Transmission, *S*-matrix, and partial densities of states for ac transport through a resonant cavity with multileads

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(Received 20 March 2002; published 25 July 2002)

We investigate the principal properties of ac transport through a resonant cavity with multileads. In terms of Green's function and the coupling strengths of the system, a set of general expressions for the partial densities of states (PDOS) can be derived in an unambiguous way. In particular we derive the PDOS with a reflection property. All the PDOS's are in an explicit and compact form. Based upon these PDOS's, the ac conductance can be calculated to a first-order frequency-dependent term. As an extension, we introduce the second-order nonlinear PDOS; then the ac conductance can be generalized to include the second-order contribution. As an example, we apply these formulas to evaluate the linear emittance and the second-order nonlinear emittance in a simplified structure. Some interesting results are obtained.

DOI: 10.1103/PhysRevB.66.045321 PACS number(s): 72.10.Bg, 73.21.−b, 11.80.−m

I. INTRODUCTION

With the advance of nanofabrications and quantum electronics it is desired to understand the properties of small electrical systems. For instance, metal-oxide-semiconductor transistors with channel lengths as small as 10 nm are now being actively studied theoretically and experimentally, and recently molecular devices have been demonstrated close to realistic functions.[1–6] These have stimulated further research into quantum logical circuits in developing quantum computing. It is clear that a quantum description of the properties of such systems is demanded. Of particular interest are the properties of ballistic electron transport through a quantum dot with leads attached to it. In order for quantum electric devices to operate effectively in the presence of logical gate-based dynamics, the devices must be subject to a source-drain bias or an alternating current, and work in nonequilibrium states.[7–9]

Following Büttiker and co-workers pioneering work, low-frequency, gauge invariant, and current conservation theories were established in a scattering framework.[10–13] In this theory certain quantities appear naturally in the response formulas. The most important are the partial densities of states (PDOS) and the local partial densities of states (LPDOS).[14–17] The characters of electron motion in mesoscopic systems are dominated by these quantities which determine the frequency-dependent conductance in the presence of slowly oscillating potentials applied to contacts of a nanostructure. As one knows that the density of states (DOS) is used to describe the equilibrium properties of a physical system, in order to treat the nonequilibrium problems the PDOS is useful by introducing injectivity and emissivity.[11,18,19] The former describes carriers injected from a reservoir regardless of which reservoir carriers exit, and the latter describes how these carriers emit to a reservoir regardless from which reservoir these carriers enter. In fact, the nondiagonal elements of the PDOS are important in describing fluctuations and correlations of carriers in transport states.[20] It can be shown that the injectivity is related to the dwell time of carriers in a conductor.[21–27] In low-frequency transport theory, the PDOS can be expressed naturally by scattering matrices. Electrical quantities such as the capacitance and the nonlinear conductance are strongly dependent on the PDOS.

In this paper we are concerned with several issues for a multiterminal conductor, such as the transmission probability, the DOS, the injectivity and emissivity, the transmission and reflection PDOS, and the dynamical admittance. We shall derive general expressions for these quantities in terms of the Green's function and the coupling strengths of a system, and then obtain an analytical expression for the ac admittance in the neutral approximation. In fact for frequencies which are not too large the mesoscopic conductor of interest here is a locally screened state at all times.

The paper is organized as follows. The model is introduced in Sec. II. Then, in Sec. III the analytical work is done to derive various densities of states in a precise way. An illustrating example is given in Sec. IV, and finally there is a brief summary.

II. MODEL AND FORMULATION

We would like to investigate the structure in which a sample is so small that the phase coherence length exceeds all of its dimensions. The sample is connected to several contacts which are all in the thermal equilibrium state, and has a large number of electrons. This means that taking out or adding in a small number of electrons does not affect the properties of reservoirs. We assume that the system consists of a cavity, such as quantum dot, quantum well, or magnetic resonator, and several leads through which carriers enter in and exit from the cavity.[28–32] The whole device is initially divided into two different parts. The first part contains an isolated conductor or a small island, while the second part includes ideal leads (waveguides) which couple the device to the measuring apparatus. The electrons (or carriers) move freely and independently inside these ideal leads. The device

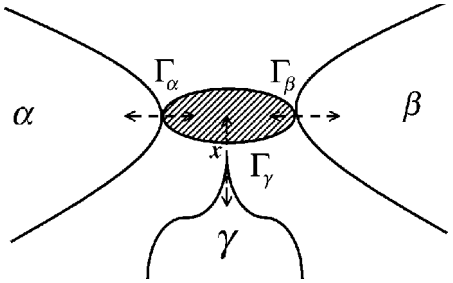

FIG. 1. The sketch of a resonant structure. α, β, and γ represent the probes connecting with reservoirs. Γ_α, Γ_β, and Γ_γ are the coupling parameters for each contact.

is controlled by external fields by means of a direct coupling to current sources or voltage sources.

In this system, only resonant transmission makes sense, so for a simple statement the structure will be referred to as a resonator, which is schematically shown in Fig. 1. It is ballistic for carriers in this open mesoscopic system. The inelastic scatterings take place only in the reservoirs. If there are N reservoirs connected to the resonator by N ideal leads, for the αth ideal lead there are N_α open channels. We consider a model Hamiltonian to describe such a resonant structure.

The first part of the Hamiltonian describing the free motion of electrons in the isolated leads is

$$\mathcal{H}_0=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}\int dE|\alpha m;E\rangle\langle\alpha m;E|E,$$

where $|\alpha m;E\rangle$ are the channel wave functions, and satisfy the normalization $\langle\alpha m;E|\beta n;E'\rangle=\delta_{\alpha\beta}\delta_{mn}\delta(E-E')$. At zero temperature the energy of free electrons in the leads is Fermi energy, i.e., $E=E_F=E_m+p^2/2m^*$. Here E_m is the transverse energy of the mth channel, and m^* is the effective mass of an electron. Then the above isolated lead Hamiltonian can be rewritten by

$$\mathcal{H}_0=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}|\alpha m\rangle\langle\alpha m|E_F, \tag{1}$$

where $\langle\alpha m|\beta n\rangle=\delta_{\alpha\beta}\delta_{mn}$.

We use the tight-binding approximation for the interior of the resonator. The resonator is discretized by N_c sites, and each site has a wave function $|x_i\rangle$. In general N_c is much larger than the number of open channels for any isolated lead, i.e., $N_c\gg N_\alpha$. Then the resonator Hamiltonian can be expressed by

$$\mathcal{H}_c=\sum_{x_i,x_j=1}^{N_c}|x_i\rangle\langle x_j|\mathcal{H}_{x_ix_j}, \tag{2}$$

where x_i is in the interior of the resonator. The bound states $|x_i\rangle$ satisfy the condition $\langle x_i|x_j\rangle=\delta_{x_ix_j}$, with $i=1,2,\ldots,N_c$. The scattering states $|\alpha m\rangle$ and the bound states $|x_i\rangle$ form the complete set of a basis in Hilbert space, i.e.,

$$1=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}|\alpha m\rangle\langle\alpha m|+\sum_{x_i=1}^{N_c}|x_i\rangle\langle x_i|.$$

To describe the scattering of electrons in the whole system we have to couple the resonator and the leads by defining the Hamiltonian $\mathcal{H}_T$,

$$\mathcal{H}_T=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}\sum_{x_i=1}^{N_c}|x_i\rangle\int dE\langle\alpha m;E|t_{x_i,\alpha m}+\text{H.c.}, \tag{3}$$

where $t_{x_i,\alpha m}$ is the coupling strength between a state in channel m in lead α and state $|x_i\rangle$ in the resonator.

Combination of the isolated Hamiltonians and the coupling Hamiltonian forms the total Hamiltonian of our system which is spanned by the complete set $\{|\alpha m\rangle,|x_i\rangle\}$ in Hilbert space:[33]

$$\mathcal{H}=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}|\alpha m\rangle\langle\alpha m|E_F+\sum_{x_i,x_j=1}^{N_c}|x_i\rangle\langle x_j|\mathcal{H}_{x_ix_j}+\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}\sum_{x_i=1}^{N_c}|x_i\rangle\int dE\langle\alpha m;E|t_{x_i,\alpha m}+\text{H.c.} \tag{4}$$

In the following we will simplify the second term on the right-hand side of Eq. (4) by conserving only the diagonal elements. It is found that $\mathcal{H}_{x_ix_i}$ includes the resonant energy level E_n, the local electrostatic potential and the self-energy due to the coupling to leads,[34]

$$\mathcal{H}_{x_ix_i}=E_n+eU(x_i)+\Delta, \tag{5}$$

where the local electrostatic potential $U(x_i)$ is produced by charge pileup or depletion in scattering processes or controlled by external gates, and Δ is the energy shift due to the coupling.

According to Büttiker and co-workers multiprobe-scattering theory,[10–12] external gates are not particular. They are also viewed as leads and can be treated the same as $|\alpha m\rangle$ states. The electrostatic potential produced by a charge distribution is determined by the Poisson equation. One should note that the approach used here is restricted to the temperatures $kT\ll\Delta_n$, where Δ_n is the single-particle level spacing of the resonator. In the mesoscopic transport regime we want to know the physical properties of the system from the scattering states in leads. Using the formal scattering theory and the Lippmann-Schwinger equation, one can relate scattering wave functions to the structure of the system. The scattering matrix $S_{\alpha\beta}(E)$ of the Hamiltonian $\mathcal{H}$ can be written using the standard technique[35–37]

$$\hat{S}=1-2\pi i\,\delta(E-\mathcal{H}_0)\hat{T}, \tag{6}$$

where $\hat{T}$ is the transition operator which relates incident and outgoing wave functions in the leads. In our model the S matrix can be reduced to[31,33,35]

$$\hat{S}=1-2\pi i\hat{W}^\dagger\hat{G}\hat{W}, \tag{7}$$

where $\hat{G}$ is the Green's function,

$$\hat{G}=(E-\mathcal{H}_c+i\pi\hat{W}\hat{W}^{\dagger})^{-1}, \tag{8}$$

and $\hat{W}$ is a coupling matrix:

$$\hat{W}=\sum_{\alpha=1}^{N}\sum_{m=1}^{N_\alpha}\sum_{x_i=1}^{N_c}|x_i\rangle\langle\alpha\, m|t_{x_i,\alpha m}. \tag{9}$$

Then the components of the *S*-matrix are

$$\begin{aligned}S_{\alpha m,\beta n}&=\langle\alpha\, m|\hat{S}|\beta\, n\rangle\\&=\delta_{\alpha\beta}\delta_{mn}-2\pi i\langle\alpha\, m|\hat{W}^{\dagger}\hat{G}\hat{W}|\beta\, n\rangle\\&=\delta_{\alpha\beta}\delta_{mn}-2\pi i\sum_{x_i,x_j}W^{\dagger}_{\alpha m,x_i}G(x_i,x_j)W_{x_j,\beta n}.\end{aligned} \tag{10}$$

We are interested in the properties of mesoscopic systems which are influenced by alternating external voltages. According to Büttiker's low-frequency and gauge invariant transport theory, the linear frequency-dependent conductance of the system is expressed by[38,39]

$$g_{\alpha\beta}(\omega)=g_{\alpha\beta}(0)-i\omega e^2E_{\alpha\beta}. \tag{11}$$

The coefficient of the frequency term, called emittance, is determined in the Thomas-Fermi approximation by

$$E_{\alpha\beta}=\int dE\left(-\frac{\partial f}{\partial E}\right)\int d\mathbf{r}\left[\frac{dn(\alpha,\mathbf{r},\beta)}{dE}-\frac{dn(\alpha,\mathbf{r})}{dE}u_\beta(\mathbf{r})\right], \tag{12}$$

where $u_\beta(\mathbf{r})$ is the characteristic potential which gives the local potential distribution profile inside the system. $dn(\alpha,\mathbf{r},\beta)/dE$ is the LPDOS, and $dn(\alpha,\mathbf{r})/dE$ is the emissivity which denotes the character of the emission at point $\mathbf{r}$ to probe α. From the above formulas one knows that the LPDOS and the internal potential determine the properties of the imaginary part of the ac conductance.

The theory provided above describes the response of current at contact α to the variation of electrochemical potential at contact β.[10,12] Due to the oscillating internal potential an electron incident with energy E may gain or lose modulation energy $\hbar\omega$ during reflection at the sample or during transmission through the sample. Equation (11) is obtained by expanding the *S*-matrix and Fermi distribution function in powers of $\hbar\omega/E$, where E is around the Fermi energy. Thus the perturbation is reasonable for the low-frequency behavior if the electrochemical potential at contact α is weak enough for transitions to neighboring levels $E+\hbar\omega$ and $E-\hbar\omega$, while electrons passing through the structure affected by a slowly oscillating potential.

Furthermore, due to the applications of the second-order nonlinear ac admittance, one needs to know the second-order nonlinear LPDOS as well. For example, in measurements of the carrier density the usual methods are to detect the ratio of the linear and the second-order nonlinear capacitances.[40–45] In mesoscopic measurements the charge response at one contact to the voltage at an other contact is determined by the emittance. The second-order emittance is[43]

$$\begin{aligned}E_{\alpha\beta\gamma}=\int dE\left(-\frac{\partial f}{\partial E}\right)\int\Bigg[&-\frac{dn(\alpha,\mathbf{r})}{dE}u_{\beta\gamma}(\mathbf{r})\\&+\frac{d^2n(\alpha,\mathbf{r},\beta)}{dE^2}\delta_{\beta\gamma}-\frac{d^2n(\alpha,\mathbf{r},\beta)}{dE^2}u_\gamma(\mathbf{r})\\&-\frac{d^2n(\alpha,\mathbf{r},\gamma)}{dE^2}u_\beta(\mathbf{r})+\frac{d^2n(\alpha,\mathbf{r})}{dE^2}u_\beta(\mathbf{r})u_\gamma(\mathbf{r})\Bigg]d\mathbf{r},\end{aligned} \tag{13}$$

where $u_{\beta\gamma}(r)$ is the second-order characteristic potential and $d^2n(\alpha,\mathbf{r},\beta)/dE^2$ is the second-order nonlinear LPDOS.

III. PARTIAL DENSITIES OF STATES

In this section we will study the LPDOS using the Green's function and the coupling matrix. For simplicity, here we consider the quasi-one-dimensional problem; then the LPDOS is[11,12,15–17,28]

$$\begin{aligned}\frac{dn(\alpha,x,\beta)}{dE}=-\frac{1}{4\pi i}\sum_{m=1}^{N_\alpha}\sum_{n=1}^{N_\beta}\Bigg\{&S^{\dagger}_{\alpha m,\beta n}[E,U(x)]\\&\times\frac{\delta S_{\alpha m,\beta n}[E,U(x)]}{\delta U(x)}-\frac{\delta S^{\dagger}_{\alpha m,\beta n}[E,U(x)]}{\delta U(x)}\\&\times S_{\alpha m,\beta n}[E,U(x)]\Bigg\}.\end{aligned} \tag{14}$$

The global PDOS is just the integral of the LPDOS, i.e., $dN(\alpha,\beta)/dE=\int dx[dn(\alpha,x,\beta)/dE]$. For the following derivation we define a potential operator in the Hartree approximation as

$$\hat{U}=\sum_{x'}|x'\rangle\langle x'|U(x'), \tag{15}$$

where x' is in the interior of the cavity, so is the potential $U(x')$. Taking a variational derivative for Eq. (15), this gives

$$\frac{\delta\hat{U}}{\delta U(x)}=|x\rangle\langle x|. \tag{16}$$

According to the definition of functional derivatives, $\delta S/\delta U(x)=\partial S/\partial\mathcal{H}_c\,\delta\mathcal{H}_c/\delta U(x)$, from Eqs. (2), (5), (8), and (10), one has

$$\frac{\delta S_{\alpha m,\beta n}}{\delta U(x)}=-2\pi i\sum_{x_i,x_j}t^{*}_{\alpha m,x_i}\langle x_i|G|x\rangle\langle x|G|x_j\rangle t_{x_j,\beta n}, \tag{17}$$

and similarly

$$\frac{\delta S^{\dagger}_{\alpha m,\beta n}}{\delta U(x)}=2\pi i\sum_{x_i,x_j}t^{*}_{\beta n,x_i}\langle x_i|G^{\dagger}|x\rangle\langle x|G^{\dagger}|x_j\rangle t_{x_j,\alpha m}. \tag{18}$$

Substituting them into Eq. (14), we have the LPDOS

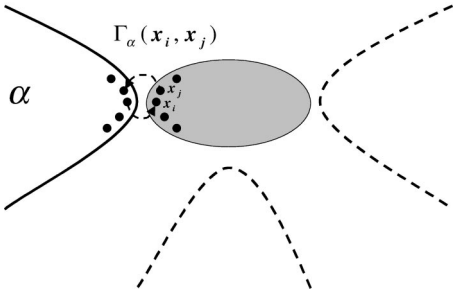

FIG. 2. The coupling between lead α and two sites x_i and x_j at the boundary. x_i and x_j are inside the cavity. The coupling strength matrix is represented by $\Gamma_\alpha(x_i,x_j)$. It is the same for the other leads β, γ, etc.

$$\frac{dn(\alpha,x,\beta)}{dE}=\frac{1}{2}\Bigg[\delta_{\alpha\beta}\sum_{m=1}^{N_\alpha}\sum_{x_1,x_2}\gamma_{\alpha m}(x_2,x_1)G(x_1,x)G(x,x_2)+\pi i\sum_{m=1}^{N_\alpha}\sum_{n=1}^{N_\beta}\sum_{x_3,x_4}\sum_{x_i,x_j}\gamma_{\beta n}(x_4,x_3)G^\dagger(x_3,x_i)\times\gamma_{\alpha m}(x_i,x_j)G(x_j,x)G(x,x_4)-\text{H.c.}\Bigg], \quad (19)$$

where we have defined the parameter

$$\gamma_{\alpha m}(x_i,x_j)=t_{x_i,\alpha m}t^*_{\alpha m,x_j},$$

and we assume that $\gamma_{\alpha m}(x_i,x_j)$ is real. We can further define two parameters

$$\gamma_\alpha(x_i,x_j)=\sum_m \gamma_{\alpha m}(x_i,x_j), \gamma(x_i,x_j)=\sum_\alpha \gamma_\alpha(x_i,x_j)$$

for later use.

For writing Eq. (19) in a more compact form, we introduce the coupling operators for a single channel,

$$\hat{\Gamma}_{\alpha m}=\sum_{x_i,x_j}|x_i\rangle\gamma_{\alpha m}(x_i,x_j)\langle x_j|, \quad (20)$$

and for a lead:

$$\hat{\Gamma}_\alpha=\sum_{m=1}^{N_\alpha}\hat{\Gamma}_{\alpha m}. \quad (21)$$

The coupling points are taken at the boundaries of the cavity, as shown in Fig. 2. Now Eq. (19) becomes[28,29]

$$\frac{dn(\alpha,x,\beta)}{dE}=\frac{1}{2}\delta_{\alpha\beta}[(G\Gamma_\alpha G)_{xx}+(G^\dagger\Gamma_\alpha G^\dagger)_{xx}]+\pi i[(G\Gamma_\beta G^\dagger\Gamma_\alpha G)_{xx}-(G^\dagger\Gamma_\alpha G\Gamma_\beta G^\dagger)_{xx}]. \quad (22)$$

To see the meaning of a transmission amplitude matrix in our system, we write a component of the S-matrix for $\alpha\neq\beta$ explicitly, i.e.,

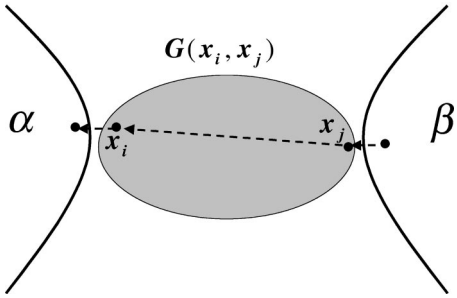

FIG. 3. The propagation of waves in a cavity. A carrier is incident from contact β and hops to site x_j by the coupling strength Γ_β. The carrier moves coherently through all paths to site x_i and then enters lead α.

$$S_{\alpha m,\beta n}=-2\pi i\sum_{x_i,x_j}t^*_{\alpha m,x_i}\langle x_i|G|x_j\rangle t_{x_j,\beta n}.$$

It relates the incident amplitude to the outgoing amplitude of a wave function. Both incident and outgoing waves suffer the scattering at the boundaries and transport coherently from site x_j to x_i. The propagator $G(x_i,x_j)$ goes all the path connecting site x_j and x_i, that is, $G(x_i,x_j)=\Sigma_p A_p(x_i,x_j)$, and p includes all Feynman paths starting from site x_j and ending at site x_i. We can see this process in Fig. 3.

In the following we need the transmission and reflection probabilities of the system. By the definition of the transmission matrix for $\alpha\neq\beta$, we have

$$T_{\alpha\beta}=\sum_{m=1}^{N_\alpha}\sum_{n=1}^{N_\beta}S^\dagger_{\alpha m,\beta n}S_{\alpha m,\beta n}=4\pi^2\sum_{m=1}^{N_\alpha}\sum_{n=1}^{N_\beta}\sum_{x_1,x_2}\sum_{x_i,x_j}\gamma_{\beta n}(x_i,x_j)G^\dagger(x_i,x_j)\times\gamma_{\alpha m}(x_1,x_2)G(x_2,x_i).$$

It is the summation of the diagonal elements of the transmission matrix. The transmission probability from contact β to contact α can be written in a simplified form[34,46,47]

$$T_{\alpha\beta}=4\pi^2\text{Tr}(\Gamma_\beta G^\dagger\Gamma_\alpha G)=4\pi^2\text{Tr}(\Gamma_\alpha G\Gamma_\beta G^\dagger). \quad (23)$$

The physical meaning is clear that for the transmission from contact β to contact α is determined by the propagator and the coupling strengths at the boundaries. In terms of the transmission and the total density of states we can express the transmission LPDOS,

$$\frac{dn(\alpha,x,\beta)}{dE}=\pi i\sum_{m=1}^{N_\alpha}\sum_{n=1}^{N_\beta}\sum_{x_3,x_4}\sum_{x_i,x_j}[\gamma_{\beta n}(x_4,x_3)G^\dagger(x_3,x_i)\times\gamma_{\alpha m}(x_i,x_j)G(x_j,x)G(x,x_4)-\text{H.c.}]$$

in a more explicit form. By noting the relation[48–50]

$$G(x_j,x_\mu)G(x_\mu,x_i')=G(x_\mu,x_\mu)G(x_j,x_i') \quad (24)$$

for wave propagation in the path $x_i'\to x_\mu\to x_j$, we have

$$\frac{dn(\alpha,x,\beta)}{dE}=\pi i[G(x,x)-G^{\dagger}(x,x)]\mathrm{Tr}(G^{\dagger}\Gamma_{\alpha}G\Gamma_{\beta}).$$

Because the local density of states is defined by

$$\frac{dn(x)}{dE}=-\frac{1}{2\pi i}[G(x,x)-G^{\dagger}(x,x)],$$

we have

$$\frac{dn(\alpha,x,\beta)}{dE}=\frac{T_{\alpha\beta}}{2}\frac{dn(x)}{dE}. \tag{25}$$

Integrating both side over x gives the global transmission PDOS as

$$\frac{dN(\alpha,\beta)}{dE}=\frac{T_{\alpha\beta}}{2}\frac{dN}{dE}.$$

Now we can see what is the local injectivity $dn(x,\beta)/dE$ by summing the LPDOS over the index α, i.e.,

$$\begin{aligned}\frac{dn(x,\beta)}{dE}&=\sum_{\alpha}\frac{dn(\alpha,x,\beta)}{dE}\\&=\frac{1}{2}[(G\Gamma_{\beta}G)_{xx}+(G^{\dagger}\Gamma_{\beta}G^{\dagger})_{xx}]\\&\quad+\pi i\sum_{n=1}^{N_{\beta}}\sum_{x_3,x_4}\sum_{x_i,x_j}[\gamma_{\beta n}(x_4,x_3)G^{\dagger}(x_3,x_i)\\&\quad\times\gamma(x_i,x_j)G(x_j,x)G(x,x_4)-\mathrm{H.c.}].\end{aligned} \tag{26}$$

To simplify this expression we need the total density of states represented by the Green's function and the coupling strengths. Using the unitary property of the *S*-matrix

$$\sum_{\gamma}S^{\dagger}_{\gamma\alpha}S_{\gamma\beta}=\delta_{\alpha\beta},$$

we have

$$\begin{aligned}&-2\pi i\sum_{m}W^{\dagger}_{\alpha m}(G-G^{\dagger})W_{\beta m}\\&\quad+4\pi^2\sum_{\gamma}\sum_{m,n}W^{\dagger}_{\alpha n}G^{\dagger}\Gamma_{\gamma m}GW_{\beta n}=0\end{aligned} \tag{27}$$

for $\alpha\neq\beta$. Combining with Eqs. (9) and (20), Eq. (27) gives

$$\begin{aligned}&G(x_j,x_i)-G^{\dagger}(x_j,x_i)\\&\quad=-2\pi i\sum_{x_1,x_2}G^{\dagger}(x_j,x_1)\gamma(x_1,x_2)G(x_2,x_i).\end{aligned} \tag{28}$$

If we define the nonlocal density of states

$$\frac{dn(x,x')}{dE}=-\frac{1}{2\pi i}[G(x,x')-G^{\dagger}(x,x')]=-\frac{1}{\pi}\mathrm{Im}\,G(x,x'), \tag{29}$$

then, for $x'=x$, the local density of states is

$$\frac{dn(x)}{dE}=\sum_{x_1,x_2}G^{\dagger}(x,x_1)\gamma(x_1,x_2)G(x_2,x).$$

This is a well-known result.[34] Substituting Eq. (28) into (26), and combining Eqs. (20) and (21), the local injectivity can be written in a compact form:

$$\frac{dn(x,\beta)}{dE}=\sum_{x_i,x_j}G(x,x_j)\gamma_{\beta}(x_j,x_i)G^{\dagger}(x_i,x)=(G\Gamma_{\beta}G^{\dagger})_{xx}. \tag{30}$$

Similarly, the emissivity can be obtained by summing the LPDOS over the another index β. In the absence of magnetic field it is equal to the injectivity.[11,38]

Furthermore, the global injectivity in the operator form is

$$\begin{aligned}\frac{d\hat{N}(\alpha)}{dE}&=\sum_{\beta}\frac{d\hat{N}(\alpha,\beta)}{dE}\\&=\frac{1}{2}(\hat{G}\hat{\Gamma}_{\alpha}\hat{G}+\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}^{\dagger})\\&\quad+\pi i(\hat{G}\hat{\Gamma}\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}-\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}\hat{\Gamma}\hat{G}^{\dagger}).\end{aligned}$$

Inserting the relation $\hat{G}^{\dagger}\hat{\Gamma}\hat{G}=\hat{G}\hat{\Gamma}\hat{G}^{\dagger}=-1/2\pi i(\hat{G}-\hat{G}^{\dagger})$ into the above expression, we find

$$\frac{d\hat{N}(\alpha)}{dE}=\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}. \tag{31}$$

Its value is the sum of the diagonal elements of the local PDOS matrix, i.e.,

$$\begin{aligned}\frac{dN(\alpha)}{dE}&=\sum_{x}\langle x|\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}|x\rangle\\&=\sum_{x}(\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G})_{xx}\\&=\sum_{x}\frac{dn(x,\alpha)}{dE},\end{aligned}$$

and for the continuous spectrum $dN(\alpha)/dE=\int dx[dn(x,\alpha)/dE]$.

Finally the total DOS is the quantity by summing over the index α as

$$\frac{d\hat{N}}{dE}=\sum_{\alpha}\frac{d\hat{N}(\alpha)}{dE}=\sum_{\alpha}\hat{G}^{\dagger}\hat{\Gamma}_{\alpha}\hat{G}=\hat{G}^{\dagger}\hat{\Gamma}\hat{G}, \tag{32}$$

where $\hat{\Gamma}=\Sigma_{\alpha}\hat{\Gamma}_{\alpha}$. Although Eq. (32) can also be obtained by other method,[34] here we show that the *S*-matrix is an effective approach to give the correct result.

Now we shall derive the expression $dn(\alpha,x,\alpha)/dE$. From Eq. (22), we find

$$\frac{dn(\alpha,x,\alpha)}{dE}=\frac{1}{2}[(G\Gamma_\alpha G)_{xx}+(G^\dagger\Gamma_\alpha G^\dagger)_{xx}] + \pi i[(G\Gamma_\alpha G^\dagger\Gamma_\alpha G)_{xx}-(G^\dagger\Gamma_\alpha G\Gamma_\alpha G^\dagger)_{xx}]. \tag{33}$$

To simplify this expression, we first consider the reflection probability of αth lead in terms of the S-matrix:

$$R_{\alpha\alpha}=S^\dagger_{\alpha\alpha}S_{\alpha\alpha}=\sum_{m,n=1}^{N_\alpha}|S_{\alpha m,\alpha n}|^2.$$

By using Eqs. (9), (10), and (21), we can write this as

$$R_{\alpha\alpha}=N_\alpha-2\pi i[\mathrm{Tr}(\Gamma_\alpha G)-\mathrm{Tr}(\Gamma_\alpha G^\dagger)] + 4\pi^2\mathrm{Tr}(\Gamma_\alpha G^\dagger\Gamma_\alpha G), \tag{34}$$

where N_α is the number of modes in lead α. On the other hand, after some algebra from Eq. (26), we can prove the relation

$$(G\Gamma_\alpha G)_{xx}+(G^\dagger\Gamma_\alpha G^\dagger)_{xx} =2\frac{dn(x,\alpha)}{dE}-4\pi^2\frac{dn(x)}{dE}\mathrm{Tr}\left[\hat\Gamma_\alpha\frac{d\hat N(\alpha)}{dE}\right]. \tag{35}$$

Substituting Eqs. (34) and (35) into Eq. (33), the final result is

$$\frac{dn(\alpha,x,\alpha)}{dE}=\frac{1}{2}(R_{\alpha\alpha}-N_\alpha)\frac{dn(x)}{dE}+\frac{dn(x,\alpha)}{dE}.$$

Furthermore, the global reflection PDOS operator is

$$\frac{d\hat N(\alpha,\alpha)}{dE}=\frac{1}{2}(R_{\alpha\alpha}-N_\alpha)\frac{d\hat N}{dE}+\frac{d\hat N(\alpha)}{dE}. \tag{36}$$

As stated in Sec. I, it is useful to know the second-order nonlinear LPDOS or the global PDOS. We can derive the second-order nonlinear PDOS in a global operator form. The local PDOS is easily obtained by inserting local projection operator. The result for the transmission PDOS is

$$\frac{d^2\hat N(\alpha,\beta)}{dE^2}=T_{\alpha\beta}\frac{d^2\hat N}{dE^2}, \tag{37}$$

and that for the reflection PDOS is

$$\frac{d^2\hat N(\alpha,\alpha)}{dE^2}=(R_{\alpha\alpha}-N_\alpha)\frac{d^2\hat N}{dE^2}+\frac{d^2\hat N(\alpha)}{dE^2}, \tag{38}$$

where d^2N/dE^2 and $d^2N(\alpha)/dE^2$ represent the energy derivatives of the total density of states and partial density of states, respectively. In our system they are

$$\frac{d^2N}{dE^2}=\mathrm{Tr}[(\hat G+\hat G^\dagger)\hat G\hat\Gamma\hat G^\dagger],$$

$$\frac{d^2N(\alpha)}{dE^2}=\mathrm{Tr}[(\hat G+\hat G^\dagger)\hat G\hat\Gamma_\alpha\hat G^\dagger]. \tag{39}$$

IV. AN APPLICATION TO A QUANTUM WELL WITH TWO LEADS

As an illustrating example, we consider a simplified case in which the system consists of a quantum well attached by two single-channel leads.[51] The quantum well corresponds to a double-barrier structure with a resonant energy E_r. We can write the Green's function as $G(E)=[(E-E_r-eU-\Delta)+i\pi\Gamma]^{-1}$, where U is the electrostatic potential away from the non-Coulomb interaction state in the well. The coupling between the left lead and the well is Γ_1, and that is for the right lead and the well is Γ_2. The total coupling strength $\Gamma=\Gamma_1+\Gamma_2$ determines the energy width of particles deviating from the resonant level E_r. To simplify the analytical treatment we take Γ to be a number by making an average over all sites. Thus all the quantities in this example are numbers rather than the matrices. Equations (31) and (32) can be expressed explicitly by

$$\frac{dN(\alpha)}{dE}=G^\dagger\Gamma_\alpha G=\frac{\Gamma_\alpha}{(E-E_r-eU-\Delta)^2+\pi^2\Gamma^2}$$

and

$$\frac{dN}{dE}=G^\dagger\Gamma G=\frac{\Gamma}{(E-E_r-eU-\Delta)^2+\pi^2\Gamma^2}.$$

In the neutral approximation the characteristic potential is

$$u_\alpha=\frac{dN(\alpha)/dE}{dN/dE}=\frac{\Gamma_\alpha}{\Gamma}.$$

Substituting these expressions into Eq. (36) and taking $R_{11}=R_{22}=R$, $M_1=M_2=1$ and $T_{12}=T_{21}=T$, we have

$$\frac{dN(1,1)}{dE}=\frac{R}{2}\frac{dN}{dE}+\frac{1}{2}\left[\frac{dN(1)}{dE}-\frac{dN(2)}{dE}\right],$$

$$\frac{dN(2,2)}{dE}=\frac{R}{2}\frac{dN}{dE}+\frac{1}{2}\left[\frac{dN(2)}{dE}-\frac{dN(1)}{dE}\right].$$

The emittances now can all be determined. In particular at zero temperature they are

$$E_{11}=\frac{R}{2}\frac{dN}{dE}+\frac{\Gamma_2-\Gamma_1}{2\Gamma}\frac{dN(1)}{dE}-\frac{1}{2}\frac{dN(2)}{dE},$$

$$E_{22}=\frac{R}{2}\frac{dN}{dE}+\frac{\Gamma_1-\Gamma_2}{2\Gamma}\frac{dN(2)}{dE}-\frac{1}{2}\frac{dN(1)}{dE},$$

$$E_{12}=\frac{T}{2}\frac{dN}{dE}-\frac{\Gamma_2}{\Gamma}\frac{dN(1)}{dE},\quad E_{21}=\frac{T}{2}\frac{dN}{dE}-\frac{\Gamma_1}{\Gamma}\frac{dN(2)}{dE}. \tag{40}$$

It is easy to confirm that $E_{11}=E_{22}=-E_{12}=-E_{21}$. In this example we can write E_{11} or E_{12} in more explicit forms. If

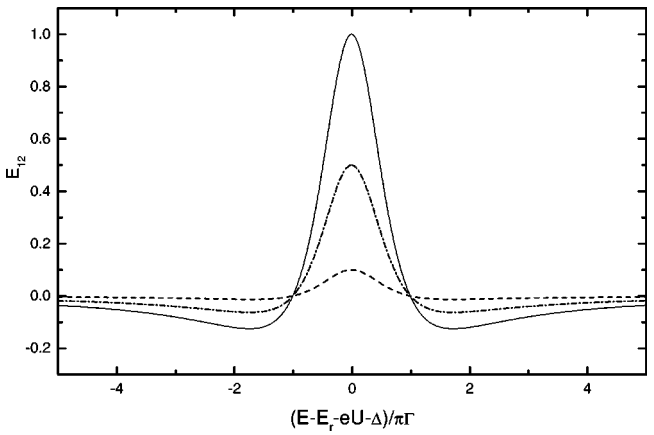

FIG. 4. The imaginary part of the dynamical conductance E_{12} vs the incident energy. The solid line is for the coupling ratio $\Gamma_1\Gamma_2/\Gamma^3=\pi^2$, while the dash-dotted line and the dashed line are for $\Gamma_1\Gamma_2/\Gamma^3=\pi^2/2$ and $\Gamma_1\Gamma_2/\Gamma^3=\pi^2/10$, respectively.

the structure is symmetric, i.e., $\Gamma_1=\Gamma_2=\Gamma/2$, substituting $dN(1)/dE$ into Eq. (40) we find

$$E_{12}=\left(\frac{T}{2}-\frac{\Gamma_1\Gamma_2}{\Gamma^2}\right)\frac{dN}{dE}=\frac{1}{4}(T-R)\frac{dN}{dE}$$

and

$$E_{11}=\frac{1}{4}(R-T)\frac{dN}{dE}.$$

It is clearly shown that in the resonant case E_{11} is negative and the crossover from negative to positive is at $R=T$. In general $\Gamma_1\neq\Gamma_2$, and Eq. (40) gives

$$E_{12}=\frac{\Gamma_1\Gamma_2}{\pi^2\Gamma^3}\frac{1-x^2}{(1+x^2)^2},$$

where

$$x=(E-E_r-eU-\Delta)/\pi\Gamma.$$

Figure 4 shows E_{12} vs x for different ratios of $\Gamma_1\Gamma_2/\Gamma^3$.

For the second-order emittance in the neutral approximation, the expression is

$$E_{\alpha\beta\gamma}=\tilde{D}_{\alpha\beta\gamma}-D_\alpha u_{\beta\gamma}, \tag{41}$$

where

$$\tilde{D}_{\alpha\beta\gamma}=\frac{d^2N(\alpha,\beta)}{dE^2}\delta_{\beta\gamma}-\frac{d^2N(\alpha,\beta)}{dE^2}u_\gamma - \frac{d^2N(\alpha,\gamma)}{dE^2}u_\beta+\frac{d^2N(\alpha)}{dE^2}u_\beta u_\gamma \tag{42}$$

and

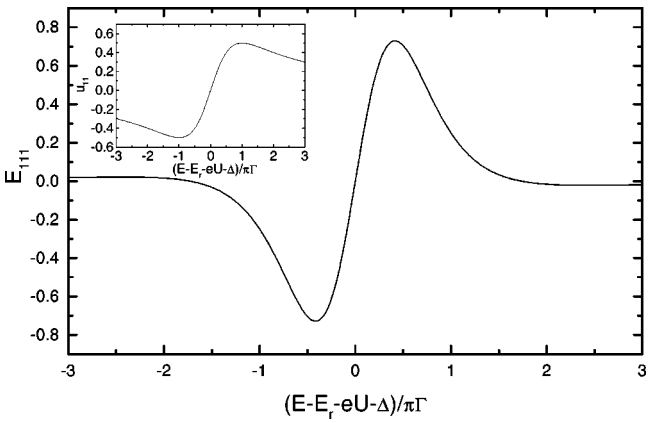

FIG. 5. The second-order nonlinear emittance E_{111} vs energy $(E-E_r-eU-\Delta)/\pi\Gamma$. The inset is the second-order characteristic potential vs the energy.

$$u_{\beta\gamma}=\frac{1}{(dN/dE)^3}\left[\frac{d^2N(\beta)}{dE^2}\left(\frac{dN}{dE}\right)^2\delta_{\beta\gamma} -2\frac{dN(\beta)}{dE}\frac{d^2N(\gamma)}{dE^2}\frac{dN}{dE}+\frac{dN(\beta)}{dE}\frac{d^2N}{dE^2}\frac{dN(\gamma)}{dE}\right]. \tag{43}$$

The second-order DOS and PDOS here can be obtained as

$$\frac{d^2N}{dE^2}=\frac{2}{\pi^3\Gamma^2}\frac{1}{(1+x^{2)^2}},\quad \frac{d^2N(\alpha)}{dE^2}=\frac{2\Gamma_\alpha}{\pi^3\Gamma^3}\frac{1}{(1+x^{2)^2}}. \tag{44}$$

Thus, inserting Eq. (44) into Eq. (43), one has

$$u_{11}=\frac{2\Gamma_1\Gamma_2}{\pi\Gamma^3}\frac{x}{1+x^2}. \tag{45}$$

In the same way we obtain the quantities

$$\frac{d^2N(1,1)}{dE^2}=\frac{2\Gamma_1}{\pi^3\Gamma^3}\frac{1}{(1+x^2)^2}\left[1-\frac{4\Gamma_2}{\Gamma(1+x^2)}\right] \tag{46}$$

and

$$\tilde{D}_{111}=\frac{2\Gamma_1\Gamma_2}{\pi^3\Gamma^5}\frac{x[(x^2-3)\Gamma_2+4\Gamma_1]}{(1+x^2)^3}. \tag{47}$$

Substituting Eqs. (45), (46), (47), and (31) into Eq. (41), we have the second-order nonlinear emittance

$$E_{111}=\frac{2\Gamma_1\Gamma_2}{\pi^3\Gamma^5}(\Gamma_1-\Gamma_2)\frac{x(3-x^2)}{(1+x^2)^3}.$$

This result shows that for the spatially symmetric structure $E_{111}=0$. For the nonsymmetric structure Fig. 5 shows E_{111} vs x. The second-order charge response at the contact 1 to the voltage variation at itself changes sign across the resonant energy E_r. From Eq. (45) one can see that the second-order

characteristic potential is not constant vs the incident energy, while the linear characteristic potential is constant.

V. SUMMARY

So far we have systematically investigated the ac transport of a small quantum structure composed of a resonant cavity with several leads. A model Hamiltonian is established for this. Based on Büttiker's and co-workers' pioneering work, we have dealt with a low-frequency conductance which is determined by a set of PDOS's. In terms of the Green's function and coupling parameters of the system, we have derived all the important formulas in a transparent way. We have also extended the PDOS to the second-order nonlinear case and derived the formulas for calculating the second-order nonlinear PDOS in terms of the Green's function and the coupling parameters. This extension is necessary and useful for the calculations of low-frequency and weakly nonlinear ac conductance. The results are in the compact and explicit form.

The theoretical results obtained are quite general and applicable for a resonant cavity connecting to an outside circuit through ideal leads. The physical meaning is clear: for instance, the transmission PDOS is a part of the total DOS and is proportional to the transmission probability. The transmission probability is related to the incident coupling strength and the outgoing coupling strength in the coherent propagation. The reflection PDOS is related to the reflection probability and the number of modes in an incident lead. This predicts that the number of modes in a lead will influence the ac transport in mesoscopic regime. The most important quantities in computing second-order nonlinear emittance are the second-order nonlinear PDOS.

It should be noted that the formulas derived in this work is based on weakly applied alternating potentials. In actual applications of these formulas one can first apply a large constant bias to reach the working point and then add a slowly oscillating voltage around the working point. This is just a typical method in classical circuits. A self-consistent calculation is needed for the alternating potential, and we require the frequencies to be far smaller than the typical sideband spacing ΔE. For example, in nanostructures composed of typical materials such as GaAs, the cutoff frequency can be as large as 100GHz.

We have applied the linear and nonlinear PDOS expressions to treat an illustrating example of ac coherent transport. For a quantum well with two single-channel leads and in the nuetral approximation, the linear and second-order nonlinear emittances were analytically derived and numerically calculated. The linear emittance is the same as the results obtained by Breit-Wigner formula.[12,13,38] The second-order nonlinear emittance is a new result, to our knowledge. We can see that it changes the sign across the resonant level of the cavity with a very sharp variation. This feature is different from the linear emittance which is no change at the resonant energy. Thus near the resonant level the electric current may decrease for an increasing the voltage difference. Such a behavior is precisely the expected nonlinear conduction character, and up to second order in the voltage difference our results can provide useful information.

ACKNOWLEDGMENTS

This work was supported by Zhejiang Provincial Natural Foundation No. 500079, the National Laboratory of Solid State Microstructures in Nanjing University No. M001509, the Educational Department of Zhejiang Province No. G20010059, and SRF for ROCS, SEM. One of the authors (G.J.) acknowledges the support from the State Key Program for Basic Research of China No. 001CB610602.

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