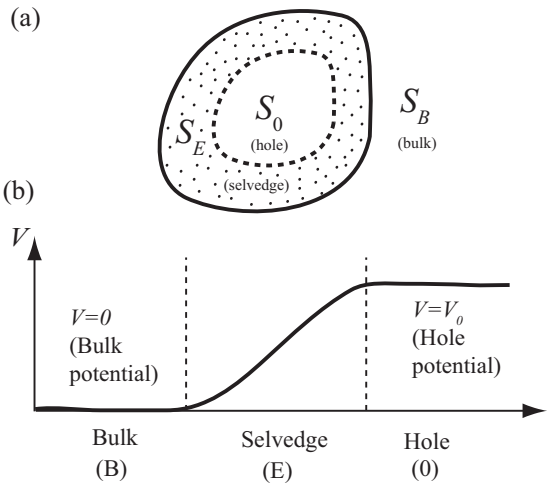

FIG. 3. (a) Vacuum hole in a 2D QW screen. The hole area denoted by S_0 is surrounded by the selvedge area S_E. Outside the selvedge the bulk area S_B of the screen extends to infinity. (b) Schematic illustration of the potential profile from the bulk through the selvedge and into the hole.

equation

$$\left[-\frac{\hbar^2}{2m}\nabla_\parallel^2 + V(\mathbf{r}_\parallel)\right]\psi^i(\mathbf{r}_\parallel) = E^i_\parallel\psi^i(\mathbf{r}_\parallel), \tag{44}$$

here written for the ith scattering state, with eigenenergy $E^i_\parallel > 0$, and $V(\mathbf{r}_\parallel)\geqslant 0$ (cf. Fig. 3). With the purpose of establishing a propagator formalism for the scattering process, we rewrite Eq. (44) as

$$[\nabla_\parallel^2 + (k^i_\parallel)^2]\psi^i(\mathbf{r}_\parallel) = \kappa^2(\mathbf{r}_\parallel)\psi^i(\mathbf{r}_\parallel), \tag{45}$$

where

$$k^i_\parallel = \left(\frac{2mE^i_\parallel}{\hbar^2}\right)^{1/2} \tag{46}$$

and

$$\kappa(\mathbf{r}_\parallel) = \left[\frac{2mV(\mathbf{r}_\parallel)}{\hbar^2}\right]^{1/2}. \tag{47}$$

Related to Eq. (45) we introduce a differential equation,

$$[\nabla_\parallel^2 + (k^i_\parallel)^2]\mathcal{G}^i(\mathbf{R}_\parallel) = -\delta(\mathbf{R}_\parallel), \tag{48}$$

for the Green's function $\mathcal{G}^i(\mathbf{R}_\parallel)$. Above, $\delta(\mathbf{R}_\parallel)$ is the 2D δ function, and $\mathbf{R}_\parallel = \mathbf{r}_\parallel - \mathbf{r}'_\parallel$. For the scattering problem at hand, the relevant solution to Eq. (48) is the outgoing (from the hole region) and retarded 2D scalar propagator

$$\mathcal{G}^i(\mathbf{R}_\parallel) = \frac{i}{4}H_0^{(1)}(k^i_\parallel|\mathbf{R}_\parallel|), \tag{49}$$

where $H_0^{(1)}$ is the Hankel function of zeroth order and first kind. In analogy to the procedure used to reach the integral theorem of Helmholtz and Kirchoff in optical diffraction, we use Eqs. (45) and (48) to establish the relation

$$\begin{aligned}\nabla_\parallel\cdot[\mathcal{G}^i(\mathbf{R}_\parallel)\nabla_\parallel\psi^i(\mathbf{r}_\parallel) - \psi^i(\mathbf{r}_\parallel)\nabla_\parallel\mathcal{G}^i(\mathbf{R}_\parallel)]\\ = \mathcal{G}^i(\mathbf{R}_\parallel)\nabla_\parallel^2\psi^i(\mathbf{r}_\parallel) - \psi^i(\mathbf{r}_\parallel)\nabla_\parallel^2\mathcal{G}^i(\mathbf{R}_\parallel)\end{aligned}$$

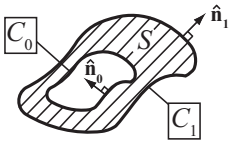

FIG. 4. Plane area S with outward-directed normal vectors $\hat{\mathbf{n}}_0$ and $\hat{\mathbf{n}}_1$ along the curves C_0 and C_1 that bound the area S.

$$= \mathcal{G}^i(\mathbf{R}_\parallel)[\nabla_\parallel^2 + (k_\parallel^i)^2]\psi^i(\mathbf{r}) - \psi^i(\mathbf{r})[\nabla_\parallel^2 + (k_\parallel^i)^2]\mathcal{G}^i(\mathbf{R}_\parallel)$$
$$= \mathcal{G}^i(\mathbf{R}_\parallel)\kappa^2(\mathbf{r}_\parallel)\psi^i(\mathbf{r}_\parallel) + \psi^i(\mathbf{r}_\parallel)\delta(\mathbf{R}_\parallel). \quad (50)$$

By integrating Eq. (50) over a plane area S, not necessarily simply connected (see Fig. 4), we get

$$\int_S \nabla'_\parallel \cdot [\mathcal{G}^i(\mathbf{R}_\parallel)\nabla'_\parallel\psi^i(\mathbf{r}'_\parallel) - \psi^i(\mathbf{r}'_\parallel)\nabla'_\parallel\mathcal{G}^i(\mathbf{R}_\parallel)]d^2r'_\parallel$$
$$= \int_S \psi^i(\mathbf{r}'_\parallel)\delta(\mathbf{R}_\parallel)d^2r'_\parallel + \int_S \mathcal{G}^i(\mathbf{R}_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel. \quad (51)$$

By means of the 2D divergence theorem, namely, $\int_S \nabla_\parallel \cdot \mathbf{f}(\mathbf{r}_\parallel)d^2r_\parallel = \oint_C \hat{\mathbf{n}}(\mathbf{r}_\parallel)\cdot\mathbf{f}(\mathbf{r}_\parallel)dr_\parallel$ we obtain the following important identity for a nonsimply connected area of the type shown in Fig. 4,

$$\int_S \psi^i(\mathbf{r}'_\parallel)\delta(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)d^2r'_\parallel$$
$$= -\int_S \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel - \Sigma_0^i(\mathbf{r}_\parallel) - \Sigma_1^i(\mathbf{r}_\parallel), \quad (52)$$

with

$$\Sigma_\beta^i(\mathbf{r}_\parallel) \equiv \oint_{C_\beta} [\psi^i(\mathbf{r}'_\parallel)\hat{\mathbf{n}}_\beta(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)$$
$$- \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\hat{\mathbf{n}}_\beta(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i(\mathbf{r}'_\parallel)]dr'_\parallel, \quad (53)$$

where β is either 0 or 1 and $\hat{\mathbf{n}}_\beta(\mathbf{r}_\parallel)$ is the local outward-directed unit (normal) vector to the closed curve C_β bounding the area S from the inside ($\beta = 0$) or outside ($\beta = 1$).

B. Extinction theorems

Extinction theorems [51–55,65–68], here microscopic and for one-electron energy eigenstates of the 2D hole geometry are derived starting from Eq. (52) using the notational details introduced in Fig. 5. We start by setting up the following three equations by integrating over the hole $S = S_0$ and setting $\mathbf{r}_\parallel = \mathbf{r}_0$, $\mathbf{r}_\parallel = \mathbf{r}_E$, and $\mathbf{r}_\parallel = \mathbf{r}_B$, respectively,

$$\psi^i(\mathbf{r}_0) = -\int_{S_0} \mathcal{G}^i(\mathbf{r}_0 - \mathbf{r}'_0)\kappa^2(\mathbf{r}'_0)\psi^i(\mathbf{r}'_0)d^2r'_0 - \Sigma_0^i(\mathbf{r}_0), \quad (54a)$$

$$0 = -\int_{S_0} \mathcal{G}^i(\mathbf{r}_E - \mathbf{r}'_0)\kappa^2(\mathbf{r}'_0)\psi^i(\mathbf{r}'_0)d^2r'_0 - \Sigma_0^i(\mathbf{r}_E), \quad (54b)$$

$$0 = -\int_{S_0} \mathcal{G}^i(\mathbf{r}_B - \mathbf{r}'_0)\kappa^2(\mathbf{r}'_0)\psi^i(\mathbf{r}'_0)d^2r'_0 - \Sigma_0^i(\mathbf{r}_B), \quad (54c)$$

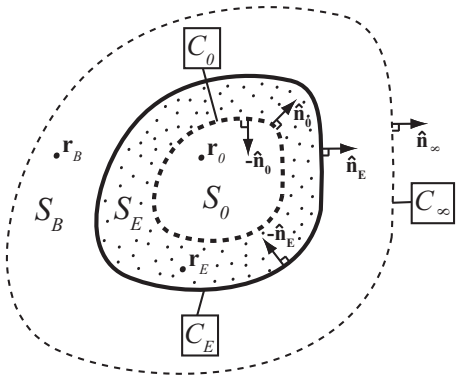

FIG. 5. The 2D hole geometry. The hole area S_0 is bounded by the curve C_0, which has an outward-directed normal vector denoted by $\hat{\mathbf{n}}_0$. The selvedge area S_E surrounds the hole area S_0 and is bounded by the curve C_0 at the inner edge and C_E at the outer edge. The outward-directed normal vector to C_E is denoted $\hat{\mathbf{n}}_E$. The bulk area S_B surrounds the selvedge area S_E and is bounded by the curves C_E and C_∞ at the inner and outer [remote (∞)] edges, respectively. The outward-directed normal vector to C_∞ is denoted by $\hat{\mathbf{n}}_\infty$. $\mathbf{r}_0$, $\mathbf{r}_E$, and $\mathbf{r}_B$ denote $\mathbf{r}_\parallel$ points inside the hole, the selvedge, and the bulk, respectively.

where

$$\Sigma_0^i(\mathbf{r}_\parallel) \equiv \oint_{C_0} [\psi^i(\mathbf{r}'_\parallel)\hat{\mathbf{n}}_0(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)$$
$$- \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\hat{\mathbf{n}}_0(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i(\mathbf{r}'_\parallel)]dr'_\parallel, \quad (55)$$

and $\kappa^2(\mathbf{r}'_0) = \kappa_0^2 = 2mV_0/\hbar^2$, which we note is independent of $\mathbf{r}'_0$.

If we integrate over the selvedge, i.e., $S = S_E$ we find

$$0 = -\int_{S_E} \mathcal{G}^i(\mathbf{r}_0 - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma_0^i(\mathbf{r}_0) - \Sigma_E^i(\mathbf{r}_0), \quad (56a)$$

$$\psi^i(\mathbf{r}_E) = -\int_{S_E} \mathcal{G}^i(\mathbf{r}_E - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma_0^i(\mathbf{r}_E) - \Sigma_E^i(\mathbf{r}_E), \quad (56b)$$

$$0 = -\int_{S_E} \mathcal{G}^i(\mathbf{r}_B - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma_0^i(\mathbf{r}_B) - \Sigma_E^i(\mathbf{r}_B), \quad (56c)$$

for $\mathbf{r}_\parallel = \mathbf{r}_0$, $\mathbf{r}_\parallel = \mathbf{r}_E$, and $\mathbf{r}_\parallel = \mathbf{r}_B$, respectively, and where

$$\Sigma_E^i(\mathbf{r}_\parallel) \equiv \oint_{C_E} [\psi^i(\mathbf{r}'_\parallel)\hat{\mathbf{n}}_E(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)$$
$$- \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\hat{\mathbf{n}}_E(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i(\mathbf{r}'_\parallel)]dr'_\parallel. \quad (57)$$

For $S = S_B$ we find for $\mathbf{r}_\parallel = \mathbf{r}_0$, $\mathbf{r}_\parallel = \mathbf{r}_E$, and $\mathbf{r}_\parallel = \mathbf{r}_B$,

$$0 = \Sigma_E^i(\mathbf{r}_0) - \Sigma_\infty^i(\mathbf{r}_0), \quad (58a)$$

$$0 = \Sigma_E^i(\mathbf{r}_E) - \Sigma_\infty^i(\mathbf{r}_E), \quad (58b)$$

$$\psi^i(\mathbf{r}_B) = \Sigma_E^i(\mathbf{r}_B) - \Sigma_\infty^i(\mathbf{r}_B), \quad (58c)$$

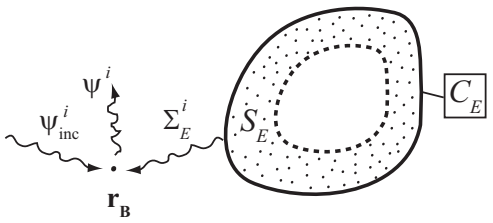

FIG. 6. Schematic illustration of the contributions to $\psi^i(\mathbf{r}_B)$.

respectively, since $\kappa^2(\mathbf{r}_B) = 0$ (the potential is flat and zero in the bulk area). Furthermore,

$$\Sigma^i_\infty(\mathbf{r}_\parallel) \equiv \oint_{C_\infty} [\psi^i(\mathbf{r}'_\parallel)\hat{\mathbf{n}}_\infty(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel) - \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\hat{\mathbf{n}}_\infty(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i(\mathbf{r}'_\parallel)]dr'_\parallel. \quad (59)$$

The incident wave function $\psi^i_{\rm inc}(\mathbf{r}_\parallel)$ may be identified as

$$\psi^i_{\rm inc}(\mathbf{r}_\parallel) = -\Sigma^i_\infty(\mathbf{r}_\parallel),\ \forall\ \mathbf{r}_\parallel, \quad (60)$$

in analogy to what is known from the optical Ewald-Oseen extinction theorem [51–54]. Readers uncertain with this identification may consult Ref. [9], e.g. A *posteriori* justification of Eq. (60) appears from the integral equation obtained below [Eq. (70)].

Using Eqs. (58c) and (60) we find

$$\psi^i(\mathbf{r}_B) = \psi^i_{\rm inc}(\mathbf{r}_B) + \Sigma^i_E(\mathbf{r}_B). \quad (61)$$

Thus, the wave function in the bulk region may be represented by the sum of the incident wave function and a "scattering" contribution from a line integral Σ^i_E around the curve bounding the selvedge C_E (see Fig. 6). Now by combining Eq. (60) with Eqs. (58a) and (58b), we obtain two *extinction theorems*,

$$\psi^i_{\rm inc}(\mathbf{r}_E) + \Sigma^i_E(\mathbf{r}_E) = 0, \quad (62)$$

$$\psi^i_{\rm inc}(\mathbf{r}_0) + \Sigma^i_E(\mathbf{r}_0) = 0, \quad (63)$$

showing that the incident wave function is extinguished in both the selvedge and the hole region by the "scattering" contribution represented by the line integral Σ^i_E (see Fig. 7). Combining Eqs. (56c) and (61) we find an expression for the wave function in the bulk, namely,

$$\psi^i(\mathbf{r}_B) = \psi^i_{\rm inc}(\mathbf{r}_B) - \int_{S_E} \mathcal{G}^i(\mathbf{r}_B - \mathbf{r}'_E) \times \kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma^i_0(\mathbf{r}_B). \quad (64)$$

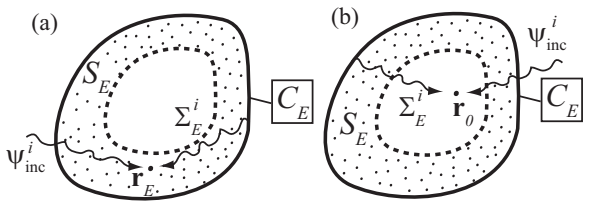

FIG. 7. Schematic illustration of the extinction theorems in Eqs. (62) and (63), (a) and (b), respectively.

Combining Eqs. (56b) and (62) we obtain an expression for the wave function in the selvedge, viz.,

$$\psi^i(\mathbf{r}_E) = \psi^i_{\rm inc}(\mathbf{r}_E) - \int_{S_E} \mathcal{G}^i(\mathbf{r}_E - \mathbf{r}'_E) \times \kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma^i_0(\mathbf{r}_E). \quad (65)$$

It is seen that the wave function in both the bulk and the selvedge can be divided into three contributions: the incident wave function, a "scattering" contribution from the selvedge, and a "scattering" contribution from the S_0 region, here written in the form of Σ^i_0, an extinction description of the wave function field originating from S_0.

Combining Eqs. (56a) and (63) we obtain a third *extinction theorem*,

$$0 = \psi^i_{\rm inc}(\mathbf{r}_0) - \int_{S_E} \mathcal{G}^i(\mathbf{r}_0 - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma^i_0(\mathbf{r}_0). \quad (66)$$

The first two terms on the right-hand side of Eq. (66) represent the total "incoming field" in S_0 from the outside: the incident wave function plus the field radiated from the selvedge. This "incoming field" is extinguished in S_0 by $\Sigma^i_0(\mathbf{r}_0)$.

Now in order to eliminate Σ^i_0 in Eqs. (64), (65), and (66), we combine these with Eqs. (54a)–(54c), obtaining

$$\psi^i(\mathbf{r}_B) = \psi^i_{\rm inc}(\mathbf{r}_B) - \int_{S_0+S_E} \mathcal{G}^i(\mathbf{r}_B - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel, \quad (67)$$

$$\psi^i(\mathbf{r}_E) = \psi^i_{\rm inc}(\mathbf{r}_E) - \int_{S_0+S_E} \mathcal{G}^i(\mathbf{r}_E - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel, \quad (68)$$

$$\psi^i(\mathbf{r}_0) = \psi^i_{\rm inc}(\mathbf{r}_0) - \int_{S_0+S_E} \mathcal{G}^i(\mathbf{r}_0 - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel. \quad (69)$$

In the equations above, it is important to note that the surface integral now extends over the hole and the selvedge regions. In compact form we may write

$$\psi^i(\mathbf{r}_\parallel) = \psi^i_{\rm inc}(\mathbf{r}_\parallel) - \int_{S_0+S_E} \mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel, \quad (70)$$

where $\mathbf{r}_\parallel \in \mathbf{r}_0,\ \mathbf{r}_E$, or $\mathbf{r}_B$. We note that Eq. (70) has the expected integral equation form of conventional scattering theory [49,50].

By applying the 2D kinetic energy operator

$$\hat{H}_{\rm kin}(\nabla_\parallel) = -\frac{\hbar^2}{2m}\nabla^2_\parallel \quad (71)$$

to Eq. (70) in the case where $\mathbf{r}_\parallel$ is a position vector in the bulk, and the incident wave function is the plane wave $\psi^i_{\rm inc}(\mathbf{r}_\parallel) = (2\pi)^{-1}\exp(i\mathbf{k}^i_\parallel\cdot\mathbf{r}_\parallel)$, one obtains

$$\hat{H}_{\rm kin}\psi^i(\mathbf{r}_\parallel) = \frac{\hbar^2}{2m}(k^i_\parallel)^2\psi^i_{\rm inc}(\mathbf{r}_\parallel) + \frac{\hbar^2}{2m}\int_{S_0+S_E}\nabla^2_\parallel\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel) \times \kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'^2_\parallel, \quad \mathbf{r}_\parallel \in \mathbf{r}_B. \quad (72)$$

With the help of the differential equation for the Green's function [Eq. (48)], which for points *outside* the domain of

integration, $S_0 + S_E$, has the form $[\nabla_\parallel^2 + (k_\parallel^i)^2]\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel) = 0$, Eq. (72) is reduced to

$$\hat{H}_{\rm kin}\psi^i(\mathbf{r}_\parallel) = \frac{\hbar^2}{2m}(k_\parallel^i)^2\left[\psi^i_{\rm inc}(\mathbf{r}_\parallel) - \int_{S_0+S_E}\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\kappa^2(\mathbf{r}'_\parallel)\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel\right] = \frac{\hbar^2}{2m}(k_\parallel^i)^2\psi^i(\mathbf{r}_\parallel), \quad \mathbf{r}_\parallel \in \mathbf{r}_B. \tag{73}$$

It appears from Eq. (73) that the total wave function $\psi^i(\mathbf{r}_\parallel)$ associated to the scattering of $\psi^i_{\rm inc}(\mathbf{r}_\parallel)$ from the selvedge (hole region) is an eigenstate for the kinetic energy operator, $\hat{H}_{\rm kin}(\nabla_\parallel)$. Due to the fact that the selvedge in the present description is assumed not to have any internal degrees of freedom, the scattering from the hole region is *elastic*. Thus, the kinetic energy of the electron is conserved in the potential scattering process. From a statistical point of view the Fermi-Dirac factors entering the analysis of the dynamics related to screens with and without a hole therefore are identical.

Provided that the potential profile through the selvedge is known, that is $\kappa^2(\mathbf{r}_E)$ a given quantity (function), (remember that the potential is flat in the hole) Eq. (70) constitutes an integral equation for the unknown wave function in the effective aperture area (selvedge + hole). Once an (approximate) solution for $\psi^i(\mathbf{r}_\parallel)$, $\mathbf{r}_\parallel \in \mathbf{r}_E$, and $\mathbf{r}_0$, has been obtained (in general, by numerical calculations), the wave function in the bulk, $\psi^i(\mathbf{r}_B)$, may be determined by direct integration. In the jellium approximation where the ionic background potential is flat, the selvedge profile is that generated by the excess electron density distribution. Hence, in general, Eq. (70) has to be supplemented by the 2D Poisson equation (longitudinal-field equation), which, written in terms of the potential $V(\mathbf{r}_\parallel)$, is

$$\nabla_\parallel^2 V(\mathbf{r}_\parallel) = -\frac{e^2}{\varepsilon_0}[n(\mathbf{r}_\parallel) - N_{\rm ion}], \tag{74}$$

where $N_{\rm ion}$ is the density of the ions (constant in the jellium screen, and zero in the hole). The potential $V(\mathbf{r}_\parallel)$ relates to $\kappa^2(\mathbf{r}_\parallel)$ via. Eq. (47). In the RPA description the electron density $n(\mathbf{r}_\parallel)$ is given by the 2D version of Eq. (8), i.e.,

$$n(\mathbf{r}_\parallel) = 2\sum_i f_i|\psi^i(\mathbf{r}_\parallel)|^2 \quad \text{(2D)}. \tag{75}$$

Thus, Eq. (70) together with Eqs. (47) and (74) constitute a set of difficult self-consistent integral equations, whose general solution for the various $\psi^i(\mathbf{r}_\parallel)$'s rely on advanced numerical techniques. It is instructive to apply the extinction-theorem formalism to the simplified case in which the barrier to the hole is assumed to be infinitely high.

C. Infinitely high potential barrier to vacuum

From a qualitative point of view an infinite-barrier model need not to be bad because one still has a selvedge region, although with a potential profile different from the one belonging to finite-barrier models. For the infinite-barrier (IB) model, $V_0 \to \infty \Rightarrow \kappa_0 \to \infty$, and $\psi^i(\mathbf{r}_0) \to 0$, $\forall\ i$. As a consequence, Eqs. (54a)–(54c), related to the electron dynamics in the hole, vanish. At an infinitely high barrier one cannot uphold the *physical requirement* that the normal derivative of the wave function is continuous. The wave function itself, however, stays continuous. Referring to Fig. 8, the following (boundary) relations now must be used in the extinction-theorem analysis:

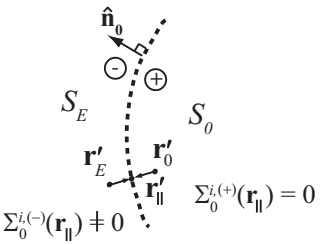

FIG. 8. Magnification of the boundary between the hole and the selvedge. + is in the hole region and − is in the selvedge region.

$$\psi^i_{(+)}(\mathbf{r}'_0 \to \mathbf{r}'_\parallel) = \psi^i_{(-)}(\mathbf{r}'_E \to \mathbf{r}'_\parallel) = 0, \tag{76}$$

$$\hat{\mathbf{n}}_0(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i_{(+)}(\mathbf{r}'_0 \to \mathbf{r}'_\parallel) = 0, \tag{77}$$

$$\hat{\mathbf{n}}_0(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i_{(-)}(\mathbf{r}'_E \to \mathbf{r}'_\parallel) \neq 0, \tag{78}$$

for a point $\mathbf{r}'_\parallel$ on the boundary. In the IB model, Eq. (66) is replaced with

$$0 = \psi^i_{\rm inc}(\mathbf{r}_0) - \int_{S_E}\mathcal{G}^i(\mathbf{r}_0 - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_E)d^2r'_E + \Sigma_0^{i,(-)}(\mathbf{r}_0), \tag{79}$$

where

$$\Sigma_0^{i,(-)}(\mathbf{r}_\parallel) = -\oint_{C_0}\mathcal{G}^i(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)\hat{\mathbf{n}}_0(\mathbf{r}'_\parallel)\cdot\nabla'_\parallel\psi^i_{(-)}(\mathbf{r}'_\parallel)dr'_\parallel. \tag{80}$$

The superscript (−) on the left-hand side of Eq. (80) is meant to remind us that the line integral along the C_0 contour must be evaluated on the selvedge side; cf. Fig. 8. From Eqs. (64) and (65) we obtain

$$\psi^i(\mathbf{r}_B) = \psi^i_{\rm inc}(\mathbf{r}_B) - \int_{S_E}\mathcal{G}^i(\mathbf{r}_B - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_\mathbf{E})d^2r'_E + \Sigma_0^{i,(-)}(\mathbf{r}_B), \tag{81}$$

$$\psi^i(\mathbf{r}_E) = \psi^i_{\rm inc}(\mathbf{r}_E) - \int_{S_E}\mathcal{G}^i(\mathbf{r}_E - \mathbf{r}'_E)\kappa^2(\mathbf{r}'_E)\psi^i(\mathbf{r}'_\mathbf{E})d^2r'_E + \Sigma_0^{i,(-)}(\mathbf{r}_E). \tag{82}$$

Equation (82) now is the central equation that needs to be solved in order to determine $\psi^i(\mathbf{r}_E)$. Subsequently, $\psi^i(\mathbf{r}_B)$ is obtained by direct integration of Eq. (81).

Equations (80) and (81) reveal that in the extreme limit where the selvedge of the hole is disregarded, the scattering contribution to the total wave function relates solely to the line integral along the hole contour. In Kottler's formulas [17] for the approximate Kirchhoff-like solution of electromagnetic diffraction by an ideal screen there also appear line integrals along the edge of the aperture (see also Ref. [15]). The integrands of Kottler involve the electromagnetic field, and

whether there exists a link between Kottler's line integrals and our involving the gradient of the electron wave function is not known.

D. Causal surface conductivity

Let us return to the integral equation for $\psi^i(\mathbf{r}_\parallel)$ [Eq. (70)]. Assuming that the incident wave function is planar, the continuum form of the equation is

$$\psi(\mathbf{r}_\parallel;\mathbf{k}_\parallel) = \frac{1}{2\pi}\exp(i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel) + \psi_{\rm scatt}(\mathbf{r}_\parallel;\mathbf{k}_\parallel), \tag{83}$$

where

$$\psi_{\rm scatt}(\mathbf{r}_\parallel;\mathbf{k}_\parallel) = -\int_{S_0+S_E} \mathcal{G}(k_\parallel|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|)\kappa^2(\mathbf{r}'_\parallel)\psi(\mathbf{r}'_\parallel;\mathbf{k}_\parallel)d^2r'_\parallel, \tag{84}$$

is the scattered part of the total wave function belonging to a *given* incident wave function with vectorial quantum index $\mathbf{k}_\parallel$. The states $\psi(\mathbf{r}_\parallel;\mathbf{k}_\parallel)$ and $\psi_{\rm scatt}(\mathbf{r}_\parallel;\mathbf{k}_\parallel)$ are *not* plane-wave states, of course. The $\mathbf{k}_\parallel$ appearing in the argument of these states is meant to remind the reader that they belong to the wave vector $\mathbf{k}_\parallel$ of the incident state.

The electron density for a screen with a hole thus is given by

$$n^0(\mathbf{r}_\parallel,z) = 2\sum_n |\Phi^n(z)|^2 \int_{-\infty}^{\infty} f_n(E(k_\parallel))|\psi(\mathbf{r}_\parallel;\mathbf{k}_\parallel)|^2 d^2k_\parallel. \tag{85}$$

As indicated, the z part of the wave functions will be different for screens with $[\Phi^n(z)]$ and without $[\phi^n(z)]$ a hole. However, when the screen is so thin that the electron dynamics essential is 2D, *and the hole is of mesoscopic size*, below we may take

$$\Phi^n(z) \simeq \phi^n(z). \tag{86}$$

In a forthcoming paper [60] on hole diffraction, in which the role of the resonance scattering between QW states is treated, we shall discuss the difference between $\phi^n(z)$ and $\Phi^n(z)$.

In the regime of dominating diamagnetic electron-field coupling the ED-ED causal surface conductivity tensor is given by

$$\mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \delta(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)\Big[(\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\int_{\rm QW}\Sigma(\mathbf{r}_\parallel,z;\omega)dz + \hat{\mathbf{z}}\hat{\mathbf{z}}\int_{\rm QW}\frac{\Sigma(\mathbf{r}_\parallel,z;\omega)dz}{1-(i\varepsilon_0\omega)^{-1}\Sigma(\mathbf{r}_\parallel,z;\omega)}\Big]. \tag{87}$$

As for the screen without a hole [Eq. (28)], we have again calculated the local-field tensor in the self-field approximation.

V. ED-ED APERTURE RESPONSE TENSOR

A. Aperture response tensor: Small-hole limit

The difference tensor

$$\mathbf{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \mathbf{S}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) - \mathbf{S}_\infty(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega), \tag{88}$$

which we call the *ED-ED causal effective aperture response tensor* is, as noted before, a fundamental quantity in the microscopic theory of light diffraction from small holes in QW screens [46]. The tensor is different from zero only in the effective aperture region ($\mathcal{A}$); see Ref. [46]. In the present diamagnetic case the surface electron density $[\mathcal{N}^0(\mathbf{r}_\parallel)]$ rapidly heals to its bulk value ($\mathcal{N}^0_\infty$) as one goes away from the hole. Qualitatively,

$$\mathcal{N}^0(\mathbf{r}_\parallel) - \mathcal{N}^0_\infty \approx 0, \tag{89}$$

when the scattered part of the wave function has become sufficiently small. The range of the scattered wave function is determined by the $\mathcal{G}(k_\parallel|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|)$'s (Hankel functions) for the various $|\mathbf{k}_\parallel|$ values and the relevant $|\mathbf{r}'_\parallel|$ in S_0+S_E.

In the ED-ED limit (here with respect to the coordinates in the plane of the screen), the integrated tensorial quantity

$$\mathbf{\Delta}(\omega) = \int_{\mathcal{A}} \mathbf{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)d^2r'_\parallel d^2r_\parallel \tag{90}$$

is the one of primary physical interest. The quantity $(i/\omega)\mathbf{\Delta}(\omega)$ is the ED polarizability tensor of the hole [46]. It appears from Eqs. (28) and (87) that $\mathbf{\Delta}(\omega)$ has the tensorial form

$$\mathbf{\Delta}(\omega) = (\mathbf{U}-\hat{\mathbf{z}}\hat{\mathbf{z}})\Delta_\parallel(\omega) + \hat{\mathbf{z}}\hat{\mathbf{z}}\Delta_\perp(\omega). \tag{91}$$

The ED polarizability hence is anisotropic, but uniaxial. The preceding analysis shows us how $\Delta_\parallel(\omega)$ and $\Delta_\perp(\omega)$ may be obtained integrating, respectively, $\Sigma-\Sigma_\infty$ and $\Sigma/[1-(i\varepsilon_0\omega)^{-1}\Sigma] - \Sigma_\infty/[1-(i\varepsilon_0\omega)^{-1}\Sigma_\infty]$ over the 2D aperture region ($\mathcal{A}$) and the QW coordinate. In Ref. [46] it was argued on general grounds that for a 2D system (screen plus hole) exhibiting rotational and reflection symmetry $\mathbf{\Delta}(\omega)$ has the tensorial form given in Eq. (91). Our jellium screen (without a hole) satisfies the above-mentioned symmetry criteria, *but* the tensorial form in Eq. (91) is obtained without symmetry demands on the geometrical form of the hole. The form of Eq. (91) reflects the common form of the local-field tensors $\mathbf{\Gamma}$ and $\mathbf{\Gamma}_\infty$ [cf. Eq. (26), and the introductory remarks to Sec. IV]. In turn, the uniaxial form may by traced back to the isotropy of the spatially local diamagnetic conductivity tensor [Eq. (6)] *and* the self-field (local) approximation for the Green's function [Eq. (21)].

B. Zeroth-order Born approximation

It readily appears from Eqs. (28), (40), (41), and (87) that the aperture response tensor $\mathbf{\Delta}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ in the zeroth-order Born approximation (0B) is given by

$$\mathbf{\Delta}^{\rm 0B}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega) = \mathbf{U}\frac{ie^2\delta(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}{m(\omega+i/\tau)}\big[\mathcal{N}^0(\mathbf{r}_\parallel)-\mathcal{N}^0_\infty\big], \tag{92}$$

and thus it is isotropic in lowest order. The result in Eq. (92) underlines the fact that the aperture response tensor is nonvanishing only in the effective optical aperture area ($\mathcal{A}$). The isotropic polarizability tensor related to Eq. (92) is given by $(i/\omega)\mathbf{\Delta}^{\rm 0B}(\omega)$, where

$$\mathbf{\Delta}^{\rm 0B}(\omega) = \mathbf{U}\frac{ie^2}{m(\omega+i/\tau)}\int\big[\mathcal{N}^0(\mathbf{r}_\parallel)-\mathcal{N}^0_\infty\big]d^2r_\parallel. \tag{93}$$

Now

$$\mathcal{N}^0(\mathbf{r}_\parallel) - \mathcal{N}^0_\infty = 2\sum_n \int_{-\infty}^{\infty} f_n(E(k_\parallel))[|\psi(\mathbf{r}_\parallel;\mathbf{k}_\parallel)|^2 - |\psi_{\rm inc}(\mathbf{r}_\parallel;\mathbf{k}_\parallel)|^2]d^2k_\parallel$$

$$= 2\sum_n \int_{-\infty}^{\infty} f_n(E(k_\parallel))\big\{|\psi_{\rm scatt}(\mathbf{r}_\parallel;\mathbf{k}_\parallel)|^2 + \big[\psi_{\rm inc}(\mathbf{r}_\parallel;\mathbf{k}_\parallel)\psi^*_{\rm scatt}(\mathbf{r}_\parallel;\mathbf{k}_\parallel) + \text{c.c.}\big]\big\} d^2k_\parallel, \tag{94}$$

a result which explicitly demonstrates that the range of $\mathbf{\Delta}^{0\rm B}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\omega)$ is given by the Hankel function $H_0^{(1)}(k_\parallel|\mathbf{r}_\parallel - \mathbf{r}'_\parallel)$ [for all relevant $k_\parallel$'s and $\mathbf{r}'_\parallel$'s]. In Eq. (94) $\psi_{\rm inc}(\mathbf{r}_\parallel;k_\parallel) = (2\pi)^{-1}\exp(i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel)$, as previously.

APPENDIX A: MICROSCOPIC DIFFRACTION THEORY

1. Classical theory and its limitations

In the framework of classical electrodynamics, theoretical studies of diffraction of an electromagnetic field from one or more holes (apertures) in a solid screen are based on a combination of the *macroscopic Maxwell equations* and an appropriate set of *macroscopic constitutive relations* usually linear. To understand the main principles of classical diffraction, it is sufficient to study a plane screen with a single hole. However, it must not be forgotten that important electromagnetic interference effects appear in diffraction from screens with two (several or many) holes. In particular, screens with regular arrays of holes may give rise to interesting coherent diffraction phenomena [18,69]. For holes sufficiently close to each other, coherent diffraction effects stemming from "hole interactions" mediated by *long-range* plasmon, polariton, or plasmariton modes or by *short-range* near-field couplings may appear. The above-mentioned partly electronic couplings cannot, in general, be treated on the basis of classical diffraction theory.

In macroscopic electrodynamics only spatial averages ($\langle\cdots\rangle$) of microscopic quantities are involved. Roughly speaking, the linear extensions of the volume element averaged over must (i) be small compared with distances over which relevant electromagnetic quantities are supposed to vary and (ii) contain many atoms and molecules. In the macroscopic Maxwell equations thus appear, for instance, spatial averages of the microscopic (also called local) electric ($\mathbf{E}$) and magnetic ($\mathbf{B}$) fields, and the microscopic current density ($\mathbf{J}$), i.e.,

$$\mathbf{E}_{\rm macro} = \langle\mathbf{E}\rangle, \quad \mathbf{B}_{\rm macro} = \langle\mathbf{B}\rangle, \tag{A1}$$

and

$$\mathbf{J}_{\rm macro} = \frac{\partial}{\partial t}\langle\mathbf{P}\rangle + \nabla\times\langle\mathbf{M}\rangle, \tag{A2}$$

where $\mathbf{P}$ and $\mathbf{M}$ are *generalized* microscopic polarization and magnetization fields. In $\mathbf{J}_{\rm macro}$ both "free" ($\mathbf{J}^{\rm free}_{\rm macro}$) and "bound" ($\partial\mathbf{D}_{\rm macro}/\partial t$) contributions are incorporated [9].

It is known that the macroscopic approach may be of limited value for studies of interfaces between different macroscopic media and for investigations of the electrodynamics of mesoscopic systems in general [57]. Since the standard (textbook) boundary (jump) conditions for the various field quantities across an interface are *derived* from the macroscopic Maxwell equations, the macroscopic constitutive relations, and *idealized* interface (sheet) charge and current densities [8,70,71], it is obvious that the standard boundary conditions become of less value for theoretical studies of mesoscopic media and interfaces.

In the macroscopic Bethe-Bouwkamp diffraction theory [13,14] (and many related works), the screen is assumed to be infinitely thin and completely opaque (with infinite conductivity). Although such two approximations may work well for metallic screens and incident microwave fields (or fields of even longer wavelength), the aforementioned approximations will fail in general. Thus, when the screen becomes sufficiently thin it behaves physically as a QW with a frequency-dispersive microscopic conductivity, and, for certainty, the screen will not be opaque. For a thin screen it may happen that its internal dynamics appears only via a double integral of the so-called causal microscopic conductivity over the well. In such cases, where the QW behaves electrodynamically as an ED absorber and radiator, the prevailing microscopic screen current density effectively exhibits δ-function confinement in the direction perpendicular to the plane of the screen, and in certain sense, the screen thus is considered as infinitely thin.

It is clear that the field-matter interaction in the vicinity of the hole must play a crucial role for a quantitatively correct description of the diffraction process. In the screen-hole surface region also called the selvedge (region), the light-unperturbed electron density varies rapidly in space, from zero in the hole region to the bulk average value in the screen. Although the selvedge length usually only is a few atomic distances, the interface electrodynamics deviates from bulk electrodynamics in a much thicker layer. If the hole is of mesocopic size and the screen is a QW sheet, it is expected that, e.g., microscopic curvature effects along the screen-hole contour will play an important role for understanding the spatial diffraction pattern and its frequency dependence.

2. General formalism

The microscopic diffraction theory established by the present authors recently is based on a combination of the *microscopic Maxwell-Lorentz equations* and a (linear) *nonlocal constitutive equation* relating the microscopic screen current density to the local electric field [46]. For a small hole it is convenient to compare the scattering from identical screens with and without a hole, assuming the incident field to be the same in the two cases. Below, a subscript ∞ is added to quantities referring to the screen without hole. A central result of Ref. [46] shows that the difference between the total (incident plus reflected) electric fields for screens with [$\mathbf{E}(\mathbf{r};\omega)$] and without [$\mathbf{E}_\infty(\mathbf{r};\omega)$] a hole is given by

$$\mathbf{E}(\mathbf{r};\omega) - \mathbf{E}_\infty(\mathbf{r};\omega) = i\mu_0\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r},\mathbf{r}'';\omega)\cdot\mathbf{\Delta}(\mathbf{r}'',\mathbf{r}';\omega)\cdot\mathbf{E}^0(\mathbf{r}';\omega)d^3r''d^3r', \tag{A3}$$

in the space ($\mathbf{r}$)-frequency (ω) domain. The tensorial quantity $\mathbf{G}(\mathbf{r},\mathbf{r}'';\omega)$ is the standard Green's function relating to vacuum,

$$\mathbf{\Delta}(\mathbf{r},\mathbf{r}';\omega) = \boldsymbol{\sigma}^{\rm cau}(\mathbf{r},\mathbf{r}';\omega) - \boldsymbol{\sigma}^{\rm cau}_\infty(\mathbf{r},\mathbf{r}';\omega) \tag{A4}$$

is the so-called causal (cau) effective aperture (hole) response tensor, and $\mathbf{E}^0(\mathbf{r}';\omega)$ is the electric field incident on the hole. The causal conductivity tensor $\boldsymbol{\sigma}^{\rm cau}(\mathbf{r},\mathbf{r}';\omega)$ is obtained from

an integral,

$$\boldsymbol{\sigma}^{\mathrm{cau}}(\mathbf{r},\mathbf{r}';\omega) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r},\mathbf{r}'';\omega)\cdot\boldsymbol{\Gamma}(\mathbf{r}'',\mathbf{r}';\omega)d^3r'', \quad \text{(A5)}$$

involving the well-known [9] microscopic conductivity tensor, $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$, and the local field tensor, $\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega)$. The last tensor satisfies the inhomogeneous integral equation

$$\boldsymbol{\Gamma}(\mathbf{r},\mathbf{r}';\omega) = \mathbf{U}\delta(\mathbf{r}-\mathbf{r}') + \int_{-\infty}^{\infty} \mathbf{K}(\mathbf{r},\mathbf{r}'';\omega)\cdot\boldsymbol{\Gamma}(\mathbf{r}'',\mathbf{r}';\omega)d^3r'', \quad \text{(A6)}$$

with kernel

$$\mathbf{K}(\mathbf{r},\mathbf{r}';\omega) = i\mu_0\omega\int_{-\infty}^{\infty}\mathbf{G}(\mathbf{r},\mathbf{r}'';\omega)\cdot\boldsymbol{\sigma}(\mathbf{r}'',\mathbf{r}';\omega)d^3r''. \quad \text{(A7)}$$

In Eq. (A6), $\mathbf{U}$ is the 3×3 unit tensor, and $\delta(\mathbf{r}-\mathbf{r}')$ is the Dirac δ function.

It appears from Eqs. (A3)–(A7) that the electric-field difference $\mathbf{E}(\mathbf{r};\omega)-\mathbf{E}_\infty(\mathbf{r};\omega)$, *in principle*, can be determined from a knowledge of the incident electric field, $\mathbf{E}^0(\mathbf{r}';\omega)$, and the microscopic conductivity tensors $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\omega)$ and $\boldsymbol{\sigma}_\infty(\mathbf{r},\mathbf{r}';\omega)$. The conductivity tensors, at a given electromagnetic angular frequency (ω), can be obtained from the field-unperturbed electronic properties of the screens with and without a hole. Quantum mechanically, these properties are determined from solutions to the time-independent Schrödinger equation and quantum statistics related to the probability that the various stationary states are occupied; see Sec. II A.

In the view of the results of Ref. [46] partly summarized above, we can make the following conclusion: The quantum-mechanical theory of diffraction only requires a preknowledge of the incident field plus the electronic properties of the screen(s). Perhaps, such a conclusion is not so surprising in itself, but the theoretical approach of Ref. [46] shows how the above-mentioned conclusion may be reached by a quite general explicit calculation.

APPENDIX B: TWO-DIMENSIONAL HARTREE-FOCK JELLIUM

Within the framework of a 2D version of the Hartree-Fock approximation, the time-independent Schrödinger equation for the ith wave function $\psi^i(\mathbf{r}_\parallel)$ (with related eigenenergy $E^i_\parallel$) takes the form

$$\left[\frac{-\hbar^2}{2m}\nabla^2_\parallel + V_{\mathrm{J}} + V_{\mathrm{H}}(\mathbf{r}_\parallel)\right]\psi^i(\mathbf{r}_\parallel) - \sum_{j(\neq i)} V^{ij}_{\mathrm{X}}(\mathbf{r}_\parallel)\psi^j(\mathbf{r}_\parallel) = E^i_\parallel\psi^i(\mathbf{r}_\parallel), \quad \text{(B1)}$$

where V_{J} is the $\mathbf{r}_\parallel$-independent jellium (J) potential,

$$V_{\mathrm{H}}(\mathbf{r}_\parallel) = \frac{e^2}{4\pi\varepsilon_0}\int\frac{1}{|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|}\sum_{j(\neq i)}|\psi^j(\mathbf{r}'_\parallel)|^2 d^2r'_\parallel, \quad \text{(B2)}$$

is the local Hartree potential [59], and

$$V^{ij}_{\mathrm{X}}(\mathbf{r}_\parallel) = \frac{e^2}{4\pi\varepsilon_0}\int\frac{1}{|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|}[\psi^j(\mathbf{r}'_\parallel)]^*\psi^i(\mathbf{r}'_\parallel)d^2r'_\parallel, \quad \text{(B3)}$$

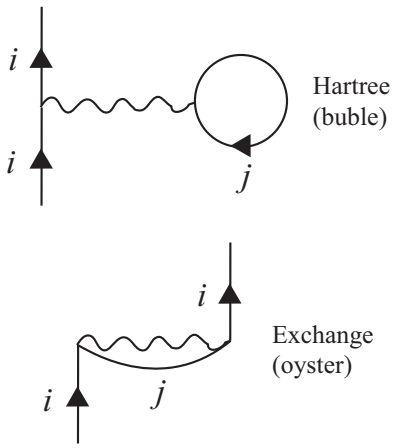

FIG. 9. Feynman diagrams related to the Hartree (top figure) and exchange (bottom figure) potential.

the ijth part of the nonlocal exchange (X) potential. In Eqs. (B1) and (B2) the summations run over all other one-electron eigenstates (j) than the ith. The factor $|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|^{-1}$ indicates that the electron-electron Coulomb interaction is nonretarded [Coulomb gauge description of longitudinal (rotational-free) field interaction]. For readers interested in the second-quantized field description of the many-body Hartree and Hartree-Fock interactions the related Feynman diagrams are shown in Fig. 9. It appears from Eqs. (17), (B1), and (B2) that the nonlocal 2D-exchange potential, $V_{\mathrm{X}}(\mathbf{r}_\parallel,\mathbf{r}'_\parallel)$, (omitting a factor of -1) is given by

$$V_X(\mathbf{r}_\parallel,\mathbf{r}'_\parallel) = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|}\sum_{j(\neq i)}\psi^j(\mathbf{r}_\parallel)[\psi^j(\mathbf{r}'_\parallel)]^*. \quad \text{(B4)}$$

For a screen without a hole, the eigenfunctions may be taken as 2D plane waves $[(2\pi)^{-1}\exp(i\mathbf{k}^i_\parallel\cdot\mathbf{r}_\parallel)]$, a fact which is well known in the 3D case [58,59]. The energy eigenvalues are modified in comparison to the free-electron-like Hartree energies. To obtain the exchange corrections to the Hartree energies, let us insert the 2D plane-wave ansatz above into the exchange term in Eq. (B1). This gives, using Eq. (B3),

$$\begin{aligned}\sum_{j(\neq i)} V^{ij}_X(\mathbf{r}_\parallel)\psi^j(\mathbf{r}_\parallel) &= \frac{e^2}{4\pi\varepsilon_0}\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{1}{|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|}e^{i(\mathbf{k}^i_\parallel-\mathbf{k}^j_\parallel)\cdot\mathbf{r}'_\parallel}e^{i\mathbf{k}^j_\parallel\cdot\mathbf{r}_\parallel}d^2r'_\parallel \\ &= \sum_{j(\neq i)} F(\mathbf{k}^i_\parallel-\mathbf{k}^j_\parallel)\frac{1}{2\pi}\exp(i\mathbf{k}^i_\parallel\cdot\mathbf{r}_\parallel), \quad \text{(B5)}\end{aligned}$$

where

$$F(\mathbf{k}^i_\parallel-\mathbf{k}^j_\parallel) = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{1}{|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|}e^{i(\mathbf{k}^j_\parallel-\mathbf{k}^i_\parallel)\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}d^2r'_\parallel. \quad \text{(B6)}$$

To calculate the integral in Eq. (B6), we use the substitution $\mathbf{r}'_\parallel = \mathbf{r}_\parallel - \mathbf{R}_\parallel$, and thereafter we carry out the integration in

polar coordinates $(R_\parallel,\phi)$. Hence,

$$\begin{aligned} F(|\mathbf{k}_\parallel^i-\mathbf{k}_\parallel^j|) &= \frac{e^2}{4\pi\varepsilon_0}\frac{1}{(2\pi)^2}\int_0^\infty\int_0^{2\pi}\frac{1}{R_\parallel}e^{i|\mathbf{k}_\parallel^j-\mathbf{k}_\parallel^i|R_\parallel\cos\phi}d\phi R_\parallel dR_\parallel \\ &= \frac{e^2}{4\pi\varepsilon_0}\frac{1}{2\pi}\int_0^\infty J_0(|\mathbf{k}_\parallel^j-\mathbf{k}_\parallel^i|R_\parallel)dR_\parallel \\ &= \frac{e^2}{8\pi^2\varepsilon_0}\frac{1}{|\mathbf{k}_\parallel^i-\mathbf{k}_\parallel^j|}. \end{aligned} \tag{B7}$$

In Eq. (B7), J_0 is the zeroth-order Bessel function. As indicated in the argument of F, this function only depends on the magnitude of the wave-vector difference $\mathbf{k}_\parallel^i-\mathbf{k}_\parallel^j$.

In the 2D Hartree-Fock approach the eigenenergy of the ith plane-wave state thus is given by

$$E_\parallel^i=\frac{\hbar^2|\mathbf{k}_\parallel^i|^2}{2m}-\sum_{j(\neq i)}F(|\mathbf{k}_\parallel^i-\mathbf{k}_\parallel^j|). \tag{B8}$$

With the explicit expression for F inserted, one reaches the result

$$E_\parallel^i=\frac{\hbar^2|\mathbf{k}_\parallel^i|^2}{2m}-\frac{e^2}{8\pi^2\varepsilon_0}\sum_{j(\neq i)}\frac{1}{|\mathbf{k}_\parallel^i-\mathbf{k}_\parallel^j|}. \tag{B9}$$

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