Conductance and density of states from the Kramers-Kronig dispersion relation

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By applying the Kramers-Kronig dispersion relation to the transmission amplitude, a direct connection of the conductance with the density of states is given in quantum scattering systems connected to two one-channel leads. Using this method we show that in the Fano resonance the peak position of the density of states is generally different from the position of the corresponding conductance peak, whereas in the Breit-Wigner resonance those peak positions coincide. The line shapes of the density of states are well described by a Lorentz type in both the resonances. These results are verified by another approach using a specific form of the scattering matrix to describe the scattering resonances.

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I. INTRODUCTION

The developments of nano-scale fabrication technique made possible confining electrons in a small region so that the system shows a discrete-energy spectrum. Such an electron system is called the quantum dot, whose characteristics have been investigated in many theoretical and experimental works.[1,2]

One way by which characteristics of a quantum dot can be investigated is to connect leads to it and to measure its conductance. Many such experiments have actually been carried out and have shown sharp peaks of the conductance as a function of the gate voltage or source-drain voltage.[1–6] These experimental results about conductance peaks have been interpreted on the hypothesis that the electric current through the quantum dot occurs if there is at least one of the energy levels of the quantum dot between chemical potentials of the reservoirs connected to the quantum dot via leads. This hypothesis is justified if the peak position of the conductance coincides with the corresponding peak position of the density of states in the quantum dot.

In this paper we investigate this hypothesis about the peak positions of the conductance and the density of states. We consider a quantum dot connected to two one-channel leads, and assume that the system has a time-reversal symmetry. In this system, from the scattering matrix the conductance and the density of states are calculated by using the Landauer conductance formula[7–11] and the Friedel sum rule,[12–14] respectively. Moreover, as will be shown in this paper, we can use the Kramers-Kronig dispersion relation in order to connect the conductance with the density of states. The Kramers-Kronig dispersion relation connects the real part of a function with its imaginary part by the Hilbert transformation, based on the analyticity of the function. By applying this relation to the logarithm of a scattering-matrix element we obtain formulas allowing us to calculate the conductance from the density of states and to calculate the density of states from the conductance. These formulas are used to investigate a relation of peak positions of the conductance and the density of states.

We consider two kinds of resonances called the Breit-Wigner resonance and the Fano resonance. The Breit-Wigner resonance is characterized by the conductance line shape

$$G_b(E)=\Lambda_b \frac{1}{(E-E_0)^2+\Delta^2} \tag{1}$$

of a Lorentz type around a resonant energy E_0 as a function of energy E, where Λ_b is a positive constant.[15] Here the real constant Δ represents a coupling strength of the quantum dot with leads, and takes a small value compared with energy-level spacings of the quantum dot in a weak coupling case with leads. This resonance line shape agreed with experimental results for conductance in some quantum dots.[6] Figure 1 shows this conductance line shape with the parameter values $E_0=100$, $\Delta=1$, and $\Lambda_b=1$. On the other hand, the Fano resonance is characterized by the conductance line shape

$$G_f(E)=\Lambda_f \frac{(E-E_0+Q)^2}{(E-E_0)^2+\Delta^2}, \tag{2}$$

around a resonant energy E_0, where Λ_f is a positive constant.[16] Here the parameter Q determines asymmetry in the conductance line shape of the Fano resonance. The Fano-resonance line shapes are drawn in Fig. 2 with the parameter values $E_0=100$ and $\Delta=1$. Here, we choose the parameter Λ_f as $\Delta^2/(\Delta^2+Q^2)$ so that the peak value of the conductance is one. The Fano resonance is caused by coupling discrete states with continuous states, and exhibits conductance

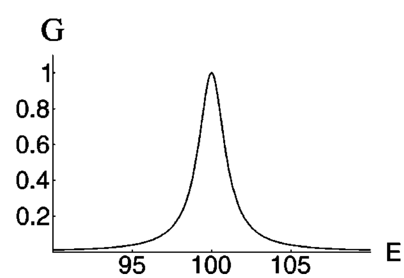

FIG. 1. Conductance line shape of the Breit-Wigner resonance as a function of energy.

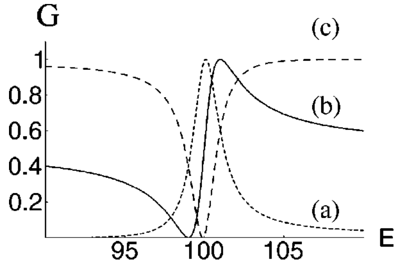

FIG. 2. Conductance line shapes of the Fano resonance as functions of energy. The graphs (a), (b), and (c) are corresponding to the cases of $Q=10$, 1, and 0.1, respectively.

zero points like the energy point $E=E_0-Q$ in Eq. (2).[17–19] It should be noted that the Fano resonance is attributed to the Breit-Wigner type in the case of $|Q/\Delta|\gg 1$ [See Fig. 2(a)]. The conductance line shape of the Fano resonance is actually observed experimentally by using the scanning-tunneling microscopy[20–22] and in the quantum dots.[23,24] These experimental results show that even the case of $|Q/\Delta|\ll 1$ like Fig. 2(c), can happen.

By applying our formula using the Kramers-Kronig dispersion relation to these two kinds of resonances we obtain the following results: (i) In the Breit-Wigner resonance, the peak position of the density of states coincides with the position $E=E_0$ of the conductance peak. (ii) In the Fano resonance, the density of states are independent of value of the asymmetric parameter Q in a weak coupling case with leads, and the peak position of the density of states is at $E=E_0$. Equation (2) shows that the peak position of the conductance depends on the asymmetric parameter Q and is given by $E=E_0+\Delta^2/Q$. Therefore, in the case of $|Q/\Delta|\gg 1$, the peak position of the density of states is close to the position of the conductance peak. On the other hand, in the case of $|Q/\Delta|\ll 1$, the peak position of the density of states is rather close to the energy E_0-Q, at which the conductance takes a local minimum value. We also show that in both the resonance types the line shapes of the density of states are a Lorentz type. These results are correct even in the case where an electron-electron interaction like the charging effect inside the quantum dot plays an important role, because the Friedel sum rule is correct even in presence of electron-electron interactions.[13]

We verify the above results by another approach that does not use the Kramers-Kronig dispersion relation. It is an approach using a specific form of the scattering matrix to describe the scattering resonances. We show that only the Breit-Wigner and the Fano resonances are derived from this scattering matrix. By applying the Landauer conductance formula and the Friedel sum rule to this specific scattering matrix we calculate the density of states and the conductance, and obtain the same results as with the dispersion-relation approach.

II. KRAMERS-KRONIG DISPERSION RELATION IN THE TRANSMISSION AMPLITUDE

The system that we consider in this paper is the quantum dot connected to the particle reservoirs via two one-channel leads. We neglect the effect of a magnetic field so that the system has the time-reversal symmetry. For such a system the scattering matrix $S(E)=[S_{ll'}(E)]$ is represented as a 2×2 symmetric and unitary matrix at any energy E. The conductance $G(E)$ is given by the Landauer conductance formula

$$G(E)=\frac{q^2}{2\pi\hbar}|t(E)|^2, \tag{3}$$

with the charge q of the particle, the Planck constant $2\pi\hbar$, and the transmission amplitude $t(E)\equiv S_{12}(E)[=S_{21}(E)]$. The density of states $\rho(E)$ is given by the Friedel sum rule

$$\rho(E)=\frac{1}{\pi}\frac{\partial\theta_f(E)}{\partial E}, \tag{4}$$

which $\theta_f(E)$ is the Friedel-phase defined by

$$\theta_f(E)\equiv\frac{1}{2i}\ln \mathrm{Det}\{S(E)\}. \tag{5}$$

It is important to note that the Friedel phase $\theta_f(E)$ and the transmission-amplitude phase $\theta_t(E)[\equiv \mathrm{Arg}\{t(E)\}]$ are not completely independent. Actually, if the conductance is not zero in any value of energy, then the transmission-amplitude phase $\theta_t(E)$ is simply given by $\theta_f(E)+\pi/2$. On the other hand, if the conductance takes zero in some energy points $E=E^{(n)}$, $n=1,2,\cdots$, then the transmission-amplitude phase can have discontinuities of $\pm\pi$ in those points, and is connected to the Friedel phase $\theta_f(E)$ as $\theta_t(E)=\theta_f(E)+\eta(E)$ with $\eta(E)\equiv\nu+\pi\Sigma_n\gamma_n\Theta(E-E^{(n)})$.[25] Here ν is an energy-independent constant, $\Theta(x)$ is the step function of x, and γ_n is a constant taking the value -1, 0, or 1 only. In this paper we treat the conductance like Eq. (2), so we should make up our formula based on the case where there is a conductance zero point.

Since the transmission-amplitude phase $\theta_t(E)$ has discontinuities in the conductance zero points, we should not assume that the logarithm of the transmission amplitude $t(E)$ itself is an analytic function of energy. Therefore, in order to apply the Kramers-Kronig dispersion relation in which the analyticity of function plays an essential role, we must carefully remove the singularity caused by the conductance zero points from the logarithm of the transmission amplitude $t(E)$. For this purpose we represent the transmission amplitude $t(E)$ as

$$t(E)=\lim_{\varepsilon\to+0} e^{i\eta(E)}e^{2^{-1}\ln[\varepsilon+|t(E)|^2]+i\theta_f(E)}. \tag{6}$$

The limit $\varepsilon\to+0$ is introduced to avoid the divergences of the function $\ln|t(E)|^2$ of E in the conductance zero points. In addition, the function $\theta_f(E)$ of E is a continuous function because its derivative gives the density of states $\rho(E)$ multiplied by π, which should be a continuous function of energy. Therefore we get the function $2^{-1}\ln(\varepsilon+|t(E)|^2)+i\theta_f(E)$, which can be assumed to be a continuous function of energy.

In the next step we separate its asymptotic form from the transmission amplitude and we make a function that goes to zero as the energy E goes to infinity. For this purpose we introduce the asymptotic forms of the functions $|t(E)|^2$ and $\theta_f(E)$ as

$$|t(E)|^2 \overset{E\to+\infty}{\sim} T^{(\infty)}(E), \tag{7}$$

$$\theta_f(E) \overset{E\to+\infty}{\sim} \theta_f^{(\infty)}(E). \tag{8}$$

As an example of the asymptotic transmission amplitude, in the one-dimensional system we may take $t(E) \overset{E\to+\infty}{\sim} \exp(ikl)$, where l is the length of the system and k is the wave vector $\sqrt{2mE}/\hbar$ with the mass m of the particle, so this gives $T^{(\infty)}(E)=1$ and $\theta_f^{(\infty)}(E)=kl$. The transmission amplitude $t(E)$ is represented as

$$t(E)=\lim_{\varepsilon\to+0} e^{2^{-1}\ln[\varepsilon+T^{(\infty)}(E)]} e^{i\{\theta_f^{(\infty)}(E)+\eta(E)\}} e^{\Phi_\varepsilon(E)}, \tag{9}$$

where $\Phi_\varepsilon(E)$ is the imaginary-function defined by

$$\Phi_\varepsilon(E)\equiv\frac{1}{2}\ln\frac{\varepsilon+|t(E)|^2}{\varepsilon+T^{(\infty)}(E)}+i[\theta_f(E)-\theta_f^{(\infty)}(E)]. \tag{10}$$

An important characteristic of the function $\Phi_\varepsilon(E)$ is that this function satisfies the condition

$$\lim_{E\to+\infty}\Phi_\varepsilon(E)=0, \tag{11}$$

and can be assumed to be a continuous function of energy. The real part of the function $\Phi_\varepsilon(E)$ gives the conductance

$$G(E)=\lim_{\varepsilon\to+0} G^{(\infty)}(E)e^{2\mathrm{Re}\{\Phi_\varepsilon(E)\}}, \tag{12}$$

by using Eq. (3), where $G^{(\infty)}(E)$ is the conductance $[q^2/(2\pi\hbar)]T^{(\infty)}(E)$ in the high-energy limit. Using Eq. (4) the density of states $\rho(E)$ is connected to the imaginary part of the function $\Phi_\varepsilon(E)$ by

$$\rho(E)=\rho^{(\infty)}(E)+\lim_{\varepsilon\to+0}\frac{1}{\pi}\frac{\partial\,\mathrm{Im}\{\Phi_\varepsilon(E)\}}{\partial E}, \tag{13}$$

where $\rho^{(\infty)}(E)$ is the asymptotic form of the density of states in the high-energy limit and is given by $(1/\pi)\partial\theta_f^{(\infty)}(E)/\partial E$. Now we finish preparing the function $\Phi_\varepsilon(E)$ to which we apply the Kramers-Kronig dispersion relation.

So far, the function $\Phi_\varepsilon(E)$ has been defined only in the real-energy region $(0,+\infty)$. (Here we took the origin of energy so that the lower bound of the energy is zero.) Now, in order to apply the Kramers-Kronig dispersion relation to the function $\Phi_\varepsilon(E)$, we extend this function so that it is defined in the whole upper-half plane of the imaginary number E including the real axis. We assume that such an extension can be done under the three conditions:

(I) The function $\Phi_\varepsilon(E)$ of E is analytic in the whole upper-half plane and in the real axis in the imaginary number E.

(II) $\lim_{|E|\to+\infty}|\Phi_\varepsilon(E)|=0$ in any energy E satisfying $\mathrm{Im}\{E\}\geqslant 0$.

(III) $\Phi_\varepsilon(-E)=\Phi_\varepsilon(E)^*$ in any real number E.

It should be noted that the condition (II) is a generalization of Eq. (11). In this paper we choose the value $\theta_f(0)-\theta_f^{(\infty)}(0)$ as 0, so that the right-hand side and the left-hand side in the equation of the condition (III) coincide at the origin $E=0$. Known as the Kramers-Kronig dispersion relation, by using the conditions (I), (II), and (III), the real part and the imaginary part of the function $\Phi_\varepsilon(E)$ are connected as

$$\mathrm{Re}\{\Phi_\varepsilon(E)\}=\frac{2}{\pi}\hat{\mathcal{P}}\int_0^{+\infty}dE'\frac{E'\,\mathrm{Im}\{\Phi_\varepsilon(E')\}}{E'^2-E^2}, \tag{14}$$

$$\mathrm{Im}\{\Phi_\varepsilon(E)\}=-\frac{2}{\pi}\hat{\mathcal{P}}\int_0^{+\infty}dE'\frac{E\,\mathrm{Re}\{\Phi_\varepsilon(E')\}}{E'^2-E^2}, \tag{15}$$

where the operator $\hat{\mathcal{P}}$ means to take the principal integral in the following integral.[26]

Using Eqs. (10), (12), and (13), the relations (14) and (15) lead to a direct connection between the conductance and the density of states:

$$G(E)=G^{(\infty)}(E)\times\exp\left\{-\int_0^{+\infty}dE'\,\mathcal{C}(E,E')[\rho(E')-\rho^{(\infty)}(E')]\right\}, \tag{16}$$

$$\rho(E)=\rho^{(\infty)}(E)+\lim_{\varepsilon\to+0}\int_0^{+\infty}dE'\,\mathcal{D}(E,E')\ln\frac{\varepsilon+G(E')}{\varepsilon+G^{(\infty)}(E')}, \tag{17}$$

where the functions $\mathcal{C}(x,y)$ and $\mathcal{D}(x,y)$ of x and y are defined by

$$\mathcal{C}(x,y)\equiv\lim_{\epsilon\to+0}\ln\{[(x-y)^2+\epsilon^2][(x+y)^2+\epsilon^2]\}, \tag{18}$$

$$\mathcal{D}(x,y)\equiv-\lim_{\epsilon\to 0}\frac{1}{2\pi^2}\left\{\frac{(x-y)^2-\epsilon^2}{[(x-y)^2+\epsilon^2]^2}+\frac{(x+y)^2-\epsilon^2}{[(x+y)^2+\epsilon^2]^2}\right\}. \tag{19}$$

(See Appendix A about the derivations of these equations.) Here, in order to derive Eq. (16) we assumed $\lim_{E\to+\infty}\{\theta_f(E)-\theta_f^{(\infty)}(E)\}\ln E=0$, which is stronger than the condition (8). Equations (16) and (17) are the key results of this paper.

As a general feature of the conductance shown by using Eq. (16) the conductance $G(E)$ is invariant under the change $\rho(E)\to\rho(E)+\alpha$ [So $\rho^{(\infty)}(E)\to\rho^{(\infty)}(E)+\alpha$] of the density of states in any constant α. Similarly Eq. (17) implies that the density of states $\rho(E)$ is invariant under the change $G(E)\to\beta G(E)$ in any constant β.

III. APPLICATION TO THE BREIT-WIGNER AND FANO RESONANCE

In this section, by using Eq. (17) we calculate the densities of states in the Breit-Wigner resonance and the Fano resonance. In the actual calculation we use the equation

$$\rho(E)-\rho^{(\infty)}(E)=-\lim_{\varepsilon\to+0}\frac{1}{\pi^2}\hat{\mathcal{P}}\int_0^{+\infty}dE'\frac{E'}{E'^2-E^2}\frac{\partial}{\partial E'}\times\ln\frac{G_\varepsilon(E')}{G_\varepsilon^{(\infty)}(E')}, \tag{20}$$

with $G_\varepsilon(E)\equiv\varepsilon+G(E)$ and $G_\varepsilon^{(\infty)}(E)\equiv\varepsilon+G^{(\infty)}(E)$. Equation (20) is equivalent with Eq. (17), as shown in the end of Appendix A.

Before calculating the density of states, we consider some problems in applications of the formula (20) to the conductances (1) and (2). First, strictly speaking, in order to obtain the density of states using the formula (20) we need to know the value of the conductance in any energy E. On the other hand Eqs. (1) and (2) are correct only around the resonant energy E_0. However the integral kernel $E'/(E'^2-E^2)$ in the formula (20) has a large absolute value only around $E'=E$, so the value of conductance around the energy E_0 is enough to obtain approximately the density of states around the energy E_0.

The second problem in applications of the formula (20) is that we do not know the general asymptotic forms of the conductance and the density of states, which is needed to calculate the exact form of the density of states $\rho(E)$ by using Eq. (20). In this section we assume that the energy dependence of the asymptotic form of the transmission amplitude is the same as with the one-dimensional case, namely, $t(E)\overset{E\to+\infty}{\sim}\exp(i\lambda\sqrt{E})$ using a constant λ. Therefore the asymptotic form of the conductance and the density of states are given by $G^{(\infty)}(E)=q^2/(2\pi\hbar)$ and $\rho^{(\infty)}(E)=\lambda/(2\pi\sqrt{E})$, respectively. We do not have to care whether the conductances (1) and (2) satisfy the condition $\lim_{E\to\infty}G(E)=q^2/(2\pi\hbar)$, because these forms of the conductances are justified only around the resonant energy E_0.

It is valuable to extract an essential part giving a peak of the density of states from the right-hand side of Eq. (20). For this purpose we rewrite Eq. (20) as

$$\rho(E)=-\lim_{\varepsilon\to+0}\frac{1}{2\pi^2}\hat{\mathcal{P}}\int_{-\infty}^{+\infty}dE'\frac{1}{E'-E}\frac{\partial\ln G_\varepsilon(E')}{\partial E'}+\mathcal{F}(E)+\frac{\lambda}{2\pi\sqrt{E}}. \tag{21}$$

Here we used the specific asymptotic form of the conductance and the density of states, and $\mathcal{F}(E)$ is defined by

$$\mathcal{F}(E)\equiv-\lim_{\varepsilon\to+0}\frac{1}{2\pi^2}\int_0^{+\infty}dE'\frac{\Xi_\varepsilon(E')}{E'+E} \tag{22}$$

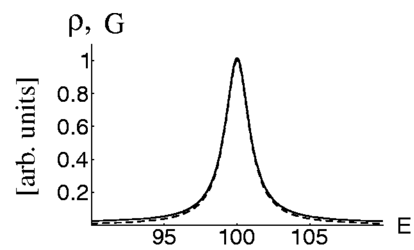

FIG. 3. Density of states (solid line) and the conductance (dashed line) as functions of energy in the Breit-Wigner resonance.

with $\Xi_\varepsilon(E)\equiv(\partial/\partial E)\ln[G_\varepsilon(E)/G_\varepsilon(-E)]$. The function $\mathcal{F}(E)$ of E is estimated as

$$|\mathcal{F}(E)|<\lim_{\varepsilon\to+0}\frac{1}{2\pi^2}\frac{1}{E}\int_0^{+\infty}dE'|\Xi_\varepsilon(E')|. \tag{23}$$

We consider a weak coupling case of the quantum dot with leads, so that we regard the constant Δ as a small parameter compared with energy-level spacings of the quantum dot. In this case we can assume that the energy value E_0 is large enough compared with the constant $|\Delta|$. Noting that it is enough for us to calculate the density of states $\rho(E)$ only around the energy E_0, we estimate that the contribution of the function $\mathcal{F}(E)$ to the density of states is negligible around the energy E_0 under the condition that the integral $\int_0^{+\infty}dE|\Xi_\varepsilon(E)|$ has a finite value, because of the small factor $1/E\simeq1/E_0$ in the right-hand side of Eq. (23). The third term in the right-hand side of Eq. (21) is a monotonous decreasing function of energy, so this part is also negligible in a large energy value $E\simeq E_0$ and almost does not contribute to changes of the peak position and the configuration of the density of states. Therefore the main contribution to the peak of the density of states comes only from the first term in the right-hand side of Eq. (21).

A. Breit-Wigner resonance

Figure 3 is the Breit-Wigner resonance line shape (1) and the corresponding density of states that is calculated by using Eq. (20). Here we choose the parameters as $\lambda=1$, and the other parameter values are the same as in Fig. 1. Figure 3 shows that the peak position of the density of states coincides with the peak position of the conductance in the Breit-Wigner resonance.

Now we check this result by the analytical consideration based on Eq. (21) neglecting its second and third terms. Substituting Eq. (1) into Eq. (21) we obtain the density of states as

$$\rho(E)\simeq\frac{1}{\pi^2}\hat{\mathcal{P}}\int_{-\infty}^{+\infty}dE'\frac{1}{E'-E}\frac{E'-E_0}{(E'-E_0)^2+\Delta^2}=\frac{1}{\pi}\frac{|\Delta|}{(E-E_0)^2+\Delta^2}. \tag{24}$$

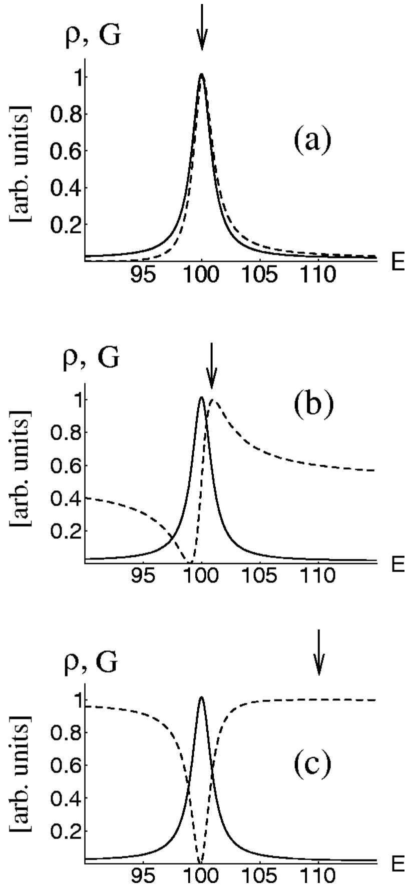

FIG. 4. Density of states (solid line) and the conductance (dashed line) as functions of energy in the Fano resonance. The graphs (a), (b), and (c) are corresponding to the cases of $Q=10$, 1, and 0.1, respectively. The arrow in each graph shows the position of the conductance peak.

This implies that the density of states is a Lorentz type whose peak position is at $E=E_0$ and is independent of the value of the prefactor Λ_b in the conductance line shape (1).

B. Fano resonance

The conductance (2) in the Fano resonance is an example in which a conductance zero occurs, so the infinitesimal constant ε in Eq. (20) plays an important role in calculating the density of states.

Figure 4 is the density of states corresponding to the Fano-resonance line shape (2), which is calculated by using Eq. (20).[27] Here, we chose the parameters as $\lambda=1$ and the other parameter values are the same as in Fig. 2. In the case of $|Q/\Delta|\gg 1$ [see Fig. 4 (a)], where the conductance line shape is close to the Breit-Wigner type, the peak position of the density of states is close to the peak position of the conductance. On the other hand, in the case of $|Q/\Delta|\ll 1$ [see Fig. 4 (c)], where the conductance line shape is a gulf rather than a peak, the peak position of the density of states is rather close to the gulf of the conductance.

Now we calculate the density of states $\rho(E)$ by using Eq. (21) neglecting its second and third terms. After a small calculation (see Appendix B for the detail of the calculation) we obtain $\rho(E)\simeq(1/\pi)|\Delta|/\{(E-E_0)^2+\Delta^2\}$, which is a Lorentz type with the peak at the energy E_0 and is the same as with the case of the Breit-Wigner resonance. It should be emphasized that this form of the density of states is independent of the value of the asymmetric parameter Q and the prefactor Λ_f in the conductance line shape (2).

IV. ANOTHER APPROACH USING A SPECIFIC SCATTERING MATRIX

In this section, by using another approach that does not use the Kramers-Kronig dispersion relation, we verify our results obtained in the previous section.

The specific form of the scattering matrix

$$S(E)=A\left(I+iB\frac{1}{E-E_0+i\Delta}\right), \tag{25}$$

around a resonant energy E_0 has been proposed to describe the scattering resonances.[28,29] Here, the 2×2 matrix $A \equiv (A_{ll'})$ is introduced as an energy-independent scattering matrix in the high-energy limit, so that it is a unitary matrix in itself: $AA^\dagger=A^\dagger A=I$. The matrix $B\equiv(B_{ll'})$ is also an energy-independent 2×2 matrix and satisfies the conditions

$$B^\dagger=B \quad \text{and} \quad B(B+2I\Delta)=0, \tag{26}$$

so that the scattering matrix $S(E)$ given by Eq. (25) becomes a unitary matrix in any energy E. It may be noted that either $B=-2I\Delta$ or $B=0$ satisfies the condition (26), but this gives an energy-independent conductance that is not pertinent to the subject of this paper. Therefore in this section we assume $B\neq -2I\Delta$ and $B\neq 0$, which lead to the parametrized representation

$$B=\Delta\begin{pmatrix} -1+\sin\phi & e^{i\varphi}\cos\phi \\ e^{-i\varphi}\cos\phi & -1-\sin\phi \end{pmatrix} \tag{27}$$

of the matrix B with real parameters ϕ and φ.

By applying the Friedel sum rule (4) to the scattering matrix (25), the density of states $\rho(E)$ is given by

$$\rho(E)=\frac{1}{\pi}\frac{\Delta}{(E-E_0)^2+\Delta^2}, \tag{28}$$

which satisfies $\lim_{\Delta\to+0}\rho(E)=\delta(E-E_0)$.[30] [See Appendix C about the derivation of Eq. (28).] Therefore the resonance line shape of the density of states is always a Lorentz type with a peak at the energy E_0. This agrees with the result concerning the line shape of the density of states in the previous section.

Now we check that the scattering matrix (25) gives the conductance line shape of the Breit-Wigner or the Fano resonance, and consider a relation between the peak positions of the conductance and the density of states. First we consider the case of $A_{12}=0$. In this case, by using Eqs. (3), (25), and $|A_{11}|=1$ the conductance $G(E)$ is represented as the Breit-Wigner type (1) with $\Lambda_b=q^2|B_{12}|^2/(2\pi\hbar)$, and the density of states is connected to the conductance simply as $\rho(E)$

$=\Delta G_b(E)/(\pi\Lambda_b)$. In this case the peak position of the conductance is at $E=E_0$ and coincides with the peak position of the density of states.

Second we consider the case of $A_{12}\neq 0$. In this case, by applying the Landauer conductance formula (3) to the scattering matrix (25) we obtain the conductance

$$G(E)=W_f+\Lambda_f\frac{(E-E_0+Q)^2}{(E-E_0)^2+\Delta^2}, \tag{29}$$

of the Fano type with parameter values

$$W_f=\frac{q^2}{2\pi\hbar}|A_{12}|^2\mathcal{K}, \tag{30}$$

$$\Lambda_f=\frac{q^2}{2\pi\hbar}|A_{12}|^2(1-\mathcal{K}), \tag{31}$$

$$Q=-\frac{d_1}{1-\mathcal{K}}. \tag{32}$$

Here $\mathcal{K}$ is defined by

$$\mathcal{K}\equiv\frac{\Delta^2+d_1^2+d_2^2-\sqrt{(\Delta^2+d_1^2-d_2^2)^2+4d_1^2d_2^2}}{2\Delta^2} \tag{33}$$

and $d_j, j=1,2$ are introduced as

$$d_1\equiv \mathrm{Im}\left\{\frac{A_{11}}{A_{12}}B_{12}\right\}, \tag{34}$$

$$d_2\equiv\Delta+B_{22}+\mathrm{Re}\left\{\frac{A_{11}}{A_{12}}B_{12}\right\}. \tag{35}$$

It is important to note that the constant $\mathcal{K}$ satisfies the inequality $0\leqslant\mathcal{K}\leqslant 1$ so the constants W_f and Λ_f given by Eqs. (30) and (31) are not negative. [In Appendix C we give outlines of the proof of this inequality and the derivation of Eq. (29).] The peak position of the conductance in this case is at $E=E_0+\Delta^2/Q$, which does not coincide with the peak position $E=E_0$ of the density of states shown by Eq. (28). The Fano conductance (29) takes a local minimum value at the energy E_0-Q. Therefore the peak position $E=E_0$ of the density of states is close to the peak position of the conductance in the case of $|Q/\Delta|\gg 1$, but as the quantity $|Q/\Delta|$ goes to 0 it moves closer to the energy at which the conductance takes a local minimum value. This is the same result as in the previous section.

The above results in this section are independent of the time-reversal symmetry of the system and are correct even in presence of a magnetic field. However if the system has the time-reversal symmetry and the conditions $S_{12}=S_{21}$ and $A_{12}=A_{21}$ are satisfied, then we obtain $W_f=0$, $\Lambda_f=[q^2/(2\pi\hbar)]|A_{12}|^2$, and $Q=-d_1$ (see Appendix D for their proofs). Therefore the conductance (29) becomes exactly the same form as Eq. (2) in the time-reversal symmetric system.

V. CONCLUSION AND REMARKS

In this paper by using the Kramers-Kronig dispersion relation, the Landauer conductance formula and the Friedel sum rule we have discussed a method to calculate the density of states from conductance and to calculate conductance from the density of states in quantum scattering systems connected to two one-channel leads. We considered the case of no magnetic field, so that the system had the time-reversal symmetry. Our formula was applied to the Breit-Wigner resonance and the Fano resonance, and led to their profiles of the density of states. In the Breit-Wigner resonance the peak positions of the conductance and the density of states coincide. On the other hand, in the Fano resonance, a relation of the peak positions of the conductance and the density of states depends on the parameter $|Q/\Delta|$ that determines asymmetry of the conductance line shape. In the case of $|Q/\Delta|\gg 1$ the peak position of the density of states is close to the position of the conductance peak, like the Breit-Wigner resonance. However in the case of $|Q/\Delta|\ll 1$ the peak position of the density of states is rather close to the energy at which the conductance takes a local minimum value. We also showed that the line shape of the density of states is a Lorentz type in both the resonances. These results are model independent, and are correct even if electron-electron interaction inside the quantum dot plays an important role. These results were verified by another consideration that does not use the Kramers-Kronig dispersion relation but uses a specific form of the scattering matrix to describe the scattering resonances.

The relation between the peak positions of the conductance and the density of states is important to explain an in-phase characteristic of the transmission-amplitude phase [see Eq. (13) in Ref. 25], which has been measured actually in an experiment.[31] Some works indicated that the Fano resonance property is important to cause this phenomenon.[32,33] In Ref. 25 it has already been shown that in a simple model consisting of a branch connected to a one-dimensional perfect wire the peak positions of the density of states are in the gulfs of the conductance.

The advantage of our approach using the Kramers-Kronig dispersion relation is that we can know the density of states directly from the conductance that can be measured in the experiments. We can also calculate the density of states from the scattering matrix itself, but it is extremely difficult for the scattering matrix itself to be measured in the experiments. On the other hand, one of the disadvantages of the dispersion relation approach is that this approach is justified only under some restrictive conditions, for example, two one-channel leads, no magnetic field, the conditions (I), (II), and (III), etc. We would get a wrong result if we neglect these conditions. For example, the approach in Sec. IV predicts a nonzero constant W_f in presence of a magnetic field, and if we were to apply the formula (17) to such a nonzero W_f case then the density of states would take a negative value in an energy region, which is not correct. To reduce the number of these conditions in our dispersion relation approach is one of the important future problems.

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APPENDIX A: DERIVATION OF THE CONNECTION BETWEEN THE CONDUCTANCE AND THE DENSITY OF STATES

In this appendix we give the derivation of Eqs. (16), (17), and (20).

First we should notice the equation

$$\hat{\mathcal{P}}\frac{1}{E'^2-E^2}=\frac{1}{2E'}\left(\hat{\mathcal{P}}\frac{1}{E'-E}+\hat{\mathcal{P}}\frac{1}{E'+E}\right)$$
$$=\lim_{\epsilon\to 0}\frac{1}{2E'}\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}+\frac{E'+E}{(E'+E)^2+\epsilon^2}\right]. \tag{A1}$$

Similarly we obtain

$$\hat{\mathcal{P}}\frac{1}{E'^2-E^2}=\lim_{\epsilon\to 0}\frac{1}{2E}\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}-\frac{E'+E}{(E'+E)^2+\epsilon^2}\right]. \tag{A2}$$

It follows from Eqs. (10), (12), (14), (18), and (A1) that

$$\ln\frac{G(E)}{G^{(\infty)}(E)}=\lim_{\varepsilon\to+0}2\mathrm{Re}\{\Phi_\varepsilon(E)\}$$
$$=\lim_{\varepsilon\to+0}\frac{4}{\pi}\hat{\mathcal{P}}\int_0^{+\infty}dE'\frac{E'\,\mathrm{Im}\{\Phi_\varepsilon(E')\}}{E'^2-E^2}$$
$$=\lim_{\varepsilon\to+0}\lim_{\epsilon\to 0}\frac{2}{\pi}\int_0^{+\infty}dE'\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}+\frac{E'+E}{(E'+E)^2+\epsilon^2}\right]\mathrm{Im}\{\Phi_\varepsilon(E')\}$$
$$=\frac{1}{\pi}\int_0^{+\infty}dE'\frac{\partial\mathcal{C}(E,E')}{\partial E'}[\theta_f(E')-\theta_f^{(\infty)}(E')]$$
$$=-\int_0^{+\infty}dE'\,\mathcal{C}(E,E')\frac{1}{\pi}\frac{\partial[\theta_f(E')-\theta_f^{(\infty)}(E')]}{\partial E'}$$
$$=-\int_0^{+\infty}dE'\,\mathcal{C}(E,E')[\rho(E')-\rho^{(\infty)}(E')], \tag{A3}$$

where we used the conditions $\theta_f(0)-\theta_f^{(\infty)}(0)=0$ and $\lim_{E'\to+\infty}\mathcal{C}(E,E')[\theta_f(E')-\theta_f^{(\infty)}(E')]=0$. This leads to Eq. (16). Similarly, by using Eqs. (10), (13), (15), (19), and (A2) we obtain

$$\rho(E)-\rho^{(\infty)}(E)=\lim_{\varepsilon\to+0}\frac{1}{\pi}\frac{\partial\,\mathrm{Im}\{\Phi_\varepsilon(E)\}}{\partial E}$$
$$=-\lim_{\varepsilon\to+0}\frac{2}{\pi^2}\frac{\partial}{\partial E}\hat{\mathcal{P}}\int_0^{+\infty}dE'\frac{E\,\mathrm{Re}\{\Phi_\varepsilon(E')\}}{E'^2-E^2}$$
$$=-\lim_{\varepsilon\to+0}\lim_{\epsilon\to 0}\frac{1}{\pi^2}\frac{\partial}{\partial E}\int_0^{+\infty}dE'\times\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}-\frac{E'+E}{(E'+E)^2+\epsilon^2}\right]\mathrm{Re}\{\Phi_\varepsilon(E')\} \tag{A4}$$
$$=\lim_{\varepsilon\to+0}\int_0^{+\infty}dE'\,\mathcal{D}(E,E')\ln\frac{\varepsilon+G(E')}{\varepsilon+G^{(\infty)}(E')}. \tag{A5}$$

This leads to Eq. (17).

Using the expression (A4) we obtain another expression for a relation between the density of states and the conductance:

$$\rho(E)-\rho^{(\infty)}(E)=\lim_{\varepsilon\to+0}\lim_{\epsilon\to 0}\frac{1}{\pi^2}\int_0^{+\infty}dE'\times\left\{\frac{\partial}{\partial E'}\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}+\frac{E'+E}{(E'+E)^2+\epsilon^2}\right]\right\}\mathrm{Re}\{\Phi_\varepsilon(E')\}$$
$$=\lim_{\varepsilon\to+0}\int_0^{+\infty}dE'\,\tilde{\mathcal{D}}(E,E')\frac{\partial}{\partial E'}\times\ln\frac{\varepsilon+G(E')}{\varepsilon+G^{(\infty)}(E')} \tag{A6}$$

where $\tilde{\mathcal{D}}(E,E')$ is defined by

$$\tilde{\mathcal{D}}(E,E')\equiv-\lim_{\epsilon\to 0}\frac{1}{2\pi^2}\left[\frac{E'-E}{(E'-E)^2+\epsilon^2}+\frac{E'+E}{(E'+E)^2+\epsilon^2}\right] \tag{A7}$$

and satisfies the condition $\tilde{\mathcal{D}}(E,0)=0$. Equations (A1) and (A5) lead to Eq. (20).

APPENDIX B: DENSITY OF STATES IN THE FANO RESONANCE

In this Appendix we calculate the density of states by using Eqs. (2) and (21).

Neglecting its second and third term, Eq. (21) leads to the density of states $\rho(E)$:

$$\rho(E)\simeq-\lim_{\varepsilon\to+0}\frac{1}{2\pi^2}\hat{\mathcal{P}}\int_{-\infty}^{+\infty}dE'\frac{\Gamma_\varepsilon(E')}{E'+E_0-E}, \qquad \text{(B1)}$$

where the function $\Gamma_\varepsilon(E)$ of E is introduced as

$$\begin{aligned}\Gamma_\varepsilon(E)&\equiv\frac{1}{G_{\varepsilon\Lambda_f}(E+E_0)}\frac{\partial G_{\varepsilon\Lambda_f}(E+E_0)}{\partial E}\\&=-2\frac{(E+Q)(QE-\Delta^2)}{(E^2+\Delta^2)[(E+Q)^2+\varepsilon(E^2+\Delta^2)]}\\&=-2\frac{E}{E^2+\Delta^2}\\&\quad+2\frac{E+\dfrac{Q}{1+\varepsilon}}{\left(E+\dfrac{Q}{1+\varepsilon}\right)^2+\varepsilon\left[\dfrac{\Delta^2}{1+\varepsilon}+\left(\dfrac{Q}{1+\varepsilon}\right)^2\right]}. \qquad \text{(B2)}\end{aligned}$$

Using the formula

$$\frac{1}{\pi}\hat{\mathcal{P}}\int_{-\infty}^{+\infty}dy\frac{1}{y-x}\frac{y}{y^2+a^2}=\frac{|a|}{x^2+a^2}, \qquad \text{(B3)}$$

for a real constant a, it follows from Eqs. (B1) and (B2) that

$$\rho(E)\simeq\frac{1}{\pi}\frac{|\Delta|}{(E-E_0)^2+\Delta^2}, \qquad \text{(B4)}$$

in $E\neq E_0-Q$.

APPENDIX C: DENSITY OF STATES AND CONDUCTANCE GIVEN BY A SPECIFIC SCATTERING MATRIX

In this appendix we derive Eqs. (28) and (29) from Eqs. (3), (4), and (25). We also give an outline of the proof of the inequality $0\leqslant\mathcal{K}\leqslant 1$.

It follows from Eq. (27) that

$$\mathrm{Tr}\{B\}=-2\Delta, \qquad \text{(C1)}$$

$$\mathrm{Det}\{B\}=0. \qquad \text{(C2)}$$

Using Eqs. (C1) and (C2) the determinant of the scattering matrix (25) is given by

$$\mathrm{Det}\{S(E)\}=\mathrm{Det}\{A\}\times\frac{E-E_0-i\Delta}{E-E_0+i\Delta}. \qquad \text{(C3)}$$

By substituting Eq. (C3) into Eq. (5) and by using Eq. (4) we obtain Eq. (28).

Now, we consider the case of $S_{12}\neq 0$ in order to derive Eq. (29) from Eqs. (3) and (25). In such a case we obtain

$$\begin{aligned}|t(E)|^2&=|S_{12}(E)|^2\\&=\left|A_{12}\frac{E-E_0-d_1+id_2}{E-E_0+i\Delta}\right|^2\\&=|A_{12}|^2\left[\mathcal{K}+(1-\mathcal{K})\frac{(E-E_0+Q)^2}{(E-E_0)^2+\Delta^2}\right], \qquad \text{(C4)}\end{aligned}$$

where we used the relation

$$\Delta^2\mathcal{K}^2-(\Delta^2+d_1^2+d_2^2)\mathcal{K}+d_2^2=0 \qquad \text{(C5)}$$

satisfied by the constant $\mathcal{K}$. By substituting Eq. (C4) into Eq. (3) and by noting Eqs. (30) and (31) we obtain Eq. (29).

The inequality $0\leqslant\mathcal{K}\leqslant 1$ is shown as follows. First we should notice that

$$\begin{aligned}(\Delta^2+d_1^2-d_2^2)^2+4d_1^2d_2^2&=(\Delta^2+d_1^2+d_2^2)^2-4\Delta^2d_2^2\\&\leqslant(\Delta^2+d_1^2+d_2^2)^2. \qquad \text{(C6)}\end{aligned}$$

By noting this fact and the form of the constant $\mathcal{K}$ given by Eq. (33) the inequality $0\leqslant\mathcal{K}$ is obtained. Second we can show that if we were to assume the inequality $\mathcal{K}>1$ then we would obtain the inequality $(\Delta d_1)^2<0$, which is incompatible with the real constant Δd_1. This means that the inequality $\mathcal{K}\leqslant 1$ must be satisfied.

APPENDIX D: TIME-REVERSAL SYMMETRY IN THE FANO RESONANCE

In this Appendix we show $d_2=0$ under the conditions $A_{12}=A_{21}\neq 0$ and $S_{12}=S_{21}$. This result $d_2=0$ leads to $\mathcal{K}=0$, so we obtain $W_f=0$, $\Lambda_f=[q^2/(2\pi\hbar)]|A_{12}|^2$, and $Q=-d_1$ by using Eqs. (30), (31), and (32).

The matrix A, which is a unitary matrix, is represented as

$$A=\begin{pmatrix} ie^{i(\tilde{\theta}+\tilde{\varphi}_1)}\sin\tilde{\phi} & e^{i(\tilde{\theta}+\tilde{\varphi}_2)}\cos\tilde{\phi}\\ e^{i(\tilde{\theta}-\tilde{\varphi}_2)}\cos\tilde{\phi} & ie^{i(\tilde{\theta}-\tilde{\varphi}_1)}\sin\tilde{\phi}\end{pmatrix}, \qquad \text{(D1)}$$

with real parameters $\tilde{\theta}$, $\tilde{\varphi}_1$, $\tilde{\varphi}_2$, and $\tilde{\phi}$. The condition $A_{12}=A_{21}$ imposes

$$\tilde{\varphi}_2=0 \quad\text{or}\quad \pi. \qquad \text{(D2)}$$

The condition $S_{12}=S_{21}$ under Eq. (D2) implies that the multiplied matrix AB is also symmetric. This leads to the condition

$$\tan\phi=-\frac{\sin(\varphi+\tilde{\varphi}_1)}{\cos\tilde{\varphi}_2}\tan\tilde{\phi}. \qquad \text{(D3)}$$

On the other hand the constant d_2 given by Eq. (35) is represented as

$$d_2=-\Delta\cos\phi[\tan\phi+\sin(\varphi+\tilde{\varphi}_1-\tilde{\varphi}_2)\tan\tilde{\phi}]. \qquad \text{(D4)}$$

Using Eqs. (D2), (D3), and (D4) we obtain $d_2=0$.

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