# Three-Channel Interference Interpretation of Fano Profile

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Fano resonance is a ubiquitous phenomenon, and it is commonly interpreted as a two-channel interference of the discrete and continuous channels. The present work investigates the Fano profile from a perspective of the temporal evolution of the wave function. By exciting the atom with a $\delta$ pulse and calculating the evolution of the wave function, the Fano formula is deduced. The results clearly show that the Fano resonance is of a three-channel interference, which is different from the traditional understanding. The three channels are revealed as the ground-continuum, ground-discrete-continuum, and a previously unmentioned third channel, i.e., ground-continuum-discrete-continuum. The present three-channel interpretation can be easily generalized to other physical systems, contributing to a deeper understanding of the Fano profile.

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Fano profiles were initially observed in molecular predissociation[1] and atomic autoionization.[2] The unusual asymmetric peak profile inspired theorists to develop the corresponding theories.[3–6] Fano's theory[6] has been widely accepted for the accuracy of its result and the simplicity of its expression. In the framework of Fano's theory, for a discrete state embedded in a continuum, "the actual stationary states may be represented as superpositions of states of different configurations which are mixed by the configuration interaction."[6] The transition cross section can be expressed as the famous Fano formula:

$$\sigma(\epsilon) = \sigma_a \frac{(q+\epsilon)^2}{1+\epsilon^2}, \tag{1}$$

where $\sigma_a$ is the cross section of the transition to the background continuum. $\epsilon = \dfrac{E-E_0}{\Gamma/2}$ is the dimensionless reduced energy, $E-E_0$ is the energy detuning with respect to the resonance energy $E_0$, and $\Gamma$ indicates the spectral width of the autoionized state. Finally, $q$ is the Fano asymmetry parameter that relates to the relative strength of the ground-discrete and ground-continuum transitions.

Fano's theory[6] has attracted much attention due to the ubiquity of the Fano resonance. Over the years, Fano resonance has been studied theoretically and experimentally in various physical systems, such as electron energy-loss spectroscopy,[7,8] x-ray cavities,[9–11] photonics,[12–14] and quantum dots.[15–17] There are two critical points of a Fano resonance, i.e., the intensity vanishes at $\epsilon = -q$ and reaches a maximum at $\epsilon = \frac{1}{q}$. In photonics, this feature allows Mie scattering to be switched from total reflection to total transmission.[12–14] In quantum dots, several different approaches have been used to achieve continuous tuning of the asymmetric parameter $q$,[15–17] which has important applications in qubit manipulations.[18,19]

The universality of the Fano resonance implies that they share the same physical essence. Many theorists have explained the Fano formula using different approaches. Fano has also investigated the Fano resonance from the viewpoint of multichannel scattering theory in 1961.[6] In the 1980s, Connerade and Lane[20–23] applied the $S$-matrix and $K$-matrix formalisms to interpret the Fano resonance, which are still in the framework of scattering theory, and they described the $q$-reversal and width vanishing effects when a Rydberg series couples with the continuum. In scattering theory, the Fano resonance is the result of the interference of the "hard sphere" scattering and the resonance.[24] Therefore, it has long been thought that the Fano profile is the result of a two-channel interference. The "hard sphere" scattering results in a continuum channel with a constant phase shift contribution, and the resonance scattering corresponds to a discrete channel with a $\pi$ change in phase shift with the energy increase. Another approach to obtain the Fano formula is the Feshbach formalism established by Feshbach[25,26] and its core spirit is to simplify the dimension of the Hamiltonian using the method of projection operators. In recent years, many experimental and theoretical works have investigated the Fano resonance in time domain.[27–33] The time-domain Fano resonance contains rich dynamical information and allows for the modulation of the Fano profile using the pump-probe technique,[30,31] and the developed theoretical methods have the ability to explain or reproduce the experimental observations. While these works focus on the evolution of the Fano line shape in the time domain, the present work focuses on the channels through which the atom reaches its final state. We restudy the Fano resonance from the perspective of time domain with the $\delta$ pulse excitation approximation, and a three-channel interpretation of the Fano resonance is revealed.

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In 1930, the Wigner–Weisskopf theory[34] was proposed to interpret spontaneous emission, in which the time-dependent Schrödinger equation can be directly solved to obtain the evolution of the wave function. The present work extends the Wigner–Weisskopf method to explain the Fano resonance, giving a clear interference interpretation of the Fano formula. We consider one discrete state embedded in one continuum of an atom, assuming that it is excited by a $\delta$ pulse, based on the Schrödinger equation, the distribution in the continuum is obtained. As is expected, the Fano formula is deduced. However, the total transition amplitude comes from the contributions of three channels, namely, ground-continuum, ground-discrete-continuum, and an interesting third channel, i.e., ground-continuum-discrete-continuum.

For an eigenstate of a multielectron atom, the electron has a definite configuration when the configuration interaction is ignored. However, when taking into account the configuration interaction, a real eigenstate of the Hamiltonian often has not a definite configuration but a superposition of several configurations. For a discrete state embedded in an ionization continuum, Fano obtained the well-known Fano formula by solving the superposition coefficients of the real eigenstates. According to Fano's theory,[6] the matrix element of the Hamiltonian in this subspace can be expressed as

$$\langle\varphi|\hat{H}|\varphi\rangle = E_0, \tag{2a}$$

$$\langle E'|\hat{H}|E''\rangle = E'\delta(E'-E''), \tag{2b}$$

$$\langle\varphi|\hat{H}|E'\rangle = V_{E'}. \tag{2c}$$

Here $|\varphi\rangle$ denotes the discrete state, and $|E'\rangle$ and $|E''\rangle$ represent the ionization continuum at energies of $E'$ and $E''$. $V_{E'}$ is the strength of configuration interactions which leads to the coupling of the discrete and continuum states.

We assume that an atom in the ground state $|G\rangle$ is excited by a $\delta$ pulse, and calculate the evolution of the wave function with time. In general, autoionization is much faster than spontaneous emission. In the case of helium, for example, the widths of the autoionized states are on the order of $10^{-3}$–$10^{-1}$ eV,[35,36] while the natural linewidths of the discrete dipole-allowed transitions are on the order of $10^{-8}$–$10^{-7}$ eV. For simplicity, we ignore the spontaneous emission of the atom, and with the $\delta$ pulse excitation approximation, we do not consider the coupling of the excited state to the ground state at $t > 0$. The wave function at time $t$ can be expanded as

$$|\Psi(t)\rangle = a(t)|\varphi\rangle + \int b_{E'}(t)|E'\rangle dE', \tag{3}$$

where $a(t)$ and $b_{E'}(t)$ represent the coefficients of the discrete and continuum states, respectively. The evolution equations in the interaction picture can be expressed as (atomic units are used throughout this study):

$$i\dot{a}(t) = \int dE' b_{E'}(t) V^*_{E'} e^{-i(E'-E_0)t}, \tag{4a}$$

$$i\dot{b}_{E'}(t) = V_{E'} a(t) e^{i(E'-E_0)t}. \tag{4b}$$

Integrating both sides of Eq. (4a) yields

$$b_{E'}(t) = b_{E'}(0) - i\int_0^t dt' V_{E'} a(t') e^{i(E'-E_0)t'}. \tag{5}$$

The first term in Eq. (5) represents the direct transition from the ground state to the continuum at $t = 0$, and the second term represents the transition through the discrete state to the continuum.

Then, we determine the paths from the ground state to the discrete state. Substituting Eq. (5) into Eq. (4a), we can obtain

$$\begin{aligned}\dot{a}(t) = & -i\int dE' b_{E'}(0) V^*_{E'} e^{-i(E'-E_0)t} \\ & - \int dE' \int_0^t dt' a(t') |V_{E'}|^2 e^{i(E'-E_0)(t'-t)}.\end{aligned} \tag{6}$$

Assume that $V_{E'}$ does not change with energy and denote it as $V_E$, which is a good approximation according to Fano's theory[4,6] and most theoretical treatments.[27–30] It is a regular procedure to extend the lower bounds on the integrals of $dE'$ to negative infinity. Considering that $V_{E'}$ is energy-independent, by using the Fourier expansion of the $\delta$-function, the second term in Eq. (6) can be written as

$$\begin{aligned}&\int_0^t dt' \int dE' a(t') |V_E|^2 e^{i(E'-E_0)(t'-t)} \\ &= 2\pi |V_E|^2 \int_0^t dt' a(t') \delta(t'-t).\end{aligned} \tag{7}$$

Notice that the singularity of $\delta(t'-t)$ is in the upper bound of the integral, and that the $\delta$-function is an even function, Eq. (7) results in

$$2\pi |V_E|^2 \int_0^t dt' a(t') \delta(t'-t) = \frac{\Gamma}{2} a(t). \tag{8}$$

Here, $\Gamma = 2\pi|V_E|^2$ is the width of the discrete state, and Eq. (6) can be rewritten as

$$\dot{a}(t) = -i\int dE' b_{E'}(0) V^*_{E'} e^{-i(E'-E_0)t} - \frac{\Gamma}{2} a(t). \tag{9}$$

Letting $a(t) = A(t) e^{-\Gamma/2}$, the equation for $A(t)$ can be reduced to

$$\dot{A}(t) = -i\int dE' b_{E'}(0) V^*_{E'} e^{-i(E'-E_0)t + \frac{\Gamma}{2}t}. \tag{10}$$

Integrating both sides of the equation yields

$$A(t) = A(0) - i\int_0^t dt' \int dE' b_{E'}(0) V^*_{E'} e^{-i(E'-E_0)t' + \frac{\Gamma}{2}t'}. \tag{11}$$

Then the solution to Eq. (6) can be obtained as follows:

$$\begin{aligned}a(t) = & \, a(0) e^{-\frac{\Gamma}{2}t} \\ & - i\int_0^t dt' \int dE' b_{E'}(0) V^*_E e^{-i(E'-E_0)t' - \frac{\Gamma}{2}(t-t')}.\end{aligned} \tag{12}$$

Equation (12) shows that there are two paths from the ground state to the discrete state: the first term is the direct excitation by the $\delta$ pulse, i.e., $|G\rangle \to |\varphi\rangle$, and the second term is the path $|G\rangle \to |E'\rangle \to |\varphi\rangle$. The exponential term ensures $a(t \to \infty) = 0$, as is expected. Substituting

Eq. (12) into Eq. (5) gives the solution in integral form for $b_{E'}(t)$:

$$b_{E'}(t) = b_{E'}(0) - i\int_0^t dt' V_E\, a(0) e^{i(E'-E_0)t' - \frac{\Gamma}{2}t'} - \int_0^t dt' \int_0^{t'} dt'' \int dE'' b_{E''}(0)|V_E|^2 \cdot e^{-i(E''-E_0)t'' + i(E'-E_0)t' - \frac{\Gamma}{2}(t'-t'')}. \quad (13)$$

The three terms in Eq. (13) represent the following channels: $|G\rangle \to |E'\rangle$, $|G\rangle \to |\varphi\rangle \to |E'\rangle$, and the third channel $|G\rangle \to |E''\rangle \to |\varphi\rangle \to |E'\rangle$, as shown in Fig. 1.

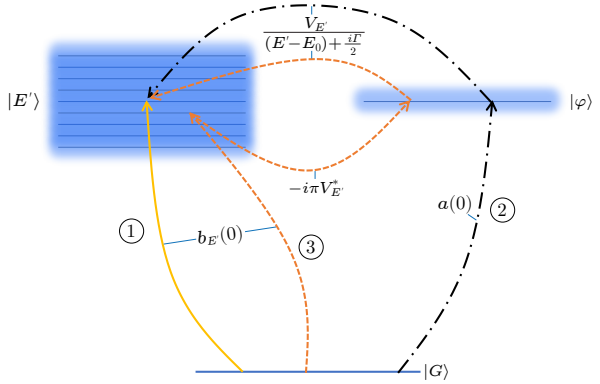


**Fig. 1.** Schematic diagram of the three-channel interference. The physical processes corresponding to the three terms in Eqs. (13) and (14) are described by different lines. The solid line indicates the direct ionization channel $|G\rangle \to |E'\rangle$, the chain dotted line represents the second channel $|G\rangle \to |\varphi\rangle \to |E'\rangle$, and the dashed line indicates the third channel $|G\rangle \to |E''\rangle \to |\varphi\rangle \to |E'\rangle$. The amplitude of every step is also marked.

Note that $b_{E'}(0)$ and $V_{E'}$ do not change significantly with the energy, and similarly using the Fourier expansion of the $\delta$-function, the integration of Eq. (13) at $t \to \infty$ is given as

$$b_{E'}(\infty) = b_{E'}(0) + V_E\, a(0)\frac{1}{(E'-E_0)+i\Gamma/2} - i\pi|V_E|^2 b_{E'}(0)\frac{1}{(E'-E_0)+i\Gamma/2}. \quad (14)$$

The form of Eq. (14) makes the three-channel picture clearer, and we define the amplitude for each step of every channel in Fig. 1, and the multiplication of the amplitude of each step will yield the corresponding amplitude of every channel in Eq. (14).

For simplicity, we use the following definition:

$$q = \frac{a(0)}{\pi V_E^* b_E(0)} = \frac{\langle\varphi|T|i\rangle}{\pi V_E^* \langle E|T|i\rangle}, \quad (15a)$$

$$\epsilon = \frac{E'-E_0}{\Gamma/2}. \quad (15b)$$

Here, $T$ is the transition operator for the $\delta$ pulse. Equation (14) can be simplified to a compact form:

$$b_{E'}(\infty) = b_{E'}(0)\Big(1 + q\frac{1}{\epsilon+i} - i\frac{1}{\epsilon+i}\Big) = b_{E'}(0)\Big(1 + \frac{q-i}{\epsilon+i}\Big). \quad (16)$$

Then, the transition probability can be obtained by its modulus squared:

$$|b_{E'}(\infty)|^2 = |b_{E'}(0)|^2 \frac{(q+\epsilon)^2}{1+\epsilon^2}. \quad (17)$$

This is the original form of the Fano formula.

In the above derivations, we have assumed that $b_{E'}(0)$ and $V_{E'}$ do not vary with the energy, which simplifies the mathematical treatments and highlights the three-channel picture. More precisely, if we consider the variation of $b_{E'}(0)$ and $V_{E'}$ with the excitation energy, a similar three-channel picture can be obtained and the derived formula is in accordance with the Fano formula.

We begin with Eq. (6) and consider the variation of $V_{E'}$ with energy. It can be expected that within the width of the discrete state, $V_{E'}$ is a slowly varying function. Using the Fourier transform of the Heaviside step function, see Ref. [37], the integral of the second term can be obtained as follows:

$$\int dE' \int_0^t dt' a(t')|V_{E'}|^2 e^{i(E'-E_0)(t'-t)} = \Big[\pi|V_{E_0}|^2 - iP\int dE' \frac{|V_{E'}|^2}{E'-E_0}\Big]a(t). \quad (18)$$

The result of Eq. (18) is equivalent to another integral:

$$\Big[\pi|V_{E_0}|^2 - iP\int dE' \frac{|V_{E'}|^2}{E'-E_0}\Big]a(t) = 2\int_0^t dt' a(t')\Big[\pi|V_{E_0}|^2 - iP\int dE' \frac{|V_{E'}|^2}{E'-E_0}\Big]\delta(t'-t). \quad (19)$$

Comparing Eq. (19) with Eq. (18), we can obtain an equivalence relation:

$$\int dE'|V_{E'}|^2 e^{i(E'-E_0)(t'-t)} \equiv 2\Big[\pi|V_{E_0}|^2 - iP\int dE' \frac{|V_{E'}|^2}{E'-E_0}\Big]\delta(t'-t). \quad (20)$$

Now we extend the form of Eq. (20) to a more general case. Suppose $f(E)$ is a slow varying function of energy $E$, then we have

$$\int dE' f(E') e^{i(E'-E_0)(t'-t)} \equiv 2\Big[\pi f(E_0) - iP\int dE' \frac{f(E')}{E'-E_0}\Big]\delta(t'-t). \quad (21)$$

The integral form for $b_{E'}(t)$ will be

$$b_{E'}(t) = b_{E'}(0) - i\int_0^t dt' V_{E'}\, a(0) e^{i(E'-E_0)t' - \frac{\kappa}{2}t'} - \int_0^t dt' \int_0^{t'} dt'' \int dE'' b_{E''}(0) V^*_{E''} V_{E'} \cdot e^{-i(E''-E_0)t'' + i(E'-E_0)t' - \frac{\kappa}{2}(t'-t'')}. \quad (22)$$

Here $\kappa = \Gamma + 2iF(E_0)$, and $F(E_0)$ is a modification to the resonance energy.

$$F(E_0) = P\int dE' \frac{|V_{E'}|^2}{E_0 - E'}. \quad (23)$$

Using the conclusion of Eq. (21) we can obtain the result for $b(\infty)$ near the resonance energy as

$$b_{E'}(\infty) = b_{E'}(0) + \frac{V_{E_0}\, a'(0)}{[E' - E_0 - F(E_0)] + i\Gamma/2} - i\pi \frac{|V_{E_0}|^2 b_{E'}(0)}{[E' - E_0 - F(E_0)] + i\Gamma/2}. \tag{24}$$

Here $a'(0)$ is the amplitude of transition to the modified discrete state $|\Phi\rangle$ at $t = 0$.

$$|\Phi\rangle = |\varphi\rangle + P \int dE' \frac{V_{E'}|E'\rangle}{E_0 - E'}. \tag{25}$$

Therefore, after considering the variation of $b_{E'}(0)$ and $V_{E'}$ with the excitation energy, the result of three channels still holds, and the original discrete state must be replaced by the modified discrete state and the resonance energy needs to de modified accordingly.

It is worth noting that the Fano formula is given regardless of whether we consider the modified discrete states or not, so that the modified discrete states are not the essence of Fano's resonance; it is a modification after consideration of more realistic models. The simplified model highlights its physical essence, and the other one is closer to the actual situation. For convenience, our subsequent discussion will not distinguish the original discrete state and the modified discrete state, as this depends on the accuracy of the model under consideration.

For a long time, the Fano resonance was understood as a result of a two-channel interference,[12,38–40] and the transition amplitude can be written as

$$f(\epsilon) \propto 1 + \frac{q - i}{\epsilon + i}. \tag{26}$$

Here, the constant term denotes the continuum, and the second term of the Lorentz response denotes the discrete channel.

It is worth mentioning that from the viewpoint of the two-channel interference, the $q - i$ in Eq. (26) characterizes the transition amplitude of the discrete channel scaled by that of the continuum,[18] which seems to conflict with the fact that $q$ relates to the ratio of the ground-discrete and ground-continuum transition amplitudes in Fano theory.[6] Another interesting question is why the imaginary part of the coefficient of the discrete channel is definitely $-i$, regardless of the transition and the target. The three-channel interpretation mentioned above can give a natural answer to these questions: the imaginary part $-i$ corresponds to the third channel, which is free from the transition amplitude $a(0)$ to the discrete state and only determined by $b_{E'}(0)$, i.e., the interaction of the discrete and continuum states results in the third channel.

It is well known that the observable quantity is the square modulus of the sum of the transition amplitudes of all channels, so in general, it is impossible to derive the information of the individual channel from the observed quantity such as the cross section. However, it is fortunate that in a particular case for the zero transition amplitude to the discrete state, which is the famous window resonance showing a symmetric dip in the measured spectrum, such as the $3s^{-1}np$ states for argon,[7] we can demonstrate the importance of the third channel. For $a(0) = 0$, which blocks the discrete channel, it is difficult to understand the interference phenomenon of the window resonance from the viewpoint of a two-channel interference since one of the two channels is blocked. However, it is natural from the viewpoint of the three-channel interpretation, since although the second channel has a zero amplitude the interference between the first and third channels results in window resonance. In this case, the transition amplitude can be expressed as

$$b_{E'}(\infty) = b_{E'}(0)\Big(1 - i\frac{1}{\epsilon + i}\Big). \tag{27}$$

The form of the window resonance is obtained by taking the modulus squared:

$$|b_{E'}(\infty)|^2 = |b_{E'}(0)|^2\Big(1 - \frac{1}{1 + \epsilon^2}\Big). \tag{28}$$

It is clear that the three-channel interpretation is necessary to naturally understand the Fano resonance.

It is interesting to compare the present three-channel interpretation with the original Fano's theory,[6] where the transition amplitude is

$$\langle \Psi_E|T|i\rangle_F = \frac{1}{\pi V_E^*}\langle \Phi|T|i\rangle \sin\Delta - \langle E|T|i\rangle \cos\Delta \tag{29}$$

Here $\Psi_E$ is the real eigenstate of the Hamiltonian, $\Phi$ is the modified discrete state, and $\Delta = -\mathrm{arccot}\epsilon$ represents the phase shift due to the configuration interactions. In Eq. (29), $\sin\Delta$ and $\cos\Delta$ can be written as

$$\sin\Delta = -e^{-i\Delta}\frac{1}{\epsilon + i}, \tag{30a}$$

$$\cos\Delta = e^{-i\Delta}\Big(1 - \frac{i}{\epsilon + i}\Big). \tag{30b}$$

Then Eqs. (16) and (29) have the relationship of

$$b_E(\infty) = -e^{i\Delta}\langle \Psi_E|T|i\rangle_F. \tag{31}$$

The factor $-e^{i\Delta}$ has no influence on the observations. It is clear that the $\cos\Delta$ term in the Fano theory corresponds to the first and third channels, and the $\sin\Delta$ term corresponds to the second channel, i.e., a clear three-channel picture is revealed by this work.

The energy spectrum of an autoionization state is deduced by the time evolution equation with the $\delta$-pulse excitation approximation, and the contributions from the different channels to the transition amplitude are elucidated. The results show that the Fano profile is an interference result of the three channels of $|G\rangle \to |E'\rangle$, $|G\rangle \to |\varphi\rangle \to |E'\rangle$, and $|G\rangle \to |E''\rangle \to |\varphi\rangle \to |E'\rangle$, which is different from the conventional understanding where the Fano profile is interpreted as a two-channel interference. It is worth mentioning that the three-channel picture of the Fano resonance has been embodied in a study of the time-domain Fano response in pump-probe scheme,[33] while the authors did not further discuss its connection with Fano's formula and no analytic results are given. Several previous works[27,28] about Fano resonance in the time-domain have also investigated the time evolution of the continuum, but differently these works focus on the continuum distributions at different times, which is different from the present work in which

we focus on the paths from the initial state to the continuum. Specifically, Mercouris *et al.*[27] calculated the time- and energy-dependent profiles of the autoionization of He $2s2p$ under a finite-length pulse excitation. Then, Chu *et al.*[28] studied the time dependence of autoionization of Be $2pns$ (embedded in multiple $2s\epsilon p$ continuum) under a short pulse excitation. Both the works calculated the time evolution of the continuum amplitude, but they both needed to use Fano's conclusions about the superposition coefficients of the eigenstates, i.e., their derivation should be developed using the eigenstates after considering the configuration interaction. In the present work, Fano formula is derived from another way, which does not require the superposition coefficient of the eigenstates in Fano's theory, but uses the wave functions of continuous and discrete states before coupling. The configuration interaction leads to the transition between the continuum and discrete states, and gives the image of the three-channel interpretation, which is helpful for in-depth understanding of Fano resonance.

The discrete channel in the two-channel interference is the result of combining the contributions of the second and third channels since they both have Lorentzian distributions. Although the present work predicts the same formula as Fano, it provides deep insight into the Fano resonance and exhibits a clear physical picture. The present three-channel interpretation will be applicable to different quantum systems.

More recently, Fano resonance has become a hot topic in broad fields, and the continuous regulation of the asymmetric parameter $q$ has been implemented in many physical systems, such as x-ray cavities,[9–11] quantum dots,[9,10,15,41] and atomic systems.[31] The results of the present work may shed new light on physical mechanisms involved in these investigations.

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