Determination of profile parameters of a Fano resonance without an ultrahigh-energy resolution

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A deconvolution procedure is proposed to determine the resonant width \( \Gamma \), the asymmetry parameter \( q \), and the background cross section \( \sigma_b \) of a Fano-type resonance in the absence of an ultrahigh-energy resolution. This procedure enables a direct extrapolation to infinite energy resolution using a set of explicit analytical relations in terms of the ratio between the width \( \Gamma \) and the experimental energy resolution \( \Omega \) in the limit of \( \Gamma/\Omega \ll 1 \).

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I. INTRODUCTION

Theoretically, the structure profile of an isolated resonance is often described by the Fano formula [1] in terms of an asymmetry parameter \( q \) and the smoothly varying background cross section \( \sigma_b \), i.e.,

\[
\sigma(E) = \sigma_b \left( \frac{q + \epsilon}{1 + \epsilon^2} \right),
\]

where \( \epsilon = (E - E_r)/(\frac{1}{2} \Gamma) \) is the reduced energy defined in terms of the energy \( E_r \) and the width \( \Gamma \) of the resonance. The cross section \( \sigma \) is expected to reach its peak value \( \sigma_{\text{max}} = \sigma_b (1 + q^2) \) and a zero at energies

\[
E_{\text{max}} = E_r + \frac{1}{2} (\Gamma/q) \quad \text{and} \quad E_{\text{min}} = E_r - \frac{1}{2} (\Gamma/q),
\]

respectively. An accurate determination of \( q \) and \( \Gamma \) is essential to the understanding of the multielectron interactions associated with an atomic resonance. For example, the \( q \) parameter measures qualitatively the interference between contributions due to transitions from initial state to the respective bound and continuum components of the final-state wave function. The width \( \Gamma \), which determines the nonradiative decay rate of a resonance through autoionization, represents the bound-continuum mixing of the resonant state [1].

In spite of the tremendous improvement in energy resolution \( \Omega \) [2,3], the widths \( \Gamma \) of some of the best known narrow resonances, e.g., the He \( sp, 2n^- \) and \( 2pnd^1P \) (or, alternatively, the \( 2,1_e \) and \( 2,1_u \)) series [2,3], remain substantially smaller than the best experimental resolution. A physical interpretation of an atomic transition involving such a narrow resonance may become unreliable based on the \( q \) and \( \Gamma \) derived from a direct numerical fit of the observed spectrum to the Fano Formula. The measured data, in fact, represent a spectrum convoluted with an experimentally determined monochromator function \( \mathcal{F} \) [1–3], i.e.,

\[
\sigma'(E; \Omega) = \int_{-\infty}^{+\infty} \sigma(E') \mathcal{F}(E' - E; \Omega) dE'.
\]

The variation of the observed \( \sigma_{\text{max}} \) effectively measures the ratio \( \Gamma/\Omega \). For example, \( \sigma_{\text{max}} \) of the He \( sp, 2n^+ 1P \) (or, \( 2,0_e \)) resonance is expected to reach a constant as the effective principal quantum number \( \nu \) increases [1,2]. In reality, the observed \( \sigma_{\text{max}} \) decreases monotonically when \( \Gamma/\Omega \) decreases rapidly as \( \Gamma \) decreases at a rate of \( \nu^{-3} \) [2,3].

The monochromator function \( \mathcal{F} \) is often approximated at the center by a Gaussian distribution \( \mathcal{G} \) and modified at its tail by a Lorentzian distribution \( \mathcal{L} \), where

\[
\mathcal{G}(E; \Omega) = \frac{e^{-E^2/\delta^2}}{\sqrt{\pi \delta^2}} \quad \text{and} \quad \mathcal{L}(E; \Omega) = \frac{1}{\pi} \left( \frac{1}{E^2 + \frac{1}{4}\Omega^2} \right),
\]

the energy resolution \( \Omega \) may be measured by the full width at half maximum (FWHM) of the distribution function and \( \delta = \Omega/(2 \ln 2) \). In general, the value of \( \Omega \) in \( \mathcal{G} \) and \( \mathcal{L} \) may be different. However, for simplicity, the same value is assumed in this study. (Use of different \( \Omega \) will not affect our proposed procedure given later, but it may lead to slightly modified analytical expressions.) Similar to Domke et al. [2], we approximate \( \mathcal{F} \) by a weighted combination of \( \mathcal{G} \) and \( \mathcal{L} \), i.e.,

\[
\mathcal{F}(E; \Omega, w_g, w_l) = w_g \mathcal{G}(E; \Omega) + w_l \mathcal{L}(E; \Omega),
\]

where the sum of the experimentally determined weighting factors \( w_g \) and \( w_l \) equals one.

Figure 1 presents a number of selected convoluted spectra \( \sigma'(E; \Omega) \) with \( \Omega \) ranging from 2 to 8 meV. The spectra \( \sigma(E) \) corresponding to infinite energy resolution (i.e., with \( \Omega = 0 \)) are derived from Eq. (1) for a fictitious resonance with \( E_r = 2.1110 \) Ry, \( \sigma_b = 1.0 \) Mb, and \( \Gamma = 5.0 \times 10^{-6} \) Ry. The \( q \) parameter varies from 0.4 to 4. For simplicity, we have chosen a monochromator function defined by a set of weighting factors \( w_g = 0.6 \) and \( w_l = 0.4 \), similar to the ones determined in recent high-resolution He experiment [2]. In practice, \( w_g \) and \( w_l \) may vary as \( \Omega \) varies.

By applying a Fourier transformation to the Gaussian distribution function, Eq. (3) becomes integrable [4] and it can be expressed in terms of an analytical formula shown explicitly in the Appendix. Whereas the term involving the Lorentzian distribution is relatively straightforward, the ones that correspond to the Gaussian distribution are highly nonlinear. As a result, it is impractical to deconvolute the observed spectra analytically for a direct determination of \( q \) and \( \Gamma \).
Alternative nonanalytical deconvolution procedures have been attempted in a limited cases with varying success [5].

II. DECONVOLUTION PROCEDURE

In this paper, we introduce a simple deconvolution procedure with the purpose of determining $\Gamma$, $q$, $\sigma_\beta$, and $E_r$ of a Fano-type resonance from the observed spectra (e.g., the ones simulated by the convoluted spectra shown in Fig. 1) in the absence of an ultrahigh energy resolution $\Omega$, i.e., when $\Gamma$ is a few orders of magnitude smaller than $\Omega$. Our proposed procedure starts with an initial estimate of $E_r$ from a plot of the observed $E_{\text{max}}$ or $E_{\text{min}}$ against $\Omega$ shown on the left of Fig. 2. By neglecting the $(\Gamma/q)$ term in Eq. (2) initially, we approximate $E_r$ by the extrapolated value of $E_{\text{max}}$ at $\Omega = 0$ for a resonance with a $|q|$ greater than one. In contrast, for a resonance with a $|q|$ smaller than one, we drop the $\Gamma/q$ term and approximate $E_r$ by $E_{\text{min}}(\Omega = 0)$. When $|q|$ is close to one, the initial $E_r$ equals the average of $E_{\text{min}}$ and $E_{\text{max}}$ estimated at $\Omega = 0$. Our calculation has shown that the value of $E_r$ determined at the end does not depend critically on the initial estimate of $E_r$.

The key step of our proposed procedure involves an expansion of the observed spectra $\sigma^r(E;\Omega)$ in terms of a set of harmonic oscillator eigenfunctions $\Psi_n$, i.e.,

$$\sigma^r(E;\Omega) = \sum_{n=0}^{\infty} c_n(\Omega)\Psi_n(\rho(E;\Omega,E_r)),$$

where $\rho = \sqrt{2\ln2(E-E_r)/(\Gamma/\Omega)}$ is a modified reduced energy and $\Psi_n(\rho)$ is a $\rho$-dependent normalized harmonic oscillator eigenfunction defined in its standard form in terms of the Hermite polynomials $H_n(\rho)$. The expansion coefficient $c_n(\Omega)$ in Eq. (6) is evaluated from the observed spectra $\sigma^r$ for each $\Omega$ by an integration

$$c_n = \int_{-\infty}^{+\infty} \sigma^r(\rho)\Psi_n(\rho)d\rho.$$  

(7)

It turns out that only the first two coefficients $c_0$ and $c_1$ at a few $\Omega$ are required to determine the values of $\Gamma$, $q$, and $\sigma_\beta$.

Mathematically, by substituting Eqs. (3) and (5) into Eq. (7) and using the generating function of the Hermite polynomials, i.e., $e^{-x^2 + 2tx} = \sum_{n=0}^{\infty} H_n(t)x^n/n!$, a straightforward calculation will lead to a simple expression for the coefficient $c_n$, i.e., $c_n/\sigma_\beta = I_{1,n}/I_{1,0}$, where

$$I_{1,n} = \frac{1}{(4\pi)^{1/4}\sqrt{2\pi n!}} \int_{-\infty}^{+\infty} \frac{(\rho + q\sqrt{2\ln2(\Gamma/\Omega)})^2}{\rho^2 + 2\ln2(\Gamma/\Omega)^2} e^{-(1/4)\rho^2} d\rho$$

and

$$I_{1,0} = \int_{-\infty}^{+\infty} \frac{\rho + q\sqrt{2\ln2(\Gamma/\Omega)}}{\rho^2 + 2\ln2(1 + \Gamma/\Omega)^2} \times \Psi_n(\rho) d\rho.$$  

(9)

Equations (8) and (9) can be evaluated analytically by applying the integral [6]

$$\int_{-\infty}^{+\infty} e^{-x^2} x^2 d\rho = \frac{\pi}{\Gamma} F_{s}(t) e^{r^2 s},$$

(10)
where $F_e(x) = 1 - (2/\sqrt{\pi})\int_0^x e^{-y^2} dy$ is the complementary error function. Both $c_0(\Omega)$ and $c_1(\Omega)$ are functions of $\Gamma/\Omega$, i.e.,

$$c_0 = (4\pi)^{1/4} + \mu(q^2 - 1) \left( \frac{\Gamma}{\Omega} \right)$$

and

$$c_1 = 2\nu \left( \frac{\Gamma}{\Omega} \right).$$

(11)

The coefficients $\mu$ and $\nu$ are given by $\mu = (f_0^{(0)}w_g + f_0^{(1)}w_l)$ and $\nu = (f_1^{(0)}w_g + f_1^{(1)}w_l)$, where

$$f_0^{(0)} = \pi^{1/4} \sqrt{\ln2} F_e(u)e^{u^2}, \quad f_0^{(1)} = \sqrt{\ln2} \pi^{3/2} F_e(v)e^{v^2},$$

and

$$f_1^{(0)} = (4\pi)^{1/4} \left( \sqrt{\ln2} - 2\sqrt{\ln2} \frac{\pi^{3/2} F_e(u)e^{u^2}}{\Gamma/\Omega} \right),$$

(12)

and

$$f_1^{(1)} = (4\pi)^{1/4} \left( \sqrt{\ln2} - 2\sqrt{\ln2} \frac{\pi^{3/2} F_e(v)e^{v^2}}{\Gamma/\Omega} \right).$$

(13)

The variables $u$ and $v$ are given by $u = \sqrt{\ln2/2}(\Gamma/\Omega)$ and $v = \sqrt{\ln2[1 + (\Gamma/\Omega)]}$, respectively. When $\Gamma \ll \Omega$, $\mu$, and $\nu$ can be expanded as

$$\mu = \sum_{n=0}^{\infty} \mu_n \left( \frac{\Gamma}{\Omega} \right)^n \quad \text{and} \quad \nu = \sum_{n=0}^{\infty} \nu_n \left( \frac{\Gamma}{\Omega} \right)^n,$$

(15)

where $\mu_n$ and $\nu_n$ can be evaluated analytically using Eqs. (12)–(14).

From Eqs. (11) and (15), the coefficients $c_0$ and $c_1$ can be expressed in terms of a power series in $\Gamma/\Omega$ when $\Gamma \ll \Omega$. Since $\Gamma$ is a constant yet to be determined, the $c_0$ and $c_1$ obtained from the observed spectra can be expanded in $\Omega^{-1}$ as

$$c_0 = \sum_{n=0}^{\infty} \alpha_n \left( \frac{1}{\Omega} \right)^n \quad \text{and} \quad c_1 = \sum_{n=1}^{\infty} \beta_n \left( \frac{1}{\Omega} \right)^n.$$  

(16)

A comparison between Eq. (16) and the analytical expressions Eqs. (11) and (15) shows that only three numerically fitted coefficients $\alpha_0$, $\alpha_1$, and $\beta_1$ are required to determine the values of $\Gamma$, $q$, and $\sigma_b$. Specifically, when $\Gamma/\Omega \ll 1$,

$$\alpha_0 = (4\pi)^{1/4}\sigma_b, \quad \alpha_1 = \mu_0\sigma_b(q^2 - 1)\Gamma,$$

and

$$\beta_1 = 2\nu_0\sigma_b\Gamma,$$

(17)

where $\mu_0 = 1.9646w_g + 1.3282w_l$ and $\nu_0 = 1.5675w_g + 0.9234w_l$.

Should $w_g$ and $w_l$ remain unchanged as $\Omega$ varies, $\Gamma$, $q$, $\sigma_b$, can be determined directly from $\alpha_0$, $\alpha_1$, and $\beta_1$ from the numerical fits of $c_0$ and $c_1$ to Eq. (16). In the limit of $\Gamma/\Omega \ll 1$, both $c_0$ and $c_1$ vary linearly as functions of $\Omega^{-1}$ (see, e.g., Fig. 2). $\sigma_b$ is determined by extrapolating $c_0$ to $\Omega^{-1} = 0$. $\Gamma$ and $q$ are calculated from the products of $q^2 - 1)\Gamma$ and $q\Gamma$ in terms of $\alpha_1$ and $\beta_1$. After $\Gamma$, $q$, and $\sigma_b$ are determined with an initial $E_r$, which excludes the $(\Gamma/q)$ and $q\Gamma$ terms, the entire procedure is repeated by starting with a more accurate $E_r$ using Eq. (2) and the extrapolated $E_{\text{max}}$ and $E_{\text{min}}$ as $\Omega \to 0$. A new $\rho$ for each $\Omega$ is introduced to evaluate $c_0$ and $c_1$ before a new set of $\Gamma$, $q$, and $\sigma_b$ are determined. The process is repeated until $E_r$, $\Gamma$, $q$, and $\sigma_b$ all converge numerically.

III. RESULTS AND DISCUSSIONS

Figure 3 compares the theoretical structure profiles to our calculated results starting from the simulated spectra shown in Fig. 1. The ratio $\Gamma/\Omega$ varies approximately from 0.007 to 0.035, $w_g$ and $w_l$ are kept unchanged for all $\Omega$. The agreement for $E_r$ is better than six digits and for $\Gamma$, $q$, and $\sigma_b$ better than three digits. To estimate the effect on $\Gamma$ and $q$ due to the uncertainty in $E_r$, we have performed a calculation by selecting an $E_r$ that is either above or below the theoretical $E_r$, by a $\Delta E = \Omega_{\text{max}}/2$, i.e., with an $E_{\text{est}} = E_r \pm 5$ meV (or, with a $\Delta E$ that is over 70 times greater than $\Gamma$). Figure 4 shows that the estimated $q$ parameter differs from the theoretical value only by about 5% whereas the effect on $\Gamma$ is greater and the difference could be as large as 12%. The effect on $\Gamma$ and $q$ is significantly reduced (to less than 1%), if $\Delta E$ is replaced by $\Omega_{\text{max}}/2$, i.e., with an $E_{\text{est}} = E_r \pm 1$ meV.

In practice, $w_g$ and $w_l$ may vary as $\Omega$ varies and $c_0$ and $c_1$ may not necessarily vary smoothly as a function of $\Omega^{-1}$. In particular, a linear extrapolation to $\Omega^{-1} = 0$ may not yield accurately the background cross section $\sigma_b$. To circumvent this difficulty, we rewrite Eq. (16) for $c_0$ as
versus $V^2$ background cross section value of $(s_s V_s)$ from a straight line as $\Gamma_1$. Gains with $E_r$ correct, approximately 50 times of the resonance width $\Gamma_1$, from the correct $E_r$. 

$$X = Y + R(q^2 - 1)\Gamma \left[ \sum_{n=1}^{\infty} \left( \frac{\mu_{n-1}}{\mu_0} \right) \left( \frac{\Gamma}{\Omega} \right)^{n-1} \right], \quad (18)$$

where $X = [(c_0/\sigma_b^{\text{est}}) - (4 \pi)^{1/2}](\Omega/\mu_0)$ and $Y = (R - 1)(4 \pi)^{1/2}(\Omega/\mu_0)$. In the limit of $\Gamma/\Omega \ll 1$, the sum in Eq. (18) is reduced to $1 + (\mu_1/\mu_0)/(\Gamma/\Omega)$. The ratio $\mu_1/\mu_0$ is approximately a constant (e.g., it varies less than 2.5% as $w_s$ increases from 0.5 to 1.0). If the estimated $\sigma_b^{\text{est}}$ is very close to its correct value $\sigma_b$, the contribution from $Y$ to $X$ approaches 0 and $X$, which decreases almost linearly as $\Omega^{-1}$ increases, approaches a value of $(q^2 - 1)\Gamma$ as $\Omega^{-1} \rightarrow 0$. On the other hand, as shown in Fig. 5, the contribution of $Y$ to $X$ is greatly amplified as $\Omega$ increases even if $\sigma_b^{\text{est}}$ is different only by as little as 1% from the correct $\sigma_b$, i.e., $X$ is expected to deviate substantially from a straight line as $\Omega^{-1} \rightarrow 0$. As a result, both $\sigma_b$ and $(q^2 - 1)\Gamma$ can be determined by a straight line from a $X$ versus $\Omega^{-1}$ plot. Once the values of $\sigma_b$ and $(q^2 - 1)\Gamma$ are determined, the product $q\Gamma$ can be estimated by plotting $Z$ against $\Omega^{-1}$ and then by extrapolating $Z$ to $\Omega^{-1} = 0$.

We have also applied the present procedure to a simulated spectra shown in Fig. 6 by introducing a random error up to 10% to the convoluted spectra for the $q=4$ resonance shown in Fig. 1. Again, both $\sigma_b$ and $(q^2 - 1)\Gamma$ are determined by the fitted straight lines from the $X$ and $Z$ versus $\Omega^{-1}$ plots shown in Fig. 7. The fitted $q$ and $\Gamma$ deviate from their corresponding input values by approximately 5% and 10%, respectively.

Finally, the present deconvolution procedure was applied to the simulated He ground-state photoionization spectra [generated from the result of a recent B-spline-based configuration interaction (BSCI) calculation [7,8]] for the $sp2n^-$ and $2pnd 1P$ resonances. The results for the $sp23^{-1}P$ resonance starting from spectra convoluted with $\Omega$ ranging from 1 to 8 meV is presented in Fig. 8. The resonance energy $E_r$ agrees with the theoretical value to better than six digits and $\Gamma$, $q$, and $\sigma_b$ to three digits or better. With a resonant width of about 0.1 meV and a best available experimental resolution of near 1 meV at a photon energy close to 60 eV [3], the He $sp23^{-1}P$ resonance represents perhaps the best candidate for a detailed experimental determination of the resonant parameters using the deconvolution procedure proposed in this paper.
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APPENDIX

Mathematically, Eq. (3) is integrable and is given by

$$\sigma^*(E; \Omega) = w_l \sigma^l(E; \Omega) + w_g \sigma^g(E; \Omega). \quad (A1)$$

The term that corresponds to the Lorentzian distribution can be evaluated by a simple change of variable and is given by

$$\sigma^l(E; \Omega) = \sigma_0 \left[ \left( \epsilon + q \right) \Gamma' / \Omega \right]^2 + \left( q^2 + 1 \right) \Gamma / \Omega + 1 \] / \left[ \left( \Gamma / \Omega \right) \epsilon \right]^2 + \left( 1 + \Gamma / \Omega \right)^2, \quad (A2)$$

where $\epsilon = (E - E_r) / (\Delta / 2)$. The second term that corresponds to the Gaussian distribution is far more complicated and can be expressed analytically by

$$\sigma^g(E; \Omega) = \sigma_0 \left[ 1 + \frac{\sqrt{\beta \pi e^{R(1-\epsilon)}}}{2} \Xi(\beta, \epsilon) \right], \quad (A3)$$

where $\beta = \ln(\Gamma / \Omega)^2$ and

$$\Xi(\beta, \epsilon) = (\epsilon^2 - 1) \Lambda(\beta, \epsilon) - 2q \Phi(\beta, \epsilon). \quad (A4)$$

$\Lambda$ and $\Phi$ are expressed in terms of a complex variable $\eta$, i.e.,

$$\Lambda(\beta, \epsilon) = \cos(2\beta\epsilon) \left[ 1 - \text{Re}(\eta) \right] + \sin(2\beta\epsilon) \text{Im}(\eta), \quad (A5)$$

and

$$\Phi(\beta, \epsilon) = \sin(2\beta\epsilon) \left[ 1 - \text{Re}(\eta) \right] - \cos(2\beta\epsilon) \text{Im}(\eta), \quad (A6)$$

where

$$\eta = \text{erf}(\gamma e^{i\theta}) \quad (A7)$$

with $\gamma = \sqrt{\beta(1+\epsilon^2)}$, $\theta = \tan^{-1} \epsilon$ and the error function erf($z$) given by

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2} dy. \quad (A8)$$

FIG. 7. Comparison between the theoretical spectra generated directly from Eq. (1) and the fitted results using the present deconvolution procedure starting from the simulated spectra shown in Fig. 7 and $X$ and $Z$ as functions of $\Omega^{-1}$ (mRy$^{-1}$) for resonance with $q = 4$.

FIG. 8. Comparison between the theoretical He ground-state photoionization spectrum near the $sp, 23^{-1}P$ resonance [8] and the fitted result using the present procedure. The photoelectron energy is expressed in terms of $\Delta$ by $E = 2.805 + \Delta \times 10^{-3}$ Ry.

where $\epsilon = (E - E_r) / (\Delta / 2)$. The second term that corresponds to the Gaussian distribution is far more complicated and can be expressed analytically by

$$\sigma^g(E; \Omega) = \sigma_0 \left[ 1 + \frac{\sqrt{\beta \pi e^{R(1-\epsilon)}}}{2} \Xi(\beta, \epsilon) \right], \quad (A3)$$

where $\beta = \ln(\Gamma / \Omega)^2$ and

$$\Xi(\beta, \epsilon) = (\epsilon^2 - 1) \Lambda(\beta, \epsilon) - 2q \Phi(\beta, \epsilon). \quad (A4)$$

$\Lambda$ and $\Phi$ are expressed in terms of a complex variable $\eta$, i.e.,

$$\Lambda(\beta, \epsilon) = \cos(2\beta\epsilon) \left[ 1 - \text{Re}(\eta) \right] + \sin(2\beta\epsilon) \text{Im}(\eta), \quad (A5)$$

and

$$\Phi(\beta, \epsilon) = \sin(2\beta\epsilon) \left[ 1 - \text{Re}(\eta) \right] - \cos(2\beta\epsilon) \text{Im}(\eta), \quad (A6)$$

where

$$\eta = \text{erf}(\gamma e^{i\theta}) \quad (A7)$$

with $\gamma = \sqrt{\beta(1+\epsilon^2)}$, $\theta = \tan^{-1} \epsilon$ and the error function erf($z$) given by

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