The quantum and classical Fano parameter $q$

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Abstract. The Fano resonance has been regarded as an important phenomenon in atomic and molecular physics for more than half a century. Typically, a combination of one quantum bound state and one or more continuum result in an asymmetric peak in the ionization spectrum. The peak-shape, called the Fano profile, can be expressed by the simple formula derived by Fano in 1935. However the interpretation of its main parameter $q$, which represents the asymmetry of the peak in the formula, is not intuitively transparent. The Fano resonance is not necessarily a quantum effect, but it is a manifestation of a certain physical mechanism in various systems, both quantum and classical. We present three intuitively transparent classical pictures and rigorously derive their Fano profiles to properly formulate the physics of the Fano parameter.

Keywords: Fano resonance, double photoexcitation, classical mechanics, science education, history of science
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1. Introduction

Typical excitation resonances in atomic physics have the well-known symmetric peak-shapes called the Lorentzian, Breit-Wigner, and Cauchy distribution. However, the helium double photoexcitation to $2s2p \ 1P^\circ$, the first experiment performed utilizing synchrotron radiation in the late sixties, presented a dramatic demonstration of asymmetric peaks in the photoabsorption spectrum. (Figure 1). (A historical note can be found in Appendix A and recent examples in Appendix B.) The first theoretical formulation of this ”Fano resonance” was developed some time before by Fano (1935) [1] and then extended and refined by Fano (1961) [2] after the photoexcitation experiment. In the latter paper, it was argued rigorously that from the superposition state consisting of a discrete state $\varphi$ and a continuum $\psi_{E'}$

$$\Psi_E = a\varphi + \int dE'b_{E'}\psi_{E'} \quad (a \neq 0) \quad (1)$$

(Fano (1961) [2] equation (2)), the Fano profile formula

$$\text{(total scattering cross-section)} \propto \frac{(q + \epsilon)^2}{1 + \epsilon^2} = 1 + \frac{q^2 - 1 + 2q\epsilon}{1 + \epsilon^2} \quad (2)$$

could be derived. Here, $\epsilon$ is the photon energy offset from the peak position and normalized by a half of the resonance width, called the reduced energy (Fano (1961) [2] equation (21)). Figure 2 plots this formula. The curve has a clear asymmetric peak with the minimum value going down to zero. (Note: If the state includes two or more continuum states, this spectrum does not necessarily go down to zero (Fano (1961)§4 [2]).)

This characteristic shape enables us to easily identify Fano resonances as conspicuous features in the experimental spectrum. Thus it is interesting both in view of
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Figure 2. Fano profile, graphical plots of Equation (2) for several values of $q$.

theory and practical utility. However, some of the important concepts in Fano’s paper [2] are not necessarily obvious. These include the basic meaning of the $q$ parameter (also called the profile index or Fano parameter) or an explanation of why the peak becomes asymmetric when a bound state is superposed on continuum. To illustrate the physical essence of the Fano resonance, we first discuss it in a classical system instead of a quantum system. Fano resonances are often regarded as a phenomenon specific to quantum mechanics, but they also occur in classical mechanics.

Recent analytical studies by Riffe (2011) [5] argued that Fano resonances occur in certain classical linear systems. However, Riffe’s paper overlooks the fact that the Fano resonance is an ubiquitous phenomenon among various physical systems rather than a concept valid only for a particular system. Some authors introduced the so-called “classical Fano resonance” as distinct from the (quantum) Fano resonance [4] [6] [7] [8]. Also, a similar line shape in the classical coupled oscillator was noted [3]. They based the analogy in terms of the similar peak-shapes. We argue for the nature of these Fano resonance in terms of the physical mechanism instead of just looking for analogy or metaphor in terms of the peak-shape. To demonstrate this, we analytically derive the Fano profile from two classical models. The first “coupled oscillator” model itself was discussed by [4] [6] [7] [8]. Then, we will introduce a second, original physical model that we formulated based on a one spring model. The latter is advantageous for grasping only the most fundamental essence of the Fano resonance without any additional details.

2. Classical Fano resonance in the coupled oscillator system

2.1. The System with Two Resonances

We have normally only a single resonance frequency in a damping simple harmonic oscillator. To discuss the interplay of the two resonance oscillations that resides close each other in resonance frequencies, we consider the system consisting of weakly connected two damping simple oscillators. We illustrate the system in figure Figure 5; Two oscillators of mass $m_1$ and $m_2$ with the stiffness constant $k_1$ and $k_2$ are connected
by a weak spring with stiffness $K$. If the values of $k_1$ and $k_2$ are close and their damping
constants are enough large, the oscillations of two harmonic oscillators will overlap and
provide us with a conspicuous anomaly in the resonance features. In the present paper,
we try to consider an extreme case in which the damping factor of $m_2$, $\gamma_2$ is zero; the
case $\gamma_1 \neq 0$, and $\gamma_2 = 0$.

The sharp one occurs on the shoulder of the broad one. We call the sharp resonances
discrete states, since the amplitude is large only in the narrow vicinity of the peak and
very small elsewhere. This sharp resonance is superimposed on the shoulder of a broad
resonance whose amplitude $A$ varies gently as the external frequency $\omega$ is changed.
At least two springs and two masses are required to produce two resonances. Let us
consider the system depicted in Figure 3. Hereafter, we set the masses $m_1 = m_2 = 1$, the
displacement $x_1$, $x_2$, the damping coefficients $\gamma_1 \neq 0$, $\gamma_2 = 0$ and the spring constants $K$, $k_2$.

To solve the equation of motion of this system,

$$\ddot{x}_1 + \gamma_1 \dot{x}_1 + K(x_1 - x_2) = F_0 \cos \omega t$$

(3)

$$\ddot{x}_2 + \gamma_2 \dot{x}_2 + k_2 x_1 - K(x_2 - x_1) = 0$$

(4)

is expressed as

$$x_1(t) = c_1(\omega) \cos \omega t,$$

(5)

and the amplitude $c_1$ of $x_1$ is

$$c_1(\omega) = \frac{\omega^2 - \omega_2^2 + i \gamma_2 \omega}{(\omega_1^2 - \omega^2 + i \gamma_1 \omega)(\omega_2^2 - \omega^2 + i \gamma_2 \omega) - v_{12}^2} F_0$$

(6)

where $\omega_1 = \sqrt{K}, \omega_2 = \sqrt{k_2 + K}, v_{12} = -K$.

(7)

We use the variable $v_{12}$ for consistency with later discussion. Plotting $|c_1(\omega)|^2$, which is
the absolute square of amplitude $c_1$, resulting in Figure 4.

The square of the frequency $\omega^2$ is placed on the horizontal axis because the energy
$E$ of a classical harmonic oscillator (one spring and one mass) is represented by

$$E = \frac{1}{2} m \omega^2.$$  

(8)

Thus, the horizontal axis is the energy provided by an external force. Incidentally, the
Fano profile can be derived as a vibration frequency as well as energy on a horizontal
axis. In a quantum system, it is clear that it can be discussed either way because
$E = \hbar \omega$, but even in a classical system, the Fano profile can be derived with either
energy $\propto \omega^2$ or frequency $\omega$ as the horizontal axis.
Compared to the previous two springs model, the frequency changes to $\omega_1 = \sqrt{k_1 + K}$. The new spring with spring constant $k_1$, can reduce the amplitude, bring two peaks closer while keeping one broad shoulder, the other one sharp and overlapping the shoulder. Substituting the solution

$$x_1(t) = c_1(\omega) \cos \omega t,$$

The vertical axis represents the square of the norm of amplitude $|c_1(\omega)|^2$ because the energy of the classical harmonic oscillator $E$ (one spring and one mass) becomes

$$E = \frac{1}{2} k A^2.$$  \hspace{1cm} (9)

In other words, the vertical axis will depend on the energy of the mass with displacement $x_1$. Taking these factors into consideration, Figure 4 shows the energy given by the external force transmitted to mass 1.

In Figure 4, two resonances can be seen. Both peaks are broad here. We would like to find the condition that makes one of them sharper, coming closer and overlapping the shoulder of the other peak that remains broad.

In order to realize this, we can consider the coupled oscillator which uses three springs and two masses (Figure 5), introduced by [4] [6] [7]. The equations of motion are similar to the previous one, with only one spring added,

$$\ddot{x}_1 + \gamma_1 \dot{x}_1 + \omega_1^2 x_1 + v_{12} x_2 = F_0 \cos \omega t$$

$$\ddot{x}_2 + \gamma_2 \dot{x}_2 + \omega_2^2 x_2 + v_{12} x_1 = 0$$

where $\omega_1 = \sqrt{k_1 + K}, \omega_2 = \sqrt{k_2 + K}, v_{12} = -K$. \hspace{1cm} (10)\hspace{1cm} (11)\hspace{1cm} (12)
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the amplitude $c_1$ becomes

$$c_1( \omega ) = \frac{\omega_2^2 - \omega^2 + i \gamma_2 \omega}{(\omega_1^2 - \omega^2 + i \gamma_1 \omega)(\omega_2^2 - \omega^2 + i \gamma_2 \omega) - \nu_{12}^2} F_0.$$  \hspace{1cm} (14)

Now, we plot $|c_1(\omega)|^2$ against $\omega^2$ (Figure 6 (left side)). As before, this graph shows how the energy provided by the external force is transmitted to mass 1. Looking at Figure 6 (left side), two peaks are found, $\omega$ the lower broader (called peak a, with angular frequency $\omega_a$) spread with a Lorentian shape, whereas the higher narrower peak $\omega$ (Called peak b, with angular frequency set as $\omega_b$) is very sharp and can be found at the foot of peak a.

Expansion of peak b looks like Figure 6 (right side). The shoulder of the gentle peak suddenly drops to 0 near $\omega^2 = \omega_2^2 = 1.44$, and after the sharp peak, it turns back into a gentle slope. It can be said that this was caused by the gentle shoulder (continuum state) interfering with the sharp peak (discrete state). The asymmetric resonance phenomenon caused by such interaction between the discrete state and the continuum state is called Fano resonance.

2.2. Intuitive interpretation of the Fano parameter $q$

In the last section, we reviewed and provided interpretation for previous discussions [4] [6] [7] [8]. Now, we increase the attenuation coefficient $\gamma_1$ without changing any other parameter. Figure 6 has the same attenuation coefficient $\gamma_1 = 0.025$ as before, and those with $\gamma_1 = 1.41$ and $\gamma_1 = 10$ in Figure 7 and 8.

Comparing the figure on the right of Figure 6–8 with the Fano profile (Figure 2), it is clearly seen that the attenuation coefficient $\gamma_1$ is related to the Fano coefficient $q$ in Fano profile’s formula

$$\sigma(\epsilon) = \frac{(q + \epsilon)^2}{1 + \epsilon^2} = 1 + \frac{q^2 - 1 + 2q\epsilon}{a + \epsilon^2}. \hspace{1cm} (15)$$

In the next section the Fano profile will actually be derived from this classical system.

2.3. Derivation of the Fano profile for the classical coupled oscillator

For the coupled oscillator (Figure 3) represented by the formula Equation (10), Equation (11), we calculate

$$|c_1(\omega)|^2 = c_1(\omega)c_1^*(\omega) \hspace{1cm} (16)$$
in the vicinity of peak b using the displacement amplitude of mass 1 $c_1$ expressed by Equation (14). For simplicity, we set $\gamma_2 = 0$ as in the previous discussions.

When diagonalizing the equations of motion Equation (10) and Equation (11) of the previous system, It can be seen that the resonance frequencies are somewhat shifted from the natural frequencies $\omega_1, \omega_2$. The case at Figure 6, shows it visually. We call these peaks peak a and peak b respectively as in the previous discussion. The diagonalized
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Figure 6. Coupled oscillator (where $\omega_1 = 1.0, \omega_2 = 1.2, \gamma_1 = 0.025, \gamma_2 = 0, v_{12} = 0.1$)

$\gamma_1 = 0.025$

Figure 7. $\gamma_1 = 1.41$

Figure 8. $\gamma_1 = 10$

result is,

\[ \omega_a^2 = \omega_1^2 - \frac{v_{12}^2}{\omega_2^2 - \omega_1^2}, \]  

\[ \omega_b^2 = \omega_2^2 + \frac{v_{12}^2}{\omega_2^2 - \omega_1^2}, \]  

which shows that both peaks are shifted by the same amount in opposite directions.
The peak $b$ position is adjusted by varying Equation (14) so that
\[ \bar{\epsilon} \overset{\text{def}}{=} \omega^2 - \omega_b^2 = \omega^2 - \omega_b^2 - \frac{v_{12}^2}{\omega_2^2 - \omega_1^2}, \] (19)
comes down to zero. Now, we used the symbol $\bar{\epsilon}$ because this variable indicates energy, recalling that
\[ E = \frac{1}{2} m \omega^2 \] (20)
is the energy of the classical harmonic oscillator.

In the expression Equation (19) since $\bar{\epsilon} = \omega^2 - \omega_b^2 = (\omega + \omega_b)(\omega - \omega_b)$, we can regard $(\omega + \omega_b)$ as a constant if we consider it in the narrow neighborhood of $\bar{\epsilon} = 0$. Therefore, since it $\bar{\epsilon} \sim (\omega - \omega_b)$, the same argument holds for the energy ((the constant multiplication of) the square of the frequency) even though the first power of the frequency is considered.

Next follows the expression for the amplitude $c_1(\omega)$ (Equation (14)) with $\bar{\epsilon}$ (Equation (19)). We replace the numerator and denominator of $c_1(\omega)$ except for $F_0$ by $A, B$ (in brief, $c_1(\omega) = \frac{A}{B} F_0$). The numerator $A = \omega_2^2 - \omega^2$ becomes
\[ A = \omega_2^2 - \omega^2 = -\frac{v_{12}^2}{\omega_2^2 - \omega_1^2}. \] (22)
Further transformation would yield
\[ A = -\gamma_1\omega_2 \frac{v_{12}^2}{(\omega_2^2 - \omega_1^2)^2} \left[ \frac{1}{\gamma_1\omega_2} \frac{(\omega_2^2 - \omega_1^2)^2}{v_{12}^2} \bar{\epsilon} + \frac{1}{\gamma_1\omega_2} (\omega_2^2 - \omega_1^2) \right]. \] (23)
The denominator $B = (\omega_1^2 - \omega^2 + i\gamma_1\omega)(\omega_2^2 - \omega^2 + i\gamma_2\omega) - v_{12}^2$ can be separated into the real part and the imaginary part using $\bar{\epsilon}$, then
\[ \Re(B) = (\omega_2^2 - \omega_1^2)\bar{\epsilon} \] (24)
\[ \Im(B) = -\gamma_1\omega_2 \left( \bar{\epsilon} + \frac{v_{12}^2}{\omega_2^2 - \omega_1^2} \right). \] (25)
Now we are examining the properties in the neighborhood of $\bar{\epsilon} = 0$.
\[ \frac{v_{12}^2}{\omega_2^2 - \omega_1^2} \gg \bar{\epsilon} \approx 0 \] (26)
leads to
\[ \Im(B) \approx -\gamma_1\omega_2 \frac{v_{12}^2}{\omega_2^2 - \omega_1^2}. \] (27)
This is the only approximation employed in this derivation. In the neighborhood the peak $b$, the real part and the imaginary part can be combined as,
\[ B \approx \gamma_1\omega_2 \frac{v_{12}^2}{\omega_2^2 - \omega_1^2} \left[ \frac{1}{\gamma_1\omega_2} \frac{(\omega_2^2 - \omega_1^2)^2}{v_{12}^2} \bar{\epsilon} - i \right]. \] (28)
Summarizing the above, the amplitude $c_1(\omega)$ can be written as
\[ c_1(\omega) \approx \frac{-\gamma_1\omega_2 \frac{v_{12}^2}{(\omega_2^2 - \omega_1^2)^2} \left[ \frac{1}{\gamma_1\omega_2} \frac{(\omega_2^2 - \omega_1^2)^2}{v_{12}^2} \bar{\epsilon} + \frac{1}{\gamma_1\omega_2} (\omega_2^2 - \omega_1^2) \right]}{\gamma_1\omega_2 \frac{v_{12}^2}{\omega_2^2 - \omega_1^2} \left[ \frac{1}{\gamma_1\omega_2} \frac{(\omega_2^2 - \omega_1^2)^2}{v_{12}^2} \bar{\epsilon} - i \right]} F_0. \] (29)
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Looking closely at the equation Equation (29), certain patterns can be observed. One of them is

$$\epsilon \defeq \frac{1}{\gamma_1 \omega_2} \frac{(\omega_2^2 - \omega_1^2)^2}{v_{12}^2} \tilde{\epsilon},$$

(proportional to the energy).

Next, define $q$ as

$$q \defeq \frac{1}{\gamma_1 \omega_2} (\omega_2^2 - \omega_1^2).$$

Then, the amplitude Equation (29) can be written as

$$c_1(\omega) \approx -\frac{\epsilon + q }{\epsilon - i \omega_2^2 - \omega_1^2} F_0.$$

Therefore, $|c_1(\omega)|^2$ can be written as

$$|c_1(\omega)|^2 \approx \frac{(\epsilon + q)^2}{\epsilon^2 + 1} \frac{F_0^2}{(\omega_2^2 - \omega_1^2)^2}.$$

Since $\frac{F_0^2}{(\omega_2^2 - \omega_1^2)^2}$ is a constant, $|c_1(\omega)|^2$ is a constant multiple of $\frac{(\epsilon + q)^2}{\epsilon^2 + 1}$.

$$|c_1(\omega)|^2 \propto \frac{(\epsilon + q)^2}{\epsilon^2 + 1}$$

This is nothing but the Fano Profile itself. That means $q$ is the Fano parameter, which produces the Figure 2.

From the above discussion, it is clear that the attenuation coefficient $\gamma_1$ is inversely proportional to the Fano parameter $q$.

$$q \propto 1/\gamma_1$$

Damping reduces the energy of the system. Therefore, it can be said that Fano parameter $q$ is an indicator of how much energy the system is retained. When $q$ is infinite, the energy of the system does not leak. Under this situation, the Fano profile turns into the Lorentzian. On the other hand, when $q$ is close to 0, the energy of the system dissipates rapidly. In this case, the Fano profile becomes a dip looking like an upside-down Lorentzian. This is called the Window Resonance [9] in absorption spectroscopy.

3. Classical Fano resonance in a system employing only one spring

3.1. Transformation from Lorentzian to Fano profile

The Fano resonance caused by the superposition of continuum states and a discrete state becomes a Lorentzian as $q \to \infty$. In other words, the superposition of continuum states reduces $q$ from infinity. We can give an interpretation to the Fano parameter $q$ illustrating the gradual deformation of the lorentzian lineshape to Fano line-shape for a harmonic oscillator system (one spring and one mass) with mechanical perturbation introduced.
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3.2. Classical harmonic oscillator (Lorentzian)

We start the discussion with the simple case of a damped driven oscillator which exhibits a near Lorentzian profile. Its equation of motion can be written as

$$\ddot{x} + 2\gamma \dot{x} + \omega_0^2 x = F_0 \cos \omega t$$

where $\gamma$ is the attenuation factor and $F_0 \cos \omega t$ is the external force.

Let us consider the following simple Lorentzian profile (probability density function of standard Cauchy distribution) (Figure 9)

$$\sigma(\epsilon) = \frac{1}{\epsilon^2 + 1}.$$ (37)

3.3. Lorentzian in terms of angular frequency, and phase difference.

The phase difference between the external force and the displacement of the mass (abbreviated as “the phase difference”) is given by

$$\theta(\omega) = \tan^{-1} \left( \frac{\gamma \omega}{\omega_0^2 - \omega^2} \right)$$

in a classical harmonic oscillator. The phase difference and the angular frequency correspond one to one, and the phase difference can be defined in the interval $-\pi/2$ to $\pi/2$ with the corresponding angular frequency extending to infinity. Therefore, using this, we can convert the horizontal axis of Lorentzian from the angular frequency $\omega$ to the phase difference $\theta$ between the external force and mass displacement.

Considering this simplest Lorentzian, the correspondence between the phase difference and the angular frequency takes a simple form

$$\theta(\omega) = \tan^{-1} \left( -\frac{1}{\omega} \right)$$

hence

$$\tan \theta(\omega) = -\frac{1}{\omega}.$$ (40)
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Figure 10. The amplitude of a driven damped one spring and one mass oscillator in terms of the phase difference

then

$$\cot \theta(\omega) = -\omega.$$  

(41)

Let’s represent the Lorentzian with phase difference by defining the new variable $\delta_\epsilon$ $(0 < \delta_\epsilon < \pi)$ satisfying $\epsilon = -\cot \delta_\epsilon$.

$$\sigma(\epsilon) = \frac{1}{\epsilon^2 + 1}$$  

(42)

$$= \frac{1}{\cot^2 \delta_\epsilon + 1}$$  

(43)

$$= \frac{\sin^2 \delta_\epsilon}{\cos^2 \delta_\epsilon + \sin^2 \delta_\epsilon}$$  

(44)

$$= \sin^2 \delta_\epsilon$$  

(45)

With phase difference the Lorentzian is represented by a simple expression (Figure 10).

What happens if this phase difference $\delta_\epsilon$ is perturbed? Let’s subtract the constant $\delta_q$, from the phase difference and include it in the expression for the Lorentzian as shown in Equation (45).

$$\sin^2(\delta_\epsilon - \delta_q) = (\sin \delta_\epsilon \cos \delta_q - \cos \delta_\epsilon \sin \delta_q)^2$$  

(46)

$$= \frac{(\sin \delta_\epsilon \cos \delta_q - \cos \delta_\epsilon \sin \delta_q)^2}{1 \times 1}$$  

(47)

$$= \frac{(\sin \delta_\epsilon \cos \delta_q - \cos \delta_\epsilon \sin \delta_q)^2}{(\sin^2 \delta_\epsilon + \cos^2 \delta_q)(\sin^2 \delta_q + \cos^2 \delta_q)}$$  

(48)

$$= \frac{(\cot \delta_\epsilon - \cot \delta_q)^2}{(1 + \cot^2 \delta_\epsilon)(1 + \cot^2 \delta_q)}$$  

(49)

$$= \frac{(\epsilon - \cot \delta_q)^2}{(1 + \epsilon^2)(1 + \cot^2 \delta_q)}$$  

(50)

From the expression Equation (41) showing the correspondence between the phase difference and the angular frequency of one spring and one mass system, it is
understood that the part cot δ₁ depends on the angular frequency. Therefore, with the transformation by \( q \overset{\text{def}}{=} -\cot \delta_q \), we can return to angular frequency picture again.

\[
\sin^2(\delta_\epsilon + \delta_q) = \frac{(\epsilon + q)^2}{(1 + \epsilon^2)(1 + q^2)}
\]  

(51)

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

(52)

Since \( q \) is a constant, \( \frac{1}{1 + q^2} \) is also a constant. We find that this expression is the Fano profile itself. (Figure 2)

\[
\sin^2(\delta_\epsilon + \delta_q) \propto \frac{(q + \epsilon)^2}{1 + \epsilon^2}
\]  

(53)

3.4. Fano resonance projected on a plane tangential to the cylinder

We proceed with the development of the geometrical interpretation from the previous section. We write the square of sine curve \( \sin^2(\delta) \) on cylindrical coordinate (Figure 11). Viewing from the origin towards the direction of the \( \delta = -\pi/2 \), we can see the Lorentzian on the tangential plane because \( \epsilon = -\cot \delta = \tan(\delta - \pi/2) \) (Figure 12). Next, by shifting the viewing angle by \( \delta_q \), the Fano profile appears on the tangential plane. The Fano parameter at this time is \( q = \cot \delta_q \) (Figure 13).

3.5. Interpretation of the Fano parameter as seen from the system of one spring and one mass

What does \( \delta_q \) mean? As shown in the cylinder’s tangential plane, \( \delta_q \) represents the rotation of the viewing angle. This rotation can be found in the previous coupled oscillator model as a sub-system. The sub-system of mass 1 and the springs on both sides (called system 1), which has a wide resonance due to the damping, imposes a phase shift of \( \delta_q \) to the other sub-system of mass 2 and the springs on both sides (called system 2).
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The resonance of system 2 appears in the value $|c_1(\omega)|^2$, which is proportional to the total energy of system 1. In other words, we see the resonance of system 2 as the effect manifests in system 1. The validity of this interpretation depends on the phase difference of system 1 at the particular force frequency. If the phase difference of system 1 is 0 or $\pi$ we cannot see an asymmetric peak due to system 2. Additionally if we see the resonance of system 1 through the total energy of system 2 ($\propto |c_2(\omega)|^2$) we cannot see any asymmetric peak because $\gamma_2 = 0$ (the phase difference of system 2 is only 0 and $\pi$ except natural frequency).

It does not have to be a coupled oscillator as long as this interplay of the shift of the phase difference occurs. Taking the two-electron excitation of helium as an example, the Fano shape occurs because the ionizing states (continuum states) cause a shift of

**Figure 12.** Lorentzian on tangential plane of cylindrical coordinate

**Figure 13.** Fano profile ($q = 1$) on tangential plane of cylindrical coordinate
the phase difference to the double photoexitation channel. The essence of the previous attempt on the derivation of Fano resonance by S-matrix scattering theory [10] can also be interpreted in terms of the shift of the phase difference in the system of one spring and one mass.

4. Conclusion

The Fano resonance is an ubiquitous phenomenon that can exist in many areas of physics and related fields. Therefore, the appearance of asymmetric peaks where there is a minimum point going down to zero could have been known since long ago. One of the important aspects of Fano’s theory was that it provided the condition that led to the phenomenon in a quantum system and gave a concise expression to the peak shape defined as the Fano profile. Previous work on classical Fano resonances emphasized only the visual appearance, without actual derivation and interpretation of the Fano parameter $q$.

The definition of the Fano parameter in the quantum system in Fano (1961) is described as

$$q = \frac{\langle \phi|T|i \rangle + PV \int dE_c \frac{\langle \phi|H|\psi_{E_c} \rangle \langle \psi_{E_c}|T|i \rangle}{E - E_c} \pi \langle \phi|H|\psi_E \rangle \langle \psi_E|T|i \rangle}{54}$$

where $|i\rangle$ is an initial state, $|\phi\rangle$ is a target discrete state with Energy $E$ and $|\psi_E\rangle$ is a target continuum state with Energy $E$. Can you understand this intuitively?

Here we rigorously derive the Fano Profile for the coupled oscillator and the (single spring) harmonic oscillator and provide physical meaning of the Fano parameter $q$ in terms of the three pictures.

The first picture is the coupled oscillator model as the system to superpose a discrete state ($\gamma_2 = 0$) to a continuum state. We can adjust the rate of superposition by $\gamma_1$, that cause the Fano parameter varying. This is the most rough sketch of the interpretation of Fano parameter. The second is a study from the interpretation that the damping coefficient $\gamma_1$ indicates the energy dissipation rate of the system to the other systems. When the energy dissipation rate is close to 0, that is, when $q$ is infinite, the peak becomes Lorentzian. As the energy dissipation rate increases, the peak becomes asymmetric, and as the energy dissipation rate approaches infinity the peak becomes an inverted Lorentzian like a dip, called the window resonance. That is, the Fano parameter $q$ can be regarded as a value proportional to the reciprocal of energy dissipation rate.

The previous two pictures are based on the coupled oscillator system. However, the foundation of the Fano resonance is not only on the coupled oscillator system or the related systems. The most essential picture is the one-spring model through the phase difference between the external force and the displacement of the mass. When the phase difference is artificially changed by $\delta_q$, it becomes increasingly asymmetric by $q = -\cot \delta_q$. It is actually impossible to artificially change the phase difference. However we can find it as a sub-system of the coupled oscillator.
We can merge these three pictures: Fano resonance cause the energy transfer from the (sub-)system with resonance to the (sub-)system with resonance having other phase difference. And Fano parameter $q$ describe the gap of the each phase difference. We viewed three pictures but it is just an “equivalent interpretation” simply because the wording is different. In quantum theory, it is not easy to understand the equivalence between the different schemes of Fano resonance (perturbation theory base / scattering theory base). The equivalence of these scheme becomes more transparent in the classical system.

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Appendix A. The prehistory of the Fano resonance

Appendix A.1. Krypton Auger processes and helium double photoexcitation

Normal resonances have a well-known symmetric peak-shape called the Lorentzian, Breit–Wigner, or Cauchy distribution. Beutler experimentally found in 1935 that some of the resonances in the krypton and xenon absorption spectra have asymmetrical peak-shapes on Kr Auger processes $(4p^5)_{1/2}nl \rightarrow (4p^5)_{3/2} + \text{free electron}$ [11]. Fano and Fermi came up with an explanation for these strange peaks—that they are the resonances due to the combination of one bound state and one or more continuum states. Their idea was successful, and Fano published a paper on this a few weeks later [1] (English translation by Guido Pupillo et al. [12]) [13].

Another important example, helium double photoexcitation to $2s2p^1P^\circ$, presented an even clearer demonstration of asymmetric peaks (Figure 1). This discovery by Madden et al. in 1965 [15] the earliest scientific result obtained by utilizing synchrotron radiation experiments. It surprised the researchers that such a clear asymmetric spectra were obtained, and they paid particular attention not only to the position and height of the peak but also to its shape. Their discovery was a good example of how new theoretical developments were driven by the emergence of new experimental techniques. In 1929, Dirac declared “The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known” [16], but atomic physics was not finished with discovering new phenomena. Instead, many new ideas entered the stage of atomic physics after that declaration was made. Thus, sustainable development of new research through the productive interplay
and cross-germination between experiments and theory characterizes progress in atomic physics.

Appendix A.2. Earlier theoretical discoveries of related phenomena

Some related studies preceded the work of Fano (and Fermi). Breit and Wigner discovered an effect similar to the Fano resonance in neutrons and published their results in 1936 [17]. It is possible that Fano’s work was inspired by their work. In the paper by Breit et al. (1936) [17], Dirac (1927) [18] is credited with finding the earliest approach for analyzing a superposition state consisting of discrete and continuum states. The first theoretical application was by Rice (1929) [19] on molecular rotational levels. In fact, a formula similar to Fano’s was derived by Dirac (1927) as equation (18) [18]. This means that Fano was not the only pioneer for this type of analyses. However, the most important practical characteristic, that the spectra should be asymmetric, was not pointed out in Dirac (1927), Rice (1929), or Breit (1936). Although in some respect, Fano’s (1935) contribution appears to be only a variation of the previous studies, his ideas were revolutionary for quantum resonances in terms of peak shape analysis and building a theory accessible to and testable by both experimentalists and theoreticians. Today, at the beginning of the 21st century, various scientific fields, such as solid-state physics and nanomaterial science, continue to benefit from our understanding of Fano resonances.

Appendix A.3. Fano (1961)

The first paper to derive the Fano profile, Fano (1935) [1] (English translation [12]), was written in Italian. Therefore, the later paper written in English, Fano (1961) [2], became better known. (There are some important differences not relevant to the current discussion.) The Fano (1961) paper achieved high recognition: as of June 2003 [14], it was 8th in citation ranking in Physical Review, in particular, ranking first for atomic and molecular physics. Fano (1961), having a big impact on physics and chemistry, was very rich in content for a relatively short 13-page paper.

Appendix B. Examples of classical Fano resonance

The fact that Fano resonance can occur in the system of spring and mass means that Fano resonance can be found in various places in everywhere and everyday life. Immediately imaginable one is the Fano resonance using the RLC resonance circuit [6] [7] [8]. For every articles cited as references on the left, they simply pointed out that as a result of plotting the voltage gain against the frequency of the input voltage for the LCR circuit equivalent to the coupled oscillator, the peak becomes asymmetric and they assert that it is a metaphor of Fano resonance. Given the series of results in our paper, these are not “metaphor”, but it can be said that Fano resonance is actually occurring because Fano profile can be derived analytically.
The quantum and classical Fano parameter \( q \)

Also, in acoustics there is also a precedent for Fano resonance by resonance tubes and the like [20] [21] [22] [23] [24]. There is another somewhat interesting example in optical engineering such that the attempt to switch light of a specific frequency at high speed by changing Fano parameter [25]. This example in optical engineering is easy to understand by assuming the waveguide in a nanoscale. When the electromagnetic wave leaks out of the waveguide from the slight gap at the joint of the waveguide (since the frequency characteristic is flat outside because it is outside the tube, it will have been through a continuum state system) and it overlaps with the one that has passed through the waveguide (It can be said that it passed through a discrete state system because it passes through a sharp Lorentian like only specific frequencies) at the end, Fano resonance occurs. In the example of [25], you can imagine that you are changing the Fano parameter by adjusting the phase of the leaked light.

Since it can be caused by the superposition of continuum states and a discrete state, similar consideration can be made even in general fields that handle linear systems such as control theory and signal processing. In these fields, a diagram called Nyquist diagram (or Nyquist plot) is frequently used to confirm the stability of the system. This is plotted for each \( \omega ( -\infty < \omega < \infty ) \) with the real part of the frequency response on the horizontal axis (In our discussion, it is the square of the amplitude of the mass 1) and the imaginary part of the frequency response on the vertical axis (Energy dissipation rate is expressed by it). There is a paper that plots the Nyquist diagram while changing the Fano parameter in the system where Fano resonance actually occurs [26].

Looking at examples of various Fano resonances, we notice an interesting difference that energy loss is represented by the real part of the impedance in the AC circuit, whereas in quantum mechanics it is represented by the imaginary part of the state energy. As we have seen, the imaginary part of the amplitude also controls energy dissipation in classical mechanics. Energy dissipation is indispensable for Fano resonance, but the representation differs between (classical and quantum) dynamics and electronic circuit regarding real and imaginary. Even if you invert real and imaginary you can build the same theory, so this does not indicate something physical facts. Depending on what you first focused on in building the theories, the real and imaginary would have been decided. The electronic circuit first focused on resistance. So in the theory the control of energy dissipation should be the real part.

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