Resonance lineshapes in quasi-one-dimensional scattering

Jens U. Nöckel and A. Douglas Stone

Applied Physics, Yale University, P.O. Box 208284, Yale Station, New Haven CT 06520-8284
(Submitted 24 November 1993)

An S matrix approach is developed to describe elastic scattering resonances of systems where the scattered particle is asymptotically confined and the scattering potential lacks continuous symmetry. Examples are conductance resonances in microstructures or transmission resonances in waveguide junctions. The generic resonance is shown to have the asymmetric Fano lineshape. The asymmetry parameter \( q \) is independent of coupling to the quasi-bound level implying a scaling property of the resonances which can be tested in transport experiments.

Although the symmetric Breit-Wigner peak \( \dagger \) is the most common resonance lineshape observed in atomic and nuclear scattering, it has been known for some time that the most general resonant lineshape is described by the asymmetric Fano function:

\[
f(\epsilon) = \frac{(\epsilon + q)^2}{\epsilon^2 + 1},
\]

Here, \( \epsilon = 2(E - E_0)/\Gamma \) is the (dimensionless) energy from resonance, \( \Gamma \) is the resonance width, and \( q \) is the asymmetry parameter. Strongly asymmetric Fano lineshapes are familiar for inelastic autoionizing resonances in atoms \( \star \); however Simpson and Fano \( \star \) explicitly noted their occurrence in spherically-symmetric elastic scattering in 1963. In fact this lineshape is implicit in much earlier work in nuclear scattering where strong asymmetries were measured in elastic neutron scattering \( \star \). To be precise one finds \( \star \) that the elastic scattering partial cross-section near a resonance in angular momentum channel \( l \) (neglecting spin) has the form

\[
\sigma_l = \frac{\lambda^2}{2\pi} \frac{(2l + 1)}{\sin^2 \theta_l} \frac{(\epsilon - \cot \theta_l)^2}{\epsilon^2 + 1},
\]

with \( \lambda \) denoting the particle wavelength and \( \theta_l \) the background phase shift in the absence of the resonance. Hence \( \sigma_l \) is proportional to the Fano function with \( q = -\cot \theta_l \).

The only assumption needed is that \( \theta_l \rightarrow 0 \) \((q \rightarrow \infty)\) of small background phase shift one recovers the Breit-Wigner lineshape; whereas \( q \rightarrow 0 \) yields a symmetric anti-resonance (BW dip). The characteristic asymmetric Fano lineshape occurs for intermediate values of \( q \) and in the inelastic case has the well-known interpretation of interference between transition amplitudes from a bound initial state to an unbound final state either directly or via a quasibound intermediate state. A similar interpretation applies for asymmetric elastic resonances in which scattering via a quasi-bound level interferes with direct (potential) scattering. An important feature of elastic Fano resonances is that the asymmetry parameter depends only on the background phase-shift and not on the strength of the coupling to the quasi-bound level; this is not true for inelastic autoionizing resonances. Note that in the spherically symmetric case \( \sigma_l \) varies between zero and \( \lambda^2(2l + 1)/\pi \), the minimum and maximum values allowed by unitarity of the S matrix.

In several recent theoretical studies of transport properties of microstructures \( \star \), asymmetric elastic conductance resonances have been encountered. Typically an impurity or geometric feature of the microstructure leads to the formation of a quasi-bound state which is degenerate with the continuum of propagating states. Although resonance lineshapes were calculated in several specific models, and the analogy to Fano resonances was discussed in an interesting paper by Tekman and Bagwell \( \star \), no general proof that these resonances have the Fano lineshape (analogous to that for spherically-symmetric continuum scattering) has been given. Unlike atomic or nuclear scattering in 3D, for electrons in microstructures or photons in waveguides one must consider geometries in which the scattering occurs between different propagating channels in leads which confine the particle asymptotically. Thus, we may assume at most discrete rotational symmetry, and the lineshape in the absence of spatial symmetry and/or time-reversal symmetry will be of great interest. We use the term quasi-one-dimensional (Q1D) scattering to emphasize the one-dimensional nature of the asymptotic motion in such systems. We note that a strong magnetic field also confines electrons asymptotically even in 3D, so our results are relevant to 3D heterostructures as well.

We obtain the following results: 1) The Fano function describes the generic lineshape for Q1D resonant scattering in the presence and absence of discrete symmetries. 2) The asymmetry parameter \( q \) again is independent of the coupling strength. This implies a scaling property of the resonances which we test on an example below. 3) Symmetric two-probe structures in the single-subband regime always show the maximum variation in the transmission through resonance allowed by unitarity. In the absence of symmetries unit reflection is maintained but unit transmission is lost. Finally, Fano resonances in microstructures have not yet been clearly seen experimentally (although some data taken on quantum point contacts is suggestive \( \star \)); we propose below a potentially
more tractable experiment for observing such resonances in 3D heterostructures.

Our discussion of Q1D resonance lineshapes exploits the fundamental relationship between resonances and poles of the S matrix in the complex energy plane, which is also the basis of Eq. (9). Consider a Q1D structure with $N$ leads and various propagating subbands per lead, the total number of subbands in all the leads being $M$. An arbitrary scattering state is then specified by $M$-vectors $\mathbf{I}$ and $\mathbf{O}$ for the amplitudes of the incoming and outgoing waves in each subband of each lead. The S matrix is defined by $\mathbf{O} = S \mathbf{I}$, and current conservation requires it to be unitary for real energies. The wavefunction of a metastable state at energy $E_0$ with decay width $\Gamma$ corresponds to a nonzero $\mathbf{O}$ with vanishing $\mathbf{I}$ at a complex energy $\bar{E} \equiv E_0 - i\Gamma/2$. For this to be possible, $S^{-1}$ must be singular at this energy, which implies that one of the eigenvalues of $S$ has a pole at $\bar{E}$. As is usually done, we assume the pole to be simple, and only a single eigenvalue to be resonant (nondegenerate resonance). With the constraint that this eigenvalue $\lambda_j(E)$ be unimodular for real energies, one can approximate

$$\lambda_j(E) \approx e^{2i\theta_j} \frac{E - E^*}{E - E_0}, \quad (3)$$

where $\theta_j$ is a real constant. This is accurate provided that the distance to other resonance poles is much larger than $\Gamma$. Introducing the eigenphase, $\lambda_j = e^{2i\theta_j}$, one arrives at

$$\theta_j \approx \theta_j - \arctan \frac{\Gamma/2}{E - E_0}. \quad (4)$$

Thus, $2\theta_j$ varies by $2\pi$ on resonance. To deduce the S matrix elements from a knowledge of its eigenvalues, one has to specify the unitary transformation that diagonalizes $S$. For the case of spherically symmetric 3D (and 2D) scattering this transformation is fixed because there is a complete set of quantum numbers $(E, \ell, m)$ that are conserved by $S$, leading to the expression in Eq. (3). In the absence of unitary and antiunitary (time-reversal) symmetries an approach which avoids specifying the diagonalizing transformation (as e.g. in multi-channel scattering theory) is to make the ansatz that each S matrix element $S_{mn}$ will itself exhibit a resonance denominator as in Eq. (3).

$$S_{mn} = S^b_{mn} - i \frac{\gamma_m \delta_n^*}{E - E_0 + i\Gamma/2}, \quad (5)$$

where $S^b$ is the background scattering matrix in the absence of the resonance and $\gamma, \delta$ are complex vectors which must satisfy $\bar{\gamma} = S^b \delta$ and $|\gamma|^2 = |\delta|^2 = \Gamma$ so that $S$ is unitary. $|\gamma_m|^2, |\delta_n|^2$ are then interpreted as partial widths for leaving and entering the resonance.

A simplified version of Eq. (5) which assumes the background S-matrix to be diagonal is often used \cite{16} and in particular was employed by B"{u}ttiker \cite{17} to derive the lineshape of resonances in Q1D structures. However this further approximation always leads to symmetric resonance lineshapes. On the other hand a general unitary $N \times N$ matrix is specified by $N^2$ real parameters, and clearly Eq. (5) contains more than $N^2$ parameters since $S^b$ is itself a general unitary matrix. It turns out that the parameterization in Eq. (3) underconstrains the S-matrix, allowing lineshapes that cannot arise in reality from a nondegenerate, simple and isolated resonance pole. For instance, according to Eq. (3) a $2 \times 2$ S-matrix with $S_{12}^b = S_{21}^b = 1$ gives rise to a non-vanishing transmission $S_{12}$ if $\gamma_2 \neq 0$. However we show below that transmission zeros are present in the most general two-probe $(2 \times 2)$ Q1D resonant S-matrix. (Exact transmission zeros have been found in various model calculations cited above and according to an argument in Ref. \cite{13} are expected to be very robust in Q1D systems).

To begin we consider a Q1D geometry with $N$ leads in the single-subband regime which is invariant under the \textit{finite} rotation group $C_N$ (an example being the symmetric cross junction \cite{8}). The symmetry will then determine the transformation which diagonalizes the S-matrix in close analogy to the 3D case. To find the eigenbasis we note that the $N$ one-dimensional irreducible representations of $C_N$ have the character system

$$\chi_i(p) = e^{-2\pi ipq/N}, \quad (p, q = 1, \ldots, N). \quad (6)$$

Here, $p$ labels the elements $R_p$ of the rotation group, and $q$ enumerates the representations. From the non-degenerate scattering states corresponding to an incoming electron in exactly one of the leads, we can form symmetrized eigenfunctions by taking the incoming waves as $\Gamma^{(q)}$ with components

$$I^{(q)}_p = \frac{1}{\sqrt{N}} \chi_i(p)^* \chi_i(p). \quad (7)$$

For any rotation $R_p$, one then has $R_p I^{(q)} = I^{(q)}(p) R^{(q)}$. But since $R_p$ leaves the system invariant, a rotation of the incoming wave amplitudes $R_p I$ leads to outgoing waves $R_p \mathbf{O}$. For the symmetrized waves this means

$$R_p \mathbf{O} = S R_p I^{(q)} = \chi_i(p) S \Gamma^{(q)} = \chi_i(p) \mathbf{O}. \quad (8)$$

Consequently, $\mathbf{O}$ transforms under the rotations in the same way as $\Gamma^{(q)}$. Since the representations are one-dimensional, it follows that $\mathbf{O} \propto \Gamma^{(q)}$, so that the $\Gamma^{(q)}$ are an eigenbasis of $S$. The unitary transformation relating the matrix elements of $S$ between incoming and outgoing waves in leads $m$ and $n$ to the diagonal elements $\lambda_j$ is then given by

$$S_{mn} = \frac{1}{N} \sum_{j=1}^{N} \chi^{(m)}(j)^* \lambda_j \chi^{(n)}(j), \quad (9)$$

$$= \frac{1}{N} \sum_{j=1}^{N} e^{2i\theta_j} e^{2\pi i(m-n)j/N}. \quad (10)$$
This is an exact expression for the multiprobe scattering amplitude. Now assume that \( \theta_1 \) is the resonant eigenphase while all other \( \theta_j \) are slowly varying with energy. Then we abbreviate the sum over the nonresonant eigenvalues by

\[
\sum_{j=2}^{N} e^{2i\theta_j} e^{2\pi i(m-n)j/N} \equiv \rho_{mn} e^{2i\tilde{\theta}_{mn}}
\]

where \( \rho \leq N-1 \). With this one obtains for the scattering probabilities

\[
|S_{mn}|^2 = \left( \frac{\rho_{mn} + 1}{N} \right)^2 - 4 \frac{\rho_{mn}}{N^2} \sin^2 (\tilde{\theta}_{mn} - \theta_1),
\]

which implies that each matrix element of \( S \) varies in modulus between \( (\rho_{mn} - 1)/N \) and \( (\rho_{mn} + 1)/N \) when crossing the resonance. From this we see immediately that the \( S_{mn} \) must take on any value between and including 0 and 1 if \( N = 2 \) (necessarily \( \rho_{mn} = 1 \)), but cannot reach all values allowed by unitarity when \( N > 2 \). To find the lineshape resulting from Eq. (11), we insert Eq. (12) for \( \theta_1 \) and get

\[
|S_{mn}|^2 = \left( \frac{\rho_{mn} + 1}{N} \right)^2 - 4 \frac{\rho_{mn}}{N^2} \sin^2 \left( \frac{\tilde{\theta}_{mn} - \theta_1 + \arctan \frac{\Gamma/2}{E - E_0}}{2} \right)
\]

\[
\equiv \left( \frac{\rho_{mn} + 1}{N} \right)^2 - 4 \frac{\rho_{mn}}{N^2} |t_{mn}|^2 \frac{\left( E - E_0 + \Delta_{mn} \right)^2}{\left( E - E_0 \right)^2 + \Gamma^2/4}. \tag{13}
\]

Here, we have identified \( |t_{mn}|^2 = \sin^2 (\tilde{\theta}_{mn} - \theta_1) \) as the (slowly varying) transmission in the absence of the resonance, and introduced the energy shift \( \Delta_{mn} = \frac{\Gamma}{2} \cot (\tilde{\theta}_{mn} - \theta_1) \). This is the Fano lineshape, Eq. (1), with \( \epsilon = (E - E_0)/(\frac{1}{2} \Gamma) \) and \( q = \Delta_{mn}/(\frac{1}{2} \Gamma) = \cot (\tilde{\theta}_{mn} - \theta_1) \), superimposed on a constant background. Owing to Eq. (11), the reflection \( |S_{mn}|^2 \) can reach unity only if all nonresonant eigenvalues are the same, in which case \( \rho_{nn} = N - 1 \). But this is automatically satisfied in the two-probe structure, \( N = 2 \), where there is only one nonresonant eigenphase, \( \tilde{\theta}_{nn} = \theta_2 \). In that special case, the transmission becomes

\[
T = 1 - |S_{11}|^2 = |t_{11}|^2 \frac{(E - E_0 + \Delta)^2}{(E - E_0)^2 + \Gamma^2/4}, \tag{14}
\]

which goes through zero and one.

We now consider the lineshape in the absence of symmetry for the multi-probe, multi-subband case. Let \( U \) be the unitary matrix that diagonalizes \( S \), and \( \theta_j \) be the resonant eigenphase, all other \( \theta_k \) being only weakly energy dependent. The reflection amplitude is

\[
S_{nn} = e^{2i\theta_1} |U_{1n}|^2 + \sum_{k>1} e^{2i\theta_k} |U_{kn}|^2. \tag{15}
\]

where the index \( k \) runs over leads and sub-bands.

Eq. (15) is completely general and implies that \( |S_{nn}|^2 \) reaches unity if and only if all the nonresonant eigenvalues are identical. As a consequence, the resonant transmission \( T \) of a two-probe structure in the single subband regime still has a zero at some energy even in the absence of symmetries. This conclusion requires no special assumptions about \( U \); however some further information is needed to obtain the lineshape. In the symmetric case Eq. (1) implies that the eigenvectors have a constant modulus of \( 1/\sqrt{N} \). If we assume that these moduli (corresponding to the incident fluxes in each lead) are only weakly dependent on energy even in the absence of symmetries, the two-probe transmission becomes

\[
T = (1 - a^2)|t_{11}|^2 \frac{(E - E_0 + \Delta)^2}{(E - E_0)^2 + \Gamma^2/4} \tag{16}
\]

where the constant \( a^2 < 1 \). Thus we recover the Fano lineshape of Eq. (14) with a reduced prefactor; this implies that perfect reflection still occurs at resonance, but not perfect transmission.

Although the Fano function, Eq. (1), is the generic lineshape for Q1D scattering it is never seen in purely 1D resonant tunneling because in this case the background transmission and lifetime of the metastable state are not independent. Well-defined resonances with small \( \Gamma \) require low background transmission, which simply gives the Breit-Wigner lineshape. On the other hand, if \( \Gamma \) is not small then the assumption of constant \( \theta \) needed in Eq. (14) is not valid over the width of the resonance. In a Q1D system, on the other hand, an electron entering the region where the quasi-bound state is localized does not necessarily enter that state itself, because the existence of a second scattering channel allows resonant and nonresonant transmission to occur in parallel as two distinct processes. The background transmission can still be large even if the coupling to the quasi-bound level (which determines \( \Gamma \)) is small, (e.g. due to approximate symmetry). Since the energy shifts \( \Delta \) in Eqs. (14), (16) are proportional to \( \Gamma \), the asymmetry parameter \( q \) defining the lineshape is actually independent of \( \Gamma \). If \( \Gamma \) can be varied while \( |t_{11}|^2 \) is roughly constant across resonance, a series of Fano lineshapes will be obtained which can be collapsed onto a curve characterized by a single asymmetry parameter \( q \) by rescaling the energy axis. This scaling property may be tested for the first time in transport experiments.

We have explored several different systems which might exhibit Fano resonances when appropriately perturbed to create a quasi-bound level in the continuum [13,14]. These include quantum point contacts, 2D electron gas systems with an in-plane magnetic field, and magnetotransport in 3D heterostructures. Here we focus
on the 3D case because epitaxial heterostructures may be grown with atomic precision so the effects of disorder are minimized. We consider a quantum well of finite depth sandwiched between bulk emitter and collector regions with a magnetic field $B$ oriented normal to the layers (see inset to Fig. 1). As noted, the motion along $B$ reduces to a 1D problem due to Landau quantization in the transverse plane (the Landau level index plays the role of the sub-band index). The well gives rise to a finite sequence of bound states which repeats itself below each Landau level threshold $E_n$. The number and binding energies of these bound states depend on well parameters which may be controlled, hence for $n > 1$ they may lie degenerate with the continuum of propagating states associated with lower LL’s. For precisely normal magnetic fields the LL wavefunctions of bound and continuum states are orthogonal and no resonance occurs, but a small tilt angle will induce inter-LL coupling at the interface and Fano resonances whose width may be tuned by varying the tilt angle $\alpha$ (see Fig. 1).

The experiment must be done at low temperature (so that thermal broadening does not distort the intrinsic lineshape) and in the linear response regime. Thus we propose tuning the Fermi energy, $E_F$ through resonance by varying the magnitude of the magnetic field, $B$. Above some threshold field $B_0$, $E_F$ will enter the lowest LL and lie slightly below $E_2$. As $B$ is increased further, $E_F$ approaches the bottom of the lowest LL, $E_1$. The quasi-bound levels also shift as a function of $B$ but $E_F$ will cross all resonances between $E_2$ and $E_1$ at some $B$. The resulting transmission curves as a function of $B$ (obtained from simulations) are shown in Fig. 1b for a particular resonance at various small tilt angles. The scaling property of the resonances is seen to be very well satisfied in this system (Fig. 1b). Discussions and simulations of this and other possible experimental geometries will be presented in detail elsewhere.

We acknowledge R. Wheeler for the important suggestion of tuning through resonance with a magnetic field. We also thank M. Büttiker, M. Reed and R. Adair for helpful discussions. This work was supported by ARO grant no. DAAH04-93-G0009.

FIG. 1. (a) Transmission of a finite well as a function of magnetic field $B$ in units of $B_0$. The resonances correspond, from left to right, to tilt angles of $\sin \alpha = 0.02, 0.01, 0.005$ (curves offset for clarity). With $\omega \equiv eB_0/mc$, the well has depth $V = 2\hbar\omega$ and width $L = 3.5\sqrt{\hbar/m\omega}$. (b) The same resonances plotted in reduced units, $\epsilon$ being defined as below Eq. (14); the Fano asymmetry parameter is $q = 0.887$. Over the width of these narrow resonances, $E_F$ is proportional to $B$ while $|t|^2$ and $\Gamma$ are independent of $B$. Inset: effective potential in the growth direction.

[1] G. Breit and E. Wigner, Phys. Rev. 49, 519 (1936)
[2] U. Fano, Phys. Rev. 124, 1866 (1961)
[3] J. A. Simpson and U. Fano, Phys. Rev. Lett. 11, 158 (1963)
[4] R. K. Adair, C. K. Bockelman and R. E. Peterson, Phys. Rev. 76, 308 (1949)
[5] J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics (Wiley, New York, 1952), chapter VIII.
[6] M. Büttiker, Phys. Rev. A 30, 1982 (1984)
[7] D. Y. K. Ko and J. C. Inkson, Semicond. Sci. Technol. 3, 791 (1988); D. Z. -Y. Zing and T. C. McGill, Phys. Rev. B 47, 7281 (1993)
[8] R. L. Schult, H. D. Wyld and D. G. Ravenhall, Phys. Rev. B 41, 12760 (1990)
[9] H. U. Baranger, Phys. Rev. B 42, 11479 (1990)
[10] W. Parodi, Zhi-an Shao and C. S. Lent, Appl. Phys. Lett. 61, 1350 (1992)
[11] P. F. Bagwell and R. K. Lake, Phys. Rev. B 46, 15329 (1992)
[12] J. U. Nöckel, Phys. Rev. B 46, 15348 (1992)
[13] E. Tekman and P. Bagwell, Phys. Rev. B 48, 2553 (1993)
[14] P. L. McEuen, B. W. Alphenaar, R. G. Wheeler and R. N. Sacks, Surf. Sci. 229, 312 (1990).
[15] J. R. Taylor, Scattering Theory (Wiley, New York, 1972)
[16] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Non-relativistic Theory (Pergamon Press, Oxford, 1977), chapter XVIII.
[17] M. Büttiker, IBM J. Res. Develop. 32, 63 (1988); Phys. Rev. B 38, 12724 (1988)
[18] S. A. Gurvitz and Y. B. Levinson, Phys. Rev. B 47, 10578 (1993)
[19] J. U. Nöckel and A. D. Stone, unpublished.