Admittance of planar two-terminal quantum systems

U. Wulf,[1,2] P. N. Racec,[2,3] and E. R. Racec[1,4]
[1]*Technische Universität Cottbus, Fakultät 1, Postfach 101344, 03013 Cottbus, Germany*
[2]*IHP/BTU JointLab, Postfach 10 13 44, 03013 Cottbus, Germany*
[3]*National Institute of Materials Physics, P.O. Box MG-7, 077125 Bucharest Magurele, Romania*
[4]*Faculty of Physics, University of Bucharest, P.O. Box MG-11, 077125 Bucharest Magurele, Romania*
(Received 26 June 2006; revised manuscript received 8 September 2006; published 12 February 2007)

We develop an approach to calculate the admittance of effectively one-dimensional open quantum systems in random-phase approximation (RPA). The stationary, unperturbed system is described within the Landauer-Büttiker formalism taking into account the Coulomb interaction in the Hartree approximation. The dynamic changes in the effective potential are calculated microscopically from the charge-charge correlation function resulting from the stationary scattering states. We provide explicit RPA expressions for the quantum admittance. As a first example the case of a quantum capacitor is considered where we can derive a small-frequency expansion for the admittance which lends itself to an experimental testing of the theory. A comparison of the low-frequency expansion with the complete RPA expression shows that for a quantum capacitor a simple classical equivalent circuit with frequency-independent elements does not describe satisfactorily the quantum admittance with increasing frequency.

DOI: 10.1103/PhysRevB.75.075320 PACS number(s): 71.10.−w, 72.10.Bg, 73.23.−b, 85.30.De

I. INTRODUCTION

The ac-transport properties of nearly ballistic devices are interesting from the point of view of basic research, as well as from the point of view of technological applications. In basic research, ac transport can provide valuable information supplementary to stationary transport. In applications, impedances are of crucial importance for the layout of ac circuits.

Recently, a number of methods for the description of time-dependent transport phenomena in mesoscopic systems have been proposed (for a recent review, see Ref. 1). Among these approaches are techniques based on nonequilibrium Green's functions,[2–5] Wigner functions,[6] bosonization schemes,[7] and phenomenological considerations.[8] If there are only small ac fields, it seems promising to calculate the linear ac response to a perturbation of the stationary system described in the successful Landauer-Büttiker formalism.[9–14] Such an approach has been developed in Refs. 15–20 and it has been used in a number of applications.[21–27] Here, the response to an external potential is derived "which prescribes the potentials (U_α) in the reservoirs only" (see Ref. 15). The reservoirs carry the charge Q_α so that the ac potential leads to a perturbation in the Hamiltonian as given by $H_1 = \Sigma_\alpha U_\alpha Q_\alpha$. This approach avoids the calculation of the time-dependent potential within the scattering area, i.e., outside the contact reservoirs. However, knowledge of the microscopic potential in the scattering area is necessary to derive a formal response theory, beyond the often invoked spatially uniform electric-field perturbation.[28] As pointed out in Refs. 27–30 the appropriate response formalism for the interacting electron system is the random-phase approximation (RPA). In our previous papers[31,32] we demonstrated the application of the complete RPA scheme to open stationary systems described in the Landauer-Büttiker formalism. A complete RPA scheme[33] requires as a central element the calculation of the irreducible polarization $\Pi_0(\boldsymbol{r},\boldsymbol{r}',\omega)$ from the self-consistent scattering functions of the stationary system. As a second necessary ingredient for the implementation of the complete RPA scheme, it was shown in Refs. 31 and 32 how the dynamic total potential in the scattering area can be determined microscopically using the calculated irreducible polarization and the Green's function for the Poisson equation with Dirichlet boundary conditions. It is explicitly shown that for a planar structure the standard three-dimensional linear-response theory in random-phase approximation reduces to an effectively one-dimensional problem.

After a formal derivation of our theoretical approach we derive in this paper explicit RPA expressions for the frequency-dependent impedance in a general two-terminal device under large dc bias. These expressions are evaluated for the case of a quantum capacitor. In the limit $\omega \to 0$ an expansion of the admittance follows as given by

$$Y = -i\omega(Y_1 + i\omega Y_2 + \cdots), \tag{1}$$

with real constants Y_1 and Y_2 that can be calculated directly from the scattering functions of the stationary system. In numerical computations we determine the admittance of a metal insulator semiconductor (MIS)-type heterostructure[32] on which measurements of the static capacitance have already been made.[34] In order to propose an experimental test of our RPA approach, we first compute the drain-source-voltage dependence of the coefficients Y_1 and Y_2 in the limit $\omega \to 0$. For higher frequencies we find numerically, first, that the expansion in Eq. (1) becomes invalid very quickly and, second, that an equivalent circuit with frequency-independent R and C elements does not reflect correctly the ac properties of the considered system. Instead, there are pronounced and systematic deviations from the equivalent circuit behavior which should be testable in experiments as well.

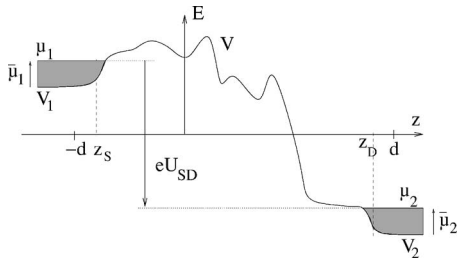

FIG. 1. Sketch of the potential energy along the growth direction in a planar two-terminal system. It can be seen that $-eU_{SD}=V_2+\bar{\mu}_2-V_1-\bar{\mu}_1$, where $\bar{\mu}_2$ and $\bar{\mu}_1$ denote the difference between the chemical potential and the bottom of the conduction band in the bulk contact.

II. GENERAL ADMITTANCE FORMULA

A. Stationary system

We consider a planar two-terminal system with a source contact ($s=1$, $z<z_S$) and a drain contact ($s=2$, $z>z_D$) under an external bias U_{SD} as shown schematically in Fig. 1. The material of the contacts can either be a strongly n-doped semiconductor or a metallization. In the mean-field theory the effective potential energy is independent of the perpendicular coordinate $\boldsymbol{r}_\perp=(x,y)$, $V=V(z)$. Because of the effective screening, the potential energy is constant in the bulk of the source contact, $V(z<-d)=V_1$, and in the bulk of the drain contact, $V(z>d)=V_2$. We write for the wave function[35]

$$\varphi(\boldsymbol{r}) = \psi^{(s)}(\epsilon,z)\frac{\exp(i\boldsymbol{k}_\perp\boldsymbol{r}_\perp)}{\sqrt{A}}, \tag{2}$$

where $\boldsymbol{k}_\perp=(n_x 2\pi/L_x, n_y 2\pi/L_y)$, n_x and n_y are integer numbers, and $A=L_xL_y$ is the cell area of periodic boundary conditions in the perpendicular directions. It follows from the time-independent Schrödinger equation $(\hat{H}_0-E)\varphi=0$, with $\hat{H}_0=-\hbar^2/(2m^*)\Delta+V(z)$, that

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V(z)-\epsilon\right]\psi^{(s)}(\epsilon,z)=0, \tag{3}$$

with

$$E=\epsilon+\frac{\hbar^2}{2m^*}k_\perp^2. \tag{4}$$

The wave function in Eq. (2) is defined by the set of quantum numbers $(s,\epsilon,\boldsymbol{k}_\perp)$ without considering the spin quantum number. Consistent with the Landauer-Büttiker formalism the $\psi^{(s)}(\epsilon,z)$ are scattering functions, where the index s defines the direction of incidence: the scattering functions incident from the source contact ($s=1$) exhibit the asymptotics

$$\psi^{(1)}(\epsilon,z)=\frac{\theta(\epsilon-V_1)}{\sqrt{2\pi}}\begin{cases}\exp[ik_1(z+d)]+\boldsymbol{S}_{11}(\epsilon)\exp[-ik_1(z+d)] & \text{for } z\leqslant -d\\ \boldsymbol{S}_{21}(\epsilon)\exp[ik_2(z-d)] & \text{for } z\geqslant d,\end{cases} \tag{5}$$

where $\boldsymbol{S}_{11}$ and $\boldsymbol{S}_{21}$ are elements of the energy-dependent 2×2 scattering matrix,[35]

$$k_s(\epsilon)=\sqrt{\frac{2m^*}{\hbar^2}(\epsilon-V_s)}, \tag{6}$$

and $\theta(\epsilon-V_1)$ is the step function. Analogous expressions hold for the drain-incident scattering functions $\psi^{(2)}(\epsilon,z)$.

As usual, the effective (total) potential energy $V(z)=V_{ext}(z)+V_{el}(z)$ contains an external part, $V_{ext}(z)$, and a second part, $V_{el}(z)$, coming from the Coulomb interaction between the electrons. The external potential arises typically from different band offsets in the used materials or from fixed external charges such as fully ionized impurities. The Coulomb interaction between the electrons is taken in the Hartree approximation so that V_{el} obeys the Poisson equation having as sources only the electronic charge density,

$$\frac{d^2}{dz^2}V_{el}(z)=-\frac{e^2}{\kappa_s}\rho(z), \tag{7}$$

where κ_s is the dielectric constant of the host material. In Appendix A we reproduce that the electron density is given by

$$\rho(z)=2\frac{m^*}{2\pi\beta\hbar^2}\sum_{s=1,2}\int_{V_s}^{\infty}d\epsilon g_s(\epsilon)|\psi^{(s)}(\epsilon,z)|^2 \times\ln\{1+\exp(\beta(\mu_s-\epsilon))\} \tag{8}$$

in a formal quantum statistical approach needed to formulate the linear-response theory which we will describe in the next section. In Eq. (8) $g_s(\epsilon)=m^*/[\hbar^2k_s(\epsilon)]$ is the one-dimensional density of states, $\beta=1/(k_BT)$, and we included a factor of 2 to account for the spin degeneracy.

B. Harmonic perturbation

1. Random-phase approximation

We consider our system with an additional small ac bias δU superimposed to the source-drain bias so that

$$U_{SD}(t)=U_{SD}+\delta U e^{-i(\omega+i\eta)t}, \tag{9}$$

where $\eta\to 0$, $\eta>0$, is an adiabatic turning-on parameter. Because of the good screening in the contacts, the applied ac bias is assumed to lead to a dynamic potential perturbation $\delta\phi(\boldsymbol{r},t)=\delta\phi(\boldsymbol{r})\exp[-i(\omega+i\eta)t]$ fulfilling the boundary conditions $\delta\phi(x,y,z\leqslant -d)=0$ and $\delta\phi(x,y,z\geqslant d)=\delta U$. Then, the

perturbation in the potential energy felt by electrons is $\delta V(\boldsymbol{r},t)=-e\,\delta\phi(\boldsymbol{r})\exp[-i(\omega+i\eta)t]$ and the time-dependent Hamiltonian becomes

$$\hat{H}=\hat{H}_0+\int d^3\boldsymbol{r}\hat{\rho}(\boldsymbol{r})\,\delta V(\boldsymbol{r},t), \tag{10}$$

where $\hat{H}_0$ describes the stationary system under static source-drain bias, see Eq. (A10), and $\hat{\rho}(\boldsymbol{r})$ is the particle density operator. Of course, Eq. (10) is only valid if retardation effects in the quantum system can be neglected, i.e., $\omega \ll c/L$, where L is the typical length of the device. For a quantum device with $L=10$ nm we find $c/L\sim 10^{16}$ Hz, which is on the upper limit of the UV radiation. The time-dependent perturbation in the electron density (induced density) $\delta\rho(\boldsymbol{r},t)$ is calculated outside the contacts in random phase approximation.[36–38] Assuming that for the planar structure $\delta V(\boldsymbol{r},t)=\delta V(z,t)$ we show in Appendix B that $\delta\rho(\boldsymbol{r},t)=\delta\rho(z,t)=\delta\rho(z)\exp(-i\omega t)$, with

$$\delta\rho(|z|\leqslant d)=\int_{-d}^{d}dz'\Pi_0(z,z',\omega)\,\delta V(z'). \tag{11}$$

Here $\Pi_0(z,z',\omega)=\Sigma_{s,s'=1}^{2}\Pi_0^{(ss')}(z,z',\omega)$,

$$\Pi_0^{(ss')}(z,z',\omega)=\lim_{\eta\to 0}\int_{V_s}^{\infty}d\epsilon\int_{V_{s'}}^{\infty}d\epsilon'\frac{F^{(ss')}(z,z',\epsilon,\epsilon')}{\epsilon-\epsilon'+\hbar(\omega+i\eta)}, \tag{12}$$

and

$$F^{(ss')}(z,z',\epsilon,\epsilon')=2\frac{m^*}{2\pi\beta\hbar^2}g_s(\epsilon)g_{s'}(\epsilon')\ln\left\{\frac{1+\exp(\beta(\mu_s-\epsilon))}{1+\exp(\beta(\mu_{s'}-\epsilon'))}\right\}(\psi^{(s)}(\epsilon,z))^*\psi^{(s')}(\epsilon',z)(\psi^{(s')}(\epsilon',z'))^*\psi^{(s)}(\epsilon,z'). \tag{13}$$

Setting the integration limits in Eq. (11) we assume that there is no phase coherence of the wave functions between the contacts and the scattering area, $\Pi_0^{(ss')}(z,|z'|>d,\omega)=0$. The perturbation of the effective potential outside the contacts which enters Eqs. (10) and (11) is determined by the Poisson equation

$$\Delta\,\delta V(z)=-\frac{e^2}{\kappa_s}\delta\rho(z). \tag{14}$$

In Eq. (14) we assume that there is no mobile charge in the interval $-d\leqslant z\leqslant d$ other than that of the tunneling electrons. The solution of Eq. (14) obeying the boundary conditions $\delta V(z\leqslant -d)=0$ and $\delta V(z\geqslant d)=-e\,\delta U$ can be written as

$$\delta V(z)=\delta V_0(z)+\int_{-d}^{d}dz'v_0(z,z')\,\delta\rho(z'), \tag{15}$$

with the homogeneous solution

$$\delta V_0(|z|\leqslant d)=-e\,\delta U\frac{z+d}{2d}. \tag{16}$$

In Eq. (15) the symmetrical Green function $v_0(z,z')=-(e^2/2\kappa_s)[|z-z'|+zz'/d-d]$ for the Poisson equation obeys the boundary condition[39] $v_0(z=\pm d,z')=0$. Using Eqs. (11) and (15) one obtains an integral equation for the total potential as given by

$$\delta V(z)=\delta V_0(z)+\int_{-d}^{d}dz'\int_{-d}^{d}dz''v_0(z,z')\Pi_0(z',z'',\omega)\,\delta V(z''). \tag{17}$$

We write the inverse of this equation in a convenient discretized form,

$$\delta\boldsymbol{V}=(\mathbf{1}-\boldsymbol{v}_0\boldsymbol{\Pi}_0)^{-1}\delta\boldsymbol{V}_0, \tag{18}$$

with $z\to z_i=-d+(i-1)\Delta z$, $i=1\cdots N+1$, $\Delta z=2d/N$, and $N\to\infty$ so that $\int_{-d}^{d}dz\to\Delta z\Sigma_{i=1}^{N+1}$. Furthermore, we define the $(N+1)\times(N+1)$ matrices $\boldsymbol{v}_0$ and $\boldsymbol{\Pi}_0(\omega)$ with $(\boldsymbol{v}_0)_{ij}=\Delta z v_0(z_i,z_j)$ and $(\boldsymbol{\Pi}_0)_{ij}=\Delta z\Pi_0(z_i,z_j,\omega)$ as well as the vectors $\delta\boldsymbol{V}_0$ and $\delta\boldsymbol{V}$ with $(\delta\boldsymbol{V}_0)_i=\delta V_0(z_i)$ and $(\delta\boldsymbol{V})_i=\delta V(z_i)$. The continuum limit of Eq. (18) can be regained using the von Neumann theorem, $(\mathbf{1}-\boldsymbol{v}_0\boldsymbol{\Pi}_0)^{-1}=\Sigma_{n=0}^{\infty}(\boldsymbol{v}_0\boldsymbol{\Pi}_0)^n$, and rewriting the obtained sums as integrals. We solve Eq. (18) numerically. Then after defining the vectors $\delta\boldsymbol{\rho}$ with $(\delta\boldsymbol{\rho})_i=\delta\rho(z_i)$ and an analogous vector $\delta\boldsymbol{j}_z$ for the z component of the particle current density, one obtains from discretization of Eq. (11)

$$\delta\boldsymbol{\rho}=\boldsymbol{\Pi}_0\delta\boldsymbol{V}=\boldsymbol{\Pi}_0(\mathbf{1}-\boldsymbol{v}_0\boldsymbol{\Pi}_0)^{-1}\delta\boldsymbol{V}_0, \tag{19}$$

and from Eq. (B5)

$$\delta\boldsymbol{j}_z=\tilde{\boldsymbol{\Pi}}_0\delta\boldsymbol{V}=\tilde{\boldsymbol{\Pi}}_0(\mathbf{1}-\boldsymbol{v}_0\boldsymbol{\Pi}_0)^{-1}\delta\boldsymbol{V}_0, \tag{20}$$

where $\tilde{\Pi}_0$ is the current-density response function defined and evaluated in Appendix B, and $\tilde{\boldsymbol{\Pi}}_0$ is the corresponding matrix obtained after discretization.

2. ac admittance

From the continuity equation $(\partial/\partial z)\delta j_z(z,t)=-(\partial/\partial t)\delta\rho(z,t)$ one obtains the relation

$$\delta j_z(z)=\delta j_z(-d)+\int_{-d}^{z}dz'\,\delta j_z'(z')=\delta j_z(-d)+i\omega\delta Q(z)$$
$$=-\delta I/Ae+i\omega\delta Q(z), \tag{21}$$

with $\delta j_z'(z)=(d/dz)\delta j_z$ and $\delta Q(z)=\int_{-d}^{z}dz'\,\delta\rho(z')$. From the

boundary conditions $\delta V(z \geqslant d) = -e\delta U$ and $\delta V(z \leqslant -d) = 0$ and the continuity of $(d/dz)\delta V(z)$, it follows that the total induced charge $\delta Q = \delta Q(d)$ vanishes. One then obtains $\delta j_z(-d) = \delta j_z(d) = -\delta I/Ae$, where δI is the induced electrical current provided by an external source and flowing through the device. The minus sign in the last step of Eq. (21) results from the current convention. The complex admittance is defined as usual by $Y = \delta I/\delta U = -Ae\delta j_z(-d)/\delta U$. Applying Eqs. (21), (20), and (16) one obtains an explicit expression for the admittance,

$$Y = \frac{\delta I}{\delta U} = Ae^2 \boldsymbol{W}_1^T \tilde{\boldsymbol{\Pi}}_0 (\mathbf{1} - \boldsymbol{v}_0 \boldsymbol{\Pi}_0)^{-1} \boldsymbol{W}_0, \tag{22}$$

where $(\boldsymbol{W}_0)_i = z_i/2d + 0.5$ and $\boldsymbol{W}_1$ is a unit vector $(\boldsymbol{W}_1)_i = \delta_{1i}$.

III. QUANTUM CAPACITOR IN RANDOM-PHASE APPROXIMATION

A. General results

We define a quantum capacitor through two conditions: First, there is basically no dc currents traversing the structure,

$$\psi^{(1)}(\epsilon, z \geqslant d) = 0, \quad \psi^{(2)}(\epsilon, z \leqslant -d) = 0. \tag{23}$$

Second, the overlap of the right-incident and the left-incident scattering functions can be neglected,

$$\psi^{(1)}(\epsilon, z)\psi^{(2)}(\epsilon', z) \sim 0, \tag{24}$$

for all ϵ, ϵ' and $z \in [-d, d]$. We then find from Eqs. (B6) and (12) that $\tilde{\boldsymbol{\Pi}}_0^{(12)} = \tilde{\boldsymbol{\Pi}}_0^{(21)} = \boldsymbol{\Pi}_0^{(12)} = \boldsymbol{\Pi}_0^{(21)} = 0$, and the induced current can be split into two independent parts, $\delta j_z = \delta j_z^{(1)} + \delta j_z^{(2)}$, with

$$\delta j_z^{(s)}(z) = \int_{-d}^{d} dz' \tilde{\Pi}_0^{(ss)}(z, z', \omega)\delta V(z'). \tag{25}$$

Since $\delta j_z^{(s)}$ results exclusively from the source-incident scattering states for $s=1$ or exclusively from the drain-incident scattering states for $s=2$ we can write for each component a separate continuity equation,

$$-i\omega\delta\rho^{(s)}(z) + \frac{d}{dz}\delta j_z^{(s)}(z) = 0, \tag{26}$$

with

$$\delta\rho^{(s)}(z) = \int_{-d}^{d} dz' \Pi_0^{(ss)}(z, z', \omega)\delta V(z'). \tag{27}$$

Integrating Eq. (26) one obtains using Eq. (23) under another form, i.e., $\delta j_z^{(1)}(d) = \delta j_z^{(2)}(-d) = 0$,

$$\frac{\delta I}{eA} = -\delta j_z^{(1)}(-d) = i\omega \int_{-d}^{d} dz \int_{-d}^{d} dz' \Pi_0^{(11)}(z, z', \omega)\delta V(z'). \tag{28}$$

With the definition of the admittance and Eqs. (18) and (16), Eq. (22) reduces after discretization to

$$Y = -e^2 A i\omega \Delta z \boldsymbol{W}_2^T \boldsymbol{\Pi}_0^{(11)} (\mathbf{1} - \boldsymbol{v}_0 \boldsymbol{\Pi}_0)^{-1} \boldsymbol{W}_0, \tag{29}$$

where $\tilde{\boldsymbol{\Pi}}_0$ is eliminated. In Eq. (29) we define the $(N+1) \times (N+1)$ matrix $(\boldsymbol{\Pi}_0^{(ss)})_{ij} = \Delta z \Pi_0^{(ss)}(z_i, z_j, \omega)$ and the vector $(\boldsymbol{W}_2)_i = 1$.

In Appendix C it is shown that for small frequencies an expansion

$$\Pi_0^{(ss)}(z, z', \omega) = P_0^{(s)}(z, z') + i\omega P_1^{(s)}(z, z') \tag{30}$$

can be derived with real functions $P_0^{(s)}(z, z')$ and $P_1^{(s)}(z, z')$. Inserting this expansion into Eq. (29) one obtains a low-frequency expansion for the admittance of a quantum capacitor as

$$Y \approx -i\omega(Y_1 + i\omega Y_2). \tag{31}$$

Here the leading order coefficient

$$Y_1 = e^2 A \Delta z \boldsymbol{W}_2^T \boldsymbol{P}_0^{(1)} (1 - \boldsymbol{v}_0 \boldsymbol{P}_0)^{-1} \boldsymbol{W}_0 \tag{32}$$

and the first correction

$$Y_2 = e^2 A \Delta z \boldsymbol{W}_2^T [\boldsymbol{P}_1^{(1)} (1 - \boldsymbol{v}_0 \boldsymbol{P}_0)^{-1} + \boldsymbol{P}_0^{(1)} (1 - \boldsymbol{v}_0 \boldsymbol{P}_0)^{-2} \boldsymbol{v}_0 \boldsymbol{P}_1] \boldsymbol{W}_0 \tag{33}$$

are real, where $\boldsymbol{P}_0 = \boldsymbol{P}_0^{(1)} + \boldsymbol{P}_0^{(2)}$, $\boldsymbol{P}_1 = \boldsymbol{P}_1^{(1)} + \boldsymbol{P}_1^{(2)}$, $(\boldsymbol{P}_0^{(s)})_{ij} = \Delta z P_0^{(s)}(z_i, z_j, \omega)$, and $(\boldsymbol{P}_1^{(s)})_{ij} = \Delta z P_1^{(s)}(z_i, z_j, \omega)$.

B. Numerical results for a MIS-type nanostructure

As a test structure for our theory we take a planar MIS-type GaAs-$Al_xGa_{1-x}As$ heterostructure with a near back gate. This structure has been analyzed in experiments,[34] the stationary system has been described theoretically within Hartree approximation,[40] and first calculations for the dynamic behavior are presented in Refs. 31 and 32. We now calculate the quantum admittance $Y(\omega)$ according to Eq. (29) up to frequencies of 100 GHz. Using Eq. (31) one can extract from the numerically (or experimentally) given data the parameters $Y_1 = -\lim_{\omega \to 0} \mathrm{Im}[Y(\omega)]/\omega$ and $Y_2 = \lim_{\omega \to 0} \mathrm{Re}[Y(\omega)]/\omega^2$. It is then possible to recast Eq. (31) in a normalized form,

$$\bar{Y} = -i\bar{\omega}(1 + i\bar{\omega}), \tag{34}$$

with $\bar{\omega} = \omega/\omega_0$, $\omega_0 = Y_1/Y_2$, and $\bar{Y} = YY_2/Y_1^2$. This normalization allows us to collapse the calculated quantum admittance at all considered source-drain voltages into one graph which is presented in Fig. 2. It is immediately seen that the expansion in Eq. (34) only holds for $\bar{\omega} \to 0$. For finite frequencies there are significant deviations from the value 1 for $\mathrm{Re}(\bar{Y})/\bar{\omega}^2$ and from the value -1 for $\mathrm{Im}(\bar{Y})/\bar{\omega}$. To discuss these deviations we compare with the admittance Y_{sg} of a classical equivalent circuit consisting of a frequency-independent resistance R and a frequency-independent capacitor C in series.[17,23,41] An inspection of the admittance $Y_{sg}(\omega \to 0)$ of this circuit yields $Y_1 = C$ and $Y_2 = RC^2$. These formulas can be regarded as quantum-mechanical expressions for the elements of the equivalent circuit. In the normalized form one then obtains

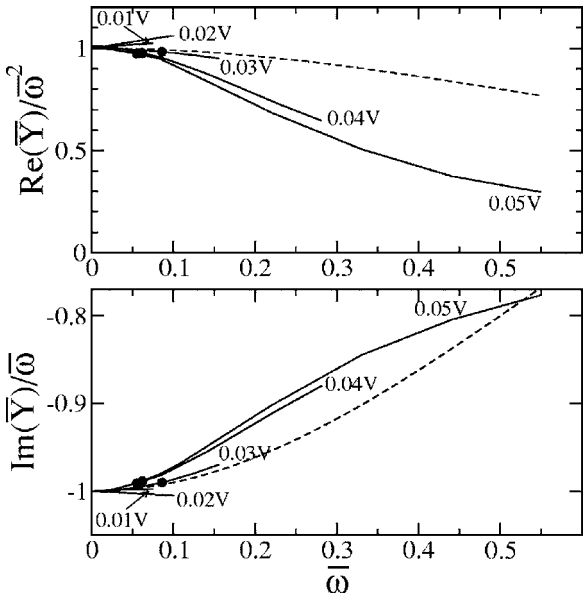

FIG. 2. Quantum admittance for MIS-type nanostructure, in a normalized representation, for different static biases U_{SD} (parameters corresponding to Fig. 1 of Ref. 40). Dashed line represents $Y_{sg}(\bar{\omega})$ for a classical RC circuit with frequency-independent elements. The symbols represent the critical frequencies (Ref. 32) up to which the approximation of the quantum result [i.e., Eq. (29)] with Y_{sg} can be considered satisfactory.

$$\bar{Y}_{sg}(\bar{\omega}) = \frac{\bar{\omega}^2}{1+\bar{\omega}^2} - i\frac{\bar{\omega}}{1+\bar{\omega}}. \tag{35}$$

It is seen from Fig. 2 that $Y_{sg}(\bar{\omega})$ generally fails to describe the numerical admittance. The numerical results show for increasing source-drain voltages a systematic enhancement of the decrease in $\mathrm{Re}(\bar{Y})$ and the increase in $\mathrm{Im}(\bar{Y})$ as the frequency is increased. This finding does not result in the classical equivalent circuit.

In Fig. 3(a) we represent the dependence of the coefficients Y_1 and Y_2 on the working point bias U_{SD}. The coefficient Y_1 is essentially identical with the low-frequency limit of the dynamic capacitance plotted in Fig. 3 of Ref. 32. As demonstrated in Ref. 32 this step in Y_1 is in good agreement with a step in the experimental capacitance curve which is caused by the formation of a two-dimensional electron gas within the quantum capacitor. The coefficient Y_2 shows a general increase with increasing bias. As a characteristic feature it is seen that the step in the capacitance of Y_1 is accompanied by a small hump in Y_2. An inspection of the scaling frequency ω_0 [Fig. 3(b)] reveals a corresponding downward hump.

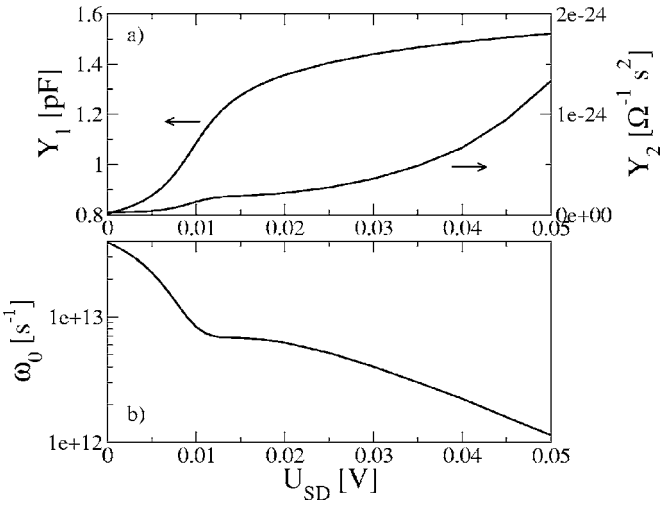

FIG. 3. (a) Y_1 and Y_2 as function of the working point U_{SD}. (b) The scaling frequency ω_0 vs U_{SD}.

IV. CONCLUSIONS

We present a quantum-mechanical model to calculate the admittance of effectively one-dimensional open quantum systems in random-phase approximation. Explicit RPA expressions for the quantum admittance of a general two-terminal system are derived. In the case of a quantum capacitor a small-frequency expansion can be obtained which lends itself to an experimental testing of the theory. A comparison of the low-frequency expansion with the complete RPA expression shows that for a quantum capacitor a simple classical equivalent circuit with frequency-independent elements does not describe satisfactorily the quantum admittance with increasing the frequency.

ACKNOWLEDGMENTS

It is a pleasure for us to acknowledge discussions with D. Robaschik. We gratefully acknowledge support by the HWP grant of the Federal Government of Germany and the State of Brandenburg. Two of us (P.N.R and E.R.R.) also acknowledge partial support from the CEEX project D-11-45 from the Romanian Ministry of Education and Research.

APPENDIX A: STATISTICAL OPERATOR FOR THE STATIONARY SYSTEM WITH FINITE SOURCE-DRAIN BIAS

1. Scattering states as a complete orthonormal single-particle basis

As shown in Refs. 35 and 42–44 the one-dimensional scattering states $\psi^{(s)}(\epsilon,z)$ defined over the entire z axes constitute a complete orthonormal system (see also Refs. 14 and 45–48), i.e.,

$$\sum_{s=1,2}\int_{V_s}^{\infty} d\epsilon g_s(\epsilon)(\psi^{(s)}(\epsilon,z))^*\psi^{(s)}(\epsilon,z') = \delta(z-z'), \tag{A1}$$

and

$$\int_{-\infty}^{\infty} dz(\psi^{(s)}(\epsilon,z))^*\psi^{(s')}(\epsilon',z) = \theta(\epsilon-V_s)\delta_{ss'}\delta(\epsilon-\epsilon')/g_s(\epsilon). \tag{A2}$$

To eliminate the weight function $g_s(\epsilon)$ we substitute for a given s in Eq. (A1) $\epsilon=\hbar^2k_s^2/(2m^*)+V_s\equiv\epsilon_s(k_s)$ [see Eq. (6)]. One obtains

$$\sum_{s=1,2}\int_0^\infty dk_s(\psi^{(s)}(\epsilon_s(k_s),z))^*\psi^{(s)}(\epsilon_s(k_s),z')=\delta(z-z'). \tag{A3}$$

According to Eq. (6) we write in Eq. (A2) $\epsilon'=\hbar^2(k'_{s'})^2/(2m^*)+V_{s'}\equiv\epsilon_{s'}(k'_{s'})$, and using the identity $\delta_{ss'}\delta(\epsilon-\epsilon')/g_s(\epsilon)=\delta_{ss'}\delta(k_s-k'_s)$ find

$$\int_{-\infty}^\infty dz(\psi^{(s)}(\epsilon_s(k_s),z))^*\psi^{(s')}(\epsilon_{s'}(k'_{s'}),z)=\theta(k_s)\delta_{ss'}\delta(k_s-k'_s). \tag{A4}$$

Since later we want to work in a number representation we introduce a k-space discretization $k_s\to k_j=j\Delta k$, $j=0,1,2,\ldots$, so that $\delta(k_s-k'_s)\to\delta_{jj'}/\Delta k$. Furthermore, we define $\psi_{sj}(z)=\sqrt{\Delta k}\psi^{(s)}(\epsilon_s(k_j),z)$. With this definition an explicit asymptotic form of the source-incident scattering wave functions ($s=1$) follows from Eq. (5) as given by

$$\psi_{1j}(z)=\sqrt{\frac{\Delta k}{2\pi}}\theta(\epsilon_1(k_j)-V_1)\begin{cases}\exp(ik_j(z+d))+S_{11}(\epsilon_1(k_j))\exp(-ik_j(z+d)) & \text{for } z\leqslant -d\\ S_{21}(\epsilon_1(k_j))\exp(i\sqrt{k_j^2+(2m^*/\hbar^2)(V_1-V_2)}(z-d)) & \text{for } z\geqslant d.\end{cases} \tag{A5}$$

For the drain-incident scattering functions ($s=2$) we find the asymptotics

$$\psi_{2j}(z)=\sqrt{\frac{\Delta k}{2\pi}}\theta(\epsilon_2(k_j)-V_2)\begin{cases}S_{12}(\epsilon_2(k_j))\exp(-i\sqrt{k_j^2+(2m^*/\hbar^2)(V_2-V_1)}(z+d)) & \text{for } z\leqslant -d\\ \exp(-ik_j(z-d))+S_{22}(\epsilon_2(k_j))\exp(ik_j(z-d)) & \text{for } z\geqslant d.\end{cases} \tag{A6}$$

After discretization we thus write for Eq. (A3)

$$\sum_{s=1}^{2}\sum_{j=0}^{\infty}\psi_{sj}^*(z)\psi_{sj}(z')=\delta(z-z'), \tag{A7}$$

and for Eq. (A4)

$$\int_{-\infty}^\infty dz\psi_{sj}^*(z)\psi_{s'j'}(z)=\delta_{ss'}\delta_{jj'}. \tag{A8}$$

In addition we introduce a complete orthonormal basis system $\phi_\nu(\boldsymbol{r}_\perp)$ for the square-integrable function in $\boldsymbol{R}^2$, $\int d\boldsymbol{r}_\perp\phi_\nu^*(\boldsymbol{r}_\perp)\phi_{\nu'}(\boldsymbol{r}_\perp)=\delta_{\nu\nu'}$ and $\Sigma_\nu\phi_\nu^*(\boldsymbol{r}_\perp)\phi_\nu(\boldsymbol{r}'_\perp)=\delta(\boldsymbol{r}_\perp-\boldsymbol{r}'_\perp)$. They are usually solutions of the time-independent Schrödinger equation in the lateral directions, $[-\hbar^2/(2m^*)\Delta_\perp+V_\perp(\boldsymbol{r}_\perp)-E_\perp^\nu]\phi_\nu(\boldsymbol{r}_\perp)=0$. Then a complete orthonormal basis for the Hilbert space of the single-particle quantum states is given by

$$\varphi_\alpha(\boldsymbol{r})=\langle\boldsymbol{r}|\varphi_\alpha\rangle=\psi_{sj}(z)\phi_\nu(\boldsymbol{r}_\perp), \tag{A9}$$

where α is the index triple $(sj\nu)$. We find the usual completeness relation $\Sigma_\alpha\varphi_\alpha^*(\boldsymbol{r})\varphi_\alpha(\boldsymbol{r}')=\delta(\boldsymbol{r}-\boldsymbol{r}')$ and the orthonormality relation is given by $\int d^3r\varphi_\alpha^*(\boldsymbol{r})\varphi_{\alpha'}(\boldsymbol{r})=\delta_{\alpha\alpha'}$.

2. Definition of the statistical operator

Because the scattering states $|\varphi_\alpha\rangle$ constitute a discrete and complete orthonormal basis it is possible to introduce the creation and annihilation operators $\hat{c}_\alpha^\dagger$ and $\hat{c}_\alpha$, respectively, with the usual anticommutation relations $\{\hat{c}_\alpha,\hat{c}_{\alpha'}^\dagger\}=\delta_{\alpha,\alpha'}$, $\{\hat{c}_\alpha,\hat{c}_{\alpha'}\}=0$, and $\{\hat{c}_\alpha^\dagger,\hat{c}_{\alpha'}^\dagger\}=0$. Based on the anticommutation relations one can formulate a particle number representation which will be described in the following.

According to standard theory[49] the field operators are given by $\hat{\Psi}(\boldsymbol{r})=\Sigma_\alpha\varphi_\alpha(\boldsymbol{r})\hat{c}_\alpha$ and $\hat{\Psi}^\dagger(\boldsymbol{r})=\Sigma_\alpha\varphi_\alpha^*(\boldsymbol{r})\hat{c}_\alpha^\dagger$. The many-particle Hamiltonian of the stationary electron system can be written as

$$\hat{H}_0=\int d^3\boldsymbol{r}\hat{\Psi}^\dagger(\boldsymbol{r})\left[-\frac{\hbar^2}{2m^*}\Delta+V_\perp(\boldsymbol{r}_\perp)+V(z)\right]\hat{\Psi}(\boldsymbol{r}),$$

$$=\sum_\alpha E_\alpha\hat{c}_\alpha^\dagger\hat{c}_\alpha, \tag{A10}$$

where $E_\alpha=E_\perp^\nu+\epsilon_s(k_i)$ is the energy of the single-particle state $|\varphi_\alpha\rangle$. Here we use the notation $\hat{H}_0$ since in Sec. II B we consider a time-dependent perturbation of this Hamiltonian. We now use as a statistical operator for the stationary system as given by

$$\hat{\rho}_0=\frac{1}{Z_0}\exp[-\beta(\hat{H}_0-\mu_1\hat{N}_1-\mu_2\hat{N}_2)], \tag{A11}$$

with the chemical potentials μ_1 and μ_2 of source and drain contacts, respectively, the particle number operators $\hat{N}_s=\Sigma_{i\nu}\hat{c}_{si\nu}^\dagger\hat{c}_{si\nu}$ with $\hat{N}=\hat{N}_1+\hat{N}_2$, and

$$Z_0=\mathrm{Tr}\{\exp[-\beta(\hat{H}_0-\mu_1\hat{N}_1-\mu_2\hat{N}_2)]\}. \tag{A12}$$

The trace is done over all states of a Fock-space basis, constructed with the help of the single-particle scattering states $|\varphi_\alpha\rangle$. The trace is easy to write in the occupation number representation,

$$Z_0 = \sum_{N=0}^{\infty} \sum_{\{n_\alpha\}} \langle N; \cdots n_\alpha \cdots | \exp\left[-\beta \sum_{\alpha'} (E_{\alpha'} - \mu_{s'}) \hat{c}^\dagger_{\alpha'} \hat{c}_{\alpha'} \right] | N; \cdots n_\alpha \cdots \rangle = \prod_{\alpha} (1 + \exp(-\beta(E_\alpha - \mu_s))). \tag{A13}$$

The occupation number n_α of the single-particle state $|\varphi_\alpha\rangle$ for electrons is 0 or 1. It is straightforward to show that the statistical operator in Eq. (A11) is stationary, i.e., $[\hat{H}_0, \hat{\rho}_0] = 0$, and that it fulfills $\mathrm{Tr}\{\hat{\rho}_0\} = 1$.

3. Expectation values

Using Eq. (A13) one finds for the equilibrium mean value $\langle n_\alpha \rangle$ of the particle number operator of a single-particle state $|\varphi_\alpha\rangle$

$$\mathrm{Tr}\{\hat{\rho}_0 \hat{c}^\dagger_\alpha \hat{c}_{\alpha'}\} = \delta_{\alpha\alpha'} \langle n_\alpha \rangle = \delta_{\alpha\alpha'} \frac{\exp(-\beta(E_\alpha - \mu_s))}{1 + \exp(-\beta(E_\alpha - \mu_s))} = \delta_{\alpha\alpha'} f_{FD}(E_\alpha - \mu_s), \tag{A14}$$

with the Fermi-Dirac distribution function

$$f_{FD}(E_\alpha - \mu_s) = \frac{1}{1 + \exp(\beta(E_\alpha - \mu_s))}. \tag{A15}$$

In agreement with the Landauer-Büttiker formalism we then find for the mean value of the particle density operator

$$\rho(\boldsymbol{r}) = 2\,\mathrm{Tr}\{\hat{\rho}_0 \hat{\Psi}^\dagger(\boldsymbol{r}) \hat{\Psi}(\boldsymbol{r})\} = 2 \sum_{\alpha} f_{FD}(E_\alpha - \mu_s) |\varphi_\alpha(\boldsymbol{r})|^2 = 2 \sum_{s\nu} \int_{V_s}^{\infty} d\epsilon g_s(\epsilon) f_{FD}(E^\nu_\perp + \epsilon - \mu_s) |\phi_\nu(\boldsymbol{r}_\perp)|^2 |\psi^{(s)}(\epsilon, z)|^2, \tag{A16}$$

where we establish the continuous limit by replacing

$$\Delta k \sum_{\alpha} \to \sum_{s\nu} \int_0^\infty dk_s \to \sum_{s\nu} \int_{V_s}^\infty d\epsilon g_s(\epsilon) \tag{A17}$$

and the factor of 2 comes from the spin degeneracy. Considering ansatz (2) one can perform the ν summation in Eq. (A16) obtaining Eq. (8).

We want to mention here that we have followed a similar scheme for the second quantization as presented by Büttiker in Ref. 45, Sec. II B. We obtain the same mean values for the occupation numbers but using an ansatz for the density operator rather than for the mean values as is done in Eq. (2.12) in Ref. 45. As we show in Appendix B, using this statistical operator for the unperturbed system, we can carry out a standard linear-response theory to obtain the polarization in the well defined standard way.

APPENDIX B: HARMONIC PERTURBATION

In this appendix we describe our approach to calculate dynamic linear-response properties of open quantum systems which are defined in Sec. II A. Starting with Eq. (10) we determine the density matrix for the perturbed system using the von Neumann equation with $\hat{H}_0$ describing the stationary open system, Eq. (A10). In linear approximation one finds[50]

$$\delta\rho(\boldsymbol{r}, \omega) = \int d^3\boldsymbol{r}' \Pi_0(\boldsymbol{r}, \boldsymbol{r}', \omega) \delta V(\boldsymbol{r}', \omega), \tag{B1}$$

where the density-density correlation function (irreducible polarization) is given by

$$\Pi_0(\boldsymbol{r}, \boldsymbol{r}', \omega) = \frac{i}{\hbar} \int_0^\infty d\tau \exp(i(\omega + i\eta)\tau) \langle [\hat{\rho}_I(\boldsymbol{r}, \tau), \hat{\rho}(\boldsymbol{r}')] \rangle_0. \tag{B2}$$

The index 0 means the thermodynamic expectation value with respect to the statistical operator $\hat{\rho}_0$ as given by Eq. (A11) and the index I means the operator in the interaction picture. The single-particle density operators $\hat{\rho}$ are now written in the second quantization using the field operators of the scattering states defined in Appendix A so that

$$\hat{\rho}_I(\boldsymbol{r}, \tau) = \sum_{\alpha,\alpha'} \varphi^*_\alpha(\boldsymbol{r}) \varphi_{\alpha'}(\boldsymbol{r}) \exp[i\hat{H}_0 \tau/\hbar] \hat{c}^\dagger_\alpha \hat{c}_{\alpha'} \exp[-i\hat{H}_0 \tau/\hbar], \tag{B3}$$

with $\alpha \equiv (sj\nu)$ and $\hat{\rho}(\boldsymbol{r}) = \hat{\rho}_I(\boldsymbol{r}, \tau = 0)$. In a standard way one uses the anticommutation relations for the $\hat{c}^\dagger_\alpha$ and $\hat{c}_\alpha$ to calculate the commutator in Eq. (B2) and obtains

$$\Pi_0(\boldsymbol{r}, \boldsymbol{r}', \omega) = 2 \lim_{\eta \to 0} \sum_{\alpha,\alpha'} \frac{f_{FD}(E_\alpha - \mu_s) - f_{FD}(E_{\alpha'} - \mu_{s'})}{E_\alpha - E_{\alpha'} + \hbar(\omega + i\eta)} \times \varphi^*_\alpha(\boldsymbol{r}) \varphi_{\alpha'}(\boldsymbol{r}) \varphi^*_{\alpha'}(\boldsymbol{r}') \varphi_\alpha(\boldsymbol{r}'), \tag{B4}$$

where we have used Eq. (A14) for the expectation values. Different from the usual expression for Π_0, the Fermi-Dirac occupation functions f_{FD} may contain different chemical potentials, either that of the source contact for $s=1$ or that of

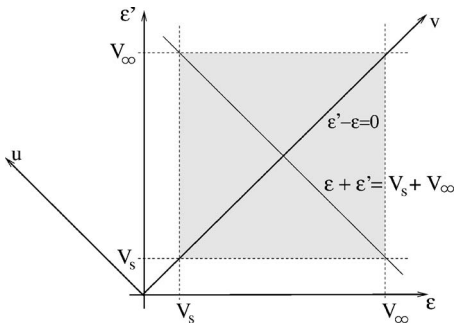

FIG. 4. Transformation of the two-dimensional integral [Eq. (C4)]. The gray area illustrates the integration domain.

the drain contact for $s=2$. Furthermore, the single-particle energies E_α are given in Eq. (A10) and the overall factor of 2 in Eq. (B4) accounts for the spin degree of freedom.

In the considered planar structure the potential perturbation depends only on z, $\delta V(\boldsymbol{r}')=\delta V(z)$. In order to develop further Eq. (B4), we take the continuous limit [Eq. (A17)], and using Eqs. (4) and (2) one can first integrate over $\boldsymbol{r}_\perp$ obtaining $\delta(\boldsymbol{k}_\perp-\boldsymbol{k}'_\perp)$ and after that sum over $\boldsymbol{k}_\perp$. As a result, a z-dependent density modulation $\delta\rho(\boldsymbol{r})=\delta\rho(z)$ is obtained which is related to the potential modulation by Eq. (11), and the polarization $\Pi_0(z,z',\omega)$ is given by Eq. (12).

Evaluating in the same procedure the perturbation of the expectation value of the z component of particle current density $\hat{j}_z(\boldsymbol{r})=(\hbar/m^*)\mathrm{Im}(\Psi^\dagger(\boldsymbol{r})\nabla_z\hat{\Psi}(\boldsymbol{r}))$, one obtains

$$\delta j_z(|z|\le d)=\int_{-d}^{d}dz'\tilde{\Pi}_0(z,z',\omega)\delta V(z'). \tag{B5}$$

The current-density response function for a planar structure has the form $\tilde{\Pi}_0(z,z',\omega)=\Sigma_{ss'}\tilde{\Pi}_0^{(ss')}(z,z',\omega)$ with

$$\tilde{\Pi}_0^{(ss')}(z,z',\omega)=\lim_{\eta\to 0}\int_{V_s}^{\infty}d\epsilon\int_{V_{s'}}^{\infty}d\epsilon'\frac{\tilde{F}^{(ss')}(z,z',\epsilon,\epsilon')}{\epsilon-\epsilon'+\hbar(\omega+i\eta)} \tag{B6}$$

and

$$\tilde{F}^{(ss')}(z,z',\epsilon,\epsilon')=2\frac{m^*}{2\pi\beta\hbar^2}g_s(\epsilon)g_{s'}(\epsilon')\ln\left\{\frac{1+\exp[\beta(\mu_s-\epsilon)]}{1+\exp[\beta(\mu_{s'}-\epsilon')]}\right\}\frac{\hbar}{2im^*}\left[(\psi^{(s)}(\epsilon,z))^*\frac{d}{dz}\psi^{(s')}(\epsilon',z)-\psi^{(s')}(\epsilon',z)\frac{d}{dz}(\psi^{(s)}(\epsilon,z))^*\right]$$
$$\times(\psi^{(s')}(\epsilon',z'))^*\psi^{(s)}(\epsilon,z'). \tag{B7}$$

APPENDIX C: LOW-FREQUENCY EXPANSION OF THE IRREDUCIBLE POLARIZATION

For small frequencies we expand in Eq. (12) for finite η

$$\frac{1}{\epsilon-\epsilon'+\hbar(\omega+i\eta)}\approx\frac{1}{\epsilon-\epsilon'+i\hbar\eta}-\frac{\hbar\omega}{(\epsilon-\epsilon'+i\hbar\eta)^2}, \tag{C1}$$

finding

$$P_0^{(s)}(z,z')=\lim_{\eta\to 0}\int_{V_s}^{\infty}d\epsilon\int_{V_s}^{\infty}d\epsilon'\frac{F^{(ss)}(z,z',\epsilon,\epsilon')}{\epsilon-\epsilon'+i\hbar\eta} \tag{C2}$$

and

$$P_1^{(s)}(z,z')=-\frac{\hbar}{i}\lim_{\eta\to 0}\int_{V_s}^{\infty}d\epsilon\int_{V_s}^{\infty}d\epsilon'\frac{F^{(ss)}(z,z',\epsilon,\epsilon')}{(\epsilon-\epsilon'+i\hbar\eta)^2}. \tag{C3}$$

We introduce a transformation $v=\epsilon+\epsilon'$ and $u=\epsilon'-\epsilon$ so that for a general function $f(\epsilon,\epsilon')$

$$\int_{V_s}^{V_\infty}d\epsilon\int_{V_s}^{V_\infty}d\epsilon' f(\epsilon,\epsilon')=\frac{1}{2}\int_{2V_s}^{2V_\infty}dv\int_{-u_0(v)}^{u_0(v)}du f(\epsilon(v,u),\epsilon'(v,u)), \tag{C4}$$

where we introduce a cutoff energy $V_\infty\to\infty$. Furthermore, as illustrated in Fig. 4, $u_0(v<V_s+V_\infty)=v-2V_s$ and $u_0(v>V_s+V_\infty)=2V_\infty-v$. For fixed z,z' we write $F^{(ss)}\times(z,z',\epsilon,\epsilon')=\alpha\chi(v,u)$ with $\alpha=2m^*/2\pi\beta\hbar^2$ and

$$\chi(v,u)=M\left(\frac{v-u}{2}\right)M^*\left(\frac{v+u}{2}\right)\left[N\left(\frac{v-u}{2}\right)-N\left(\frac{v+u}{2}\right)\right], \tag{C5}$$

where

$$M(v)=g_s(v)(\psi^{(s)}(v,z))^*\psi^{(s)}(v,z') \tag{C6}$$

and

$$N(v)=\ln\{1+\exp(\beta(\mu_s-v))\}. \tag{C7}$$

It is easy to see that $\chi(v,u)=\chi_1(v,u)+i\chi_2(v,u)=-\chi^*(v,-u)$ so that $\chi_1(v,u)=-\chi_1(v,-u)$ and $\chi_2(v,u)=\chi_2(v,-u)$. Furthermore, since $\chi(v,0)=0$ one finds for small $|u|$ the expansion

$$\chi(v,u\to 0)\approx u\chi_u(v,0), \tag{C8}$$

where we obtain a real function for the partial derivative with respect to u at $u=0$,

$$\chi_u(v,0)=\beta\left|M\left(\frac{v}{2}\right)\right|^2 f_{FD}\left(\frac{v}{2}-\mu_s\right), \tag{C9}$$

with the Fermi-Dirac distribution function given by Eq. (A15). This means that in expansion (C8), the leading term in the real part is linear in u while the leading term in the imaginary part is parabolic in u. Writing $\lim_{\eta\to 0}(\epsilon-\epsilon'+i\hbar\eta)^{-1}=-\mathrm{PV}(1/u)-i\pi\delta(u)$, where PV denotes the Cauchy principal value, and using the symmetry properties of the functions χ_1 and χ_2, one obtains

$$P_0^{(s)}(z,z') = -\frac{\alpha}{2}\int_{2V_s}^{2V_\infty} dv \int_{-u_0(v)}^{u_0(v)} du \frac{\chi_1(v,u)}{u} = \int_{V_s}^{V_\infty} d\epsilon \int_{V_s}^{V_\infty} d\epsilon' \frac{F_1^{(ss)}(z,z',\epsilon,\epsilon')}{\epsilon-\epsilon'}, \quad \text{(C10)}$$

where $F^{(ss)}(z,z',\epsilon,\epsilon') = F_1^{(ss)}(z,z',\epsilon,\epsilon') + iF_2^{(ss)}(z,z',\epsilon,\epsilon')$. In Eq. (C10) we omitted the principal-value operation because one obtains in $u=0$ a regular integrand due to the expansion in Eq. (C8). Writing[51] $\lim_{\eta\to 0}(\epsilon-\epsilon'+i\hbar\eta)^{-2} = \mathrm{PV}(1/u^2) - i\pi(d/du)\delta(u)$ it follows from Eq. (C3) that

$$P_1^{(s)}(z,z') = -\frac{\alpha\hbar}{2}\int_{2V_s}^{2V_\infty} dv \int_{-u_0(v)}^{u_0(v)} du \frac{\chi_2(v,u)}{u^2} - \frac{\alpha\hbar}{2}\pi\int_{2V_s}^{2V_\infty} dv\,\chi_u(v,0) = -\hbar\int_{V_s}^{V_\infty} d\epsilon \int_{V_s}^{V_\infty} d\epsilon' \frac{F_2^{(ss)}(z,z',\epsilon,\epsilon')}{(\epsilon-\epsilon')^2} - \alpha\beta\hbar\pi\int_{V_s}^{V_\infty} d\epsilon g_s^2(\epsilon) \times |\psi^{(s)}(\epsilon,z)|^2 |\psi^{(s)}(\epsilon,z')|^2 f_{FD}(\epsilon-\mu_s). \quad \text{(C11)}$$

Here we omitted the principal-value operation in the first integral since the integrand is regular at $u=0$ because the leading order term in $\chi_2(v,u\to 0)$ is parabolic in u.

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