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 Γ, the asymmetry parameter q, and the background cross section σ_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 Γ and the experimental energy resolution Ω in the limit of $\Gamma/\Omega \ll 1$. [S1050-2947(98)04906-3]

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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 σ_b, i.e.,

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

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

$$E_{\max}=E_r+\tfrac{1}{2}(\Gamma/q) \quad \text{and} \quad E_{\min}=E_r-\tfrac{1}{2}(\Gamma q), \tag{2}$$

respectively. An accurate determination of q and Γ 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 Γ, 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 Ω [2,3], the widths Γ of some of the best known narrow resonances, e.g., the He $sp,2n^-$ and $2pnd\ ^1P$ (or, alternatively, the $2,1_n$ and $2,-1_n$) 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 Γ 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.,

$$\sigma^c(E;\Omega)=\int_{-\infty}^{+\infty}\sigma(E')\mathcal{F}(E'-E;\Omega)dE'. \tag{3}$$

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

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

The energy resolution Ω may be measured by the full width at half maximum (FWHM) of the distribution function and $\delta=\Omega/(2\sqrt{\ln 2})$. In general, the value of Ω in $\mathcal{G}$ and $\mathcal{L}$ may be different. However, for simplicity, the same value is assumed in this study. (Use of different Ω 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.,

$$\mathcal{F}(E;\Omega,w_g,w_l)=w_g\mathcal{G}(E;\Omega)+w_l\mathcal{L}(E;\Omega), \tag{5}$$

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 $\sigma^c(E;\Omega)$ with Ω 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 $\Gamma=5.0\times10^{-6}$ 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 Ω 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 Γ.

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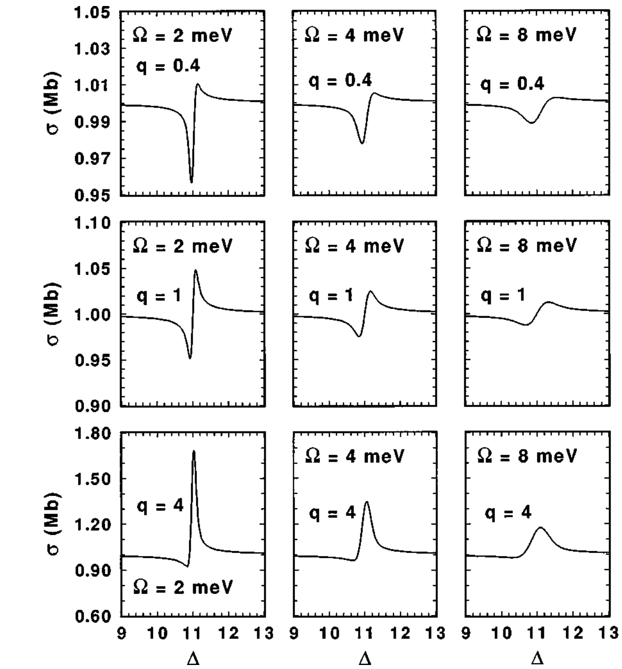

FIG. 1. Convoluted spectra $\sigma^c(E;\Omega)$ derived from Eq. (3) with energy resolutions Ω ranging from 2 to 8 meV. The spectra corresponding to infinite energy resolution, i.e., $\sigma(E)$ defined by Eq. (1), are generated by using a set of profile parameters $E_r = 2.1110$ Ry, $\sigma_b = 1.0$ Mb, and $\Gamma = 5.0\times10^{-6}$ Ry. The q parameter varies from 0.4 to 4. The photoelectron energy is expressed in terms of Δ by $k^2 = 2.10 + \Delta\times10^{-3}$ Ry. The monochromator function is defined by a set of weighting factors $w_g = 0.6$ and $w_l = 0.4$.

Alternative nonanalytical deconvolution precesses 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 Γ, q, σ_b, 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 Ω, i.e., when Γ is a few orders of magnitude smaller than Ω. Our proposed procedure starts with an initial estimate of E_r from a plot of the observed $E_{\max}$ or $E_{\min}$ against Ω shown on the left of Fig. 2. By neglecting the (Γ/q) term in Eq. (2) initially, we approximate E_r by the extrapolated value of $E_{\max}$ 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 Γq term and approximate E_r by $E_{\min}(\Omega=0)$. When $|q|$ is close to one, the initial E_r equals the average of $E_{\min}$ and $E_{\max}$ 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 $\sigma^c(E;\Omega)$ in terms of a set of *harmonic oscillator* eigenfunctions Ψ_n, i.e.,

$$\sigma^c(E;\Omega) = \sum_{n=0}^{\infty} c_n(\Omega)\Psi_n(\rho(E;\Omega,E_r)), \tag{6}$$

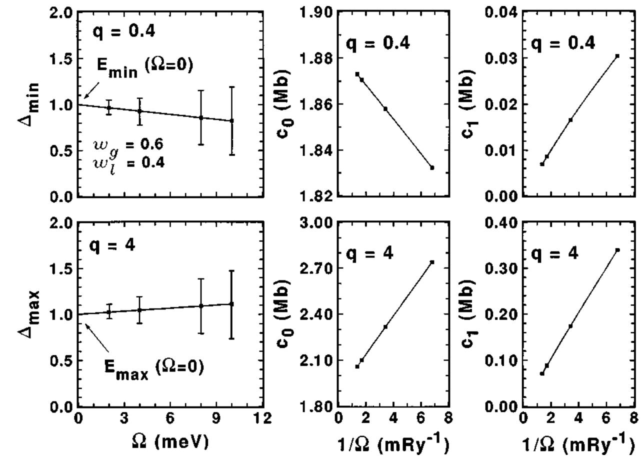

FIG. 2. The observed $E_{\max}$ and $E_{\min}$ in terms of Δ as functions of Ω (meV) and the expansion coefficients c_0 and c_1 as functions of Ω^{-1} (mRy^{-1}). The error bar represents the experimental Ω. The photoelectron energy is expressed in terms of Δ by $E = 2.110 + \Delta \times 10^{-3}$ Ry, $E_{\min}(\Omega=0) = 2.110\,9993$ Ry, and $E_{\max}(\Omega=0) = 2.111\,0005$ Ry. The weighting factors $w_g = 0.6$ and $w_l = 0.4$ remain unchanged for all Ω.

where $\rho = \sqrt{2\ln 2}(E - E_r)/(\frac{1}{2}\Omega)$ is a modified reduced energy and $\Psi_n(\rho)$ is a ρ-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 σ^c for each Ω by an integration

$$c_n = \int_{-\infty}^{+\infty} \sigma^c \Psi_n(\rho) d\rho. \tag{7}$$

It turns out that only the first two coefficients c_0 and c_1 at *a few* Ω are required to determine the values of Γ, q, and σ_b.

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

$$I_{g,n} = \frac{1}{(4\pi)^{1/4}\sqrt{2^n n!}} \int_{-\infty}^{+\infty} \frac{[\rho + q\sqrt{2\ln 2}(\Gamma/\Omega)]^2}{\rho^2 + 2\ln 2(\Gamma/\Omega)^2} e^{-(1/4)\rho^2} \rho^n d\rho \tag{8}$$

and

$$I_{l,n} = \int_{-\infty}^{+\infty} \frac{[\rho + q\sqrt{2\ln 2}(\Gamma/\Omega)]^2 + 2\ln 2[(q^2+1)\Gamma/\Omega + 1]}{\rho^2 + 2\ln 2(1 + \Gamma/\Omega)^2} \times \Psi_n(\rho) d\rho. \tag{9}$$

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

$$\int_{-\infty}^{+\infty} \frac{e^{-s^2x^2}}{x^2 + t^2} dx = \frac{\pi}{t} F_c(ts) e^{t^2 s^2}, \tag{10}$$

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

$$\frac{c_0}{\sigma_b}=(4\pi)^{1/4}+\mu(q^2-1)\left(\frac{\Gamma}{\Omega}\right) \quad \text{and} \quad \frac{c_1}{\sigma_b}=2\nu q\left(\frac{\Gamma}{\Omega}\right). \tag{11}$$

The coefficients μ and ν are given by $\mu=(f_0^{(g)}w_g+f_0^{(l)}w_l)$ and $\nu=(f_1^{(g)}w_g+f_1^{(l)}w_l)$, where

$$f_0^{(g)}=\pi^{3/4}\sqrt{\ln 2}F_c(u)e^{u^2}, \quad f_0^{(l)}=\sqrt{2\ln 2}\,\pi^{3/4}F_c(v)e^{v^2}, \tag{12}$$

$$f_1^{(g)}=(4\pi)^{1/4}\left[\sqrt{\ln 2}-\ln 2\sqrt{\frac{\pi}{2}}F_c(u)e^{u^2}\left(\frac{\Gamma}{\Omega}\right)\right], \tag{13}$$

and

$$f_1^{(l)}=(4\pi)^{1/4}2\left[\sqrt{\ln 2}-\ln 2\sqrt{\pi}F_c(v)e^{v^2}\left(1+\frac{\Gamma}{\Omega}\right)\right]. \tag{14}$$

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

$$\mu=\sum_{n=0}^{\infty}\mu_n\left(\frac{\Gamma}{\Omega}\right)^n \quad \text{and} \quad \nu=\sum_{n=0}^{\infty}\nu_n\left(\frac{\Gamma}{\Omega}\right)^n, \tag{15}$$

where μ_n and ν_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 Γ/Ω when $\Gamma\ll\Omega$. Since Γ is a constant yet to be determined, the c_0 and c_1 obtained from the *observed* spectra can be expanded in Ω^{-1} as

$$c_0=\sum_{n=0}^{\infty}\alpha_n\left(\frac{1}{\Omega}\right)^n \quad \text{and} \quad c_1=\sum_{n=1}^{\infty}\beta_n\left(\frac{1}{\Omega}\right)^n. \tag{16}$$

A comparison between Eq. (16) and the analytical expressions Eqs. (11) and (15) shows that only three numerically fitted coefficients α_0, α_1, and β_1 are required to determine the values of Γ, q, and σ_b. Specifically, when $\Gamma/\Omega\ll 1$,

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

and

$$\beta_1=2\nu_0 q\sigma_b\Gamma, \tag{17}$$

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 Ω varies, Γ, q, and σ_b can be determined directly from α_0, α_1, and β_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 Ω^{-1} (see, e.g., Fig. 2). σ_b is determined by extrapolating c_0 to $\Omega^{-1}=0$. Γ and q are calculated from the products $(q^2-1)\Gamma$ and $q\Gamma$ in terms of α_1 and β_1. After Γ, q, and σ_b are determined with an initial E_r, which excludes the (Γ/q) and $q\Gamma$ terms, the entire procedure is repeated by starting with a more accurate E_r using Eq. (2) and the extrapolated $E_{\max}$ and $E_{\min}$ as $\Omega\to 0$. A new ρ for each Ω is introduced to evaluate c_0 and c_1 before a new set of Γ, q, and σ_b are determined. The process is repeated until E_r, Γ, q, and σ_b all converge numerically.

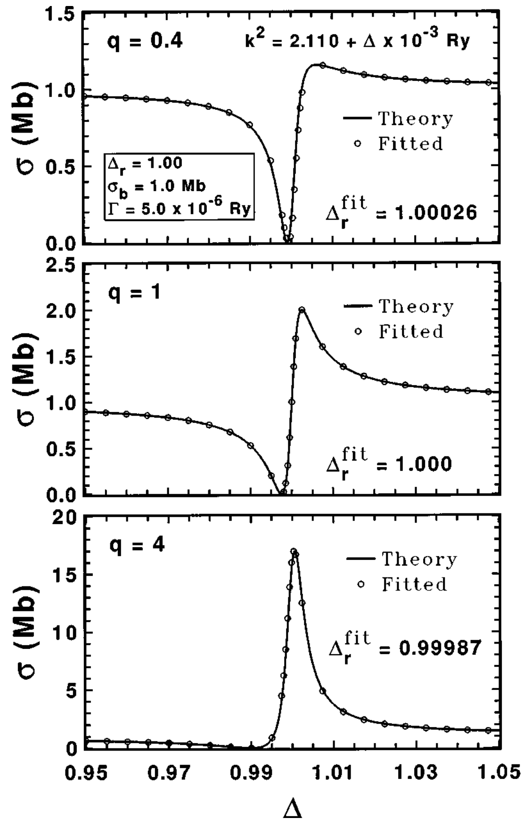

FIG. 3. Comparison between the theoretical spectra generated directly from Eq. (1) and the fitted results using the present deconvolution procedure starting from the simulated spectra shown in Fig. 1.

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 Γ/Ω varies approximately from 0.007 to 0.035. w_g and w_l are kept unchanged for all Ω. The agreement for E_r is better than six digits and for Γ, q, and σ_b better than three digits. To estimate the effect on Γ 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 $\Delta E=\Omega_{\max}/2$, i.e., with an $E_{\rm est}\simeq E_r\pm 5$ meV (or, with a ΔE that is over 70 times greater than Γ). Figure 4 shows that the estimated q parameter differs from the theoretical value only by about 5% whereas the effect on Γ is greater and the difference could be as large as 12%. The effect on Γ and q is significantly reduced (to less than 1%), if ΔE is replaced by $\Omega_{\min}/2$, i.e., with an $E_{\rm est}\simeq E_r\pm 1$meV.

In practice, w_g and w_l may vary as Ω varies and c_0 and c_1 may not necessarily vary smoothly as a function of Ω^{-1}. In particular, a linear extrapolation to $\Omega^{-1}=0$ may not yield accurately the backgraound cross section σ_b. To circumvent this difficulty, we rewrite Eq. (16) for c_0 as

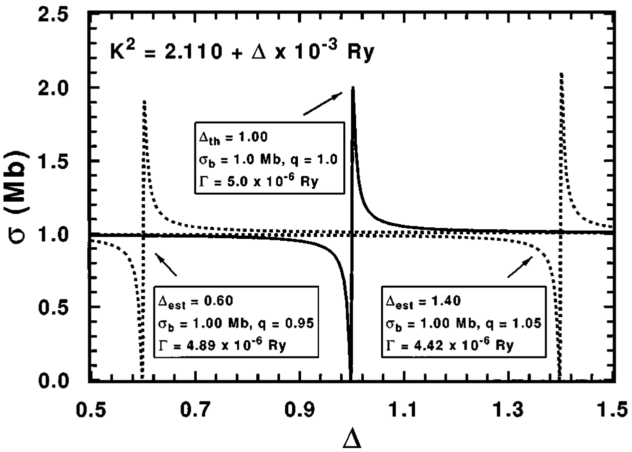

FIG. 4. Comparison between the theoretical spectra (center) and the fitted spectra using an estimated E_r, which is displaced by an ΔE, approximately 50 times of the resonance width Γ, from the correct E_r.

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

where $X=[(c_0/\sigma_b^{\rm est})-(4\pi)^{1/4}](\Omega/\mu_0)$ and $Y=(R-1)(4\pi)^{1/4}(\Omega/\mu_0)$ are expressed in terms of an estimated background cross section $\sigma_b^{\rm est}$ and a ratio $R=\sigma_b/\sigma_b^{\rm est}$. 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 μ_1/μ_0 is approximately a constant (e.g., it varies less than 2.5% as w_g increases from 0.5 to 1.0). If the estimated $\sigma_b^{\rm est}$ is very close to its correct value σ_b, the contribution from Y to X approaches 0 and X, which decreases almost linearly as Ω^{-1} increases, approaches a value of $(q^2-1)\Gamma$ as $\Omega^{-1}\to 0$. On the other hand, as shown in Fig. 5, the contribution of Y to X is greatly amplified as Ω increases even if $\sigma_b^{\rm est}$ is different only by as little as 1% from the correct σ_b, i.e., X is expected to deviate substantially from a straight line as $\Omega^{-1}\to 0$. As a result, both σ_b and $(q^2-1)\Gamma$ can be determined by a straight line from a X versus Ω^{-1} plot. Once the values of σ_b and $(q^2-1)\Gamma$ are determined, the product $q\Gamma$ can be estimated by plotting $Z=c_1\Omega/(2\sigma_b\nu_0)$ against Ω^{-1} and then by extrapolating Z to $\Omega^{-1}=0$.

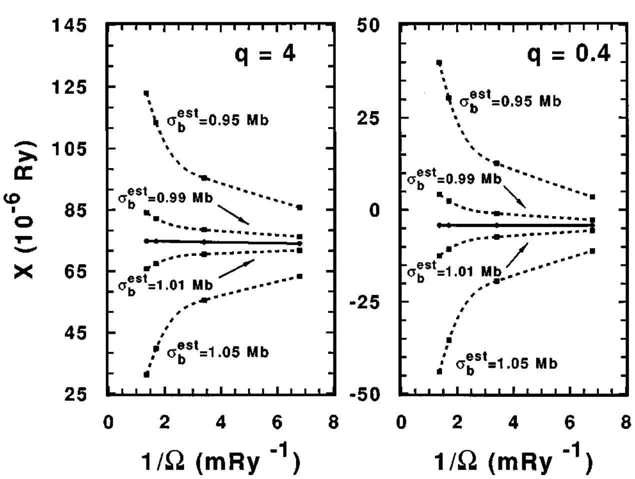

FIG. 5. $X(10^{-6}$ Ry) as a function of Ω^{-1} (mRy^{-1}) for resonances with $q=0.4$ and 4. The solid straight line corresponds to $\sigma_b^{\rm est}=\sigma_b$.

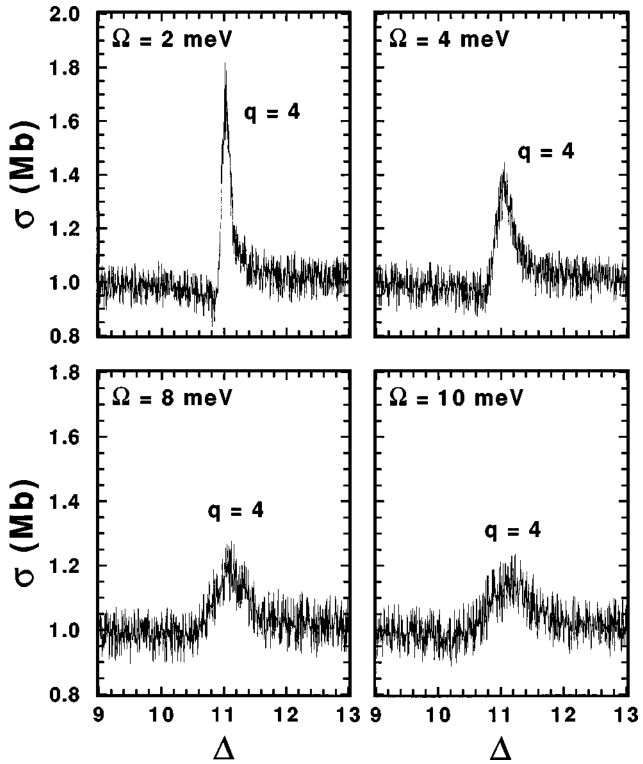

FIG. 6. Convoluted spectra $\sigma^c(E;\Omega)$ derived from Eq. (3) with energy resolutions Ω ranging from 2 to 10 meV. A random error up to 10% is introduced to simulate the experimental uncertainty. Similar to the spectra given in Fig. 1, the spectra corresponding to infinite energy resolution, i.e., $\sigma(E)$ defined by Eq. (1), are generated by using a set of profile parameters $E_r=2.1110$ Ry, $\sigma_b=1.0$ Mb, $q=4$, and $\Gamma=5.0\times10^{-6}$ Ry. The photoelectron energy is expressed in terms of Δ by $k^2=2.10+\Delta\times10^{-3}$ Ry.

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 σ_b and $(q^2-1)\Gamma$ are determined by the fitted straight lines from the X and Z versus Ω^{-1} plots shown in Fig. 7. The fitted q and Γ 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 $sp,2n^-$ and $2pnd\ ^1P$ resonances. The results for the $sp,23^-\ ^1P$ resonance starting from spectra convoluted with Ω 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 Γ, q, and σ_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 $sp,23^{-\ 1}P$ resonance represents perhaps the best candidate for a detailed experimental determination of the resonant parameters using the deconvolution procedure proposed in this paper.

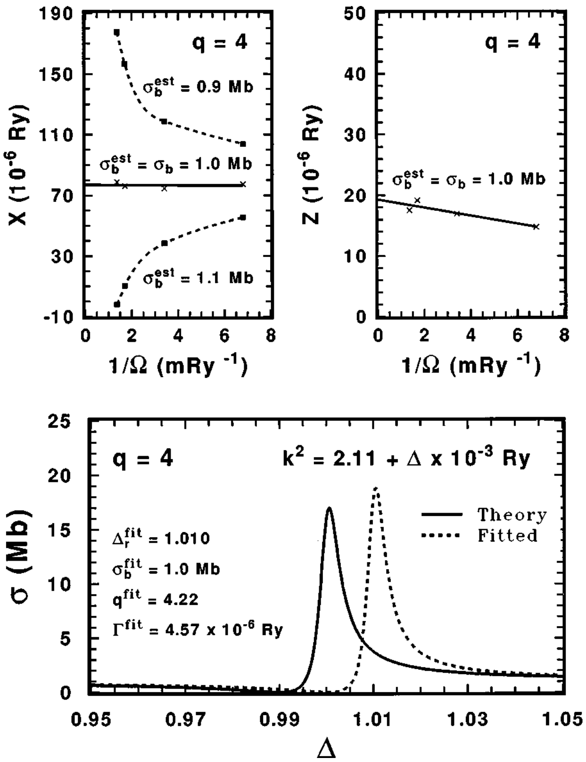

FIG. 7. Comparison between the theoretical spectra generated directly from Eq. (1) and the fitted results using the present deconvolution procedure starting from the simulated spectra shown in Fig. 7 and X and Z as functions of Ω^{-1} (mRy^{-1}) for resonance with $q=4$.

ACKNOWLEDGMENT

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APPENDIX

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

$$\sigma^c(E;\Omega)=w_l\sigma_l^c(E;\Omega)+w_g\sigma_g^c(E;\Omega). \qquad \text{(A1)}$$

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

$$\sigma_l^c(E;\Omega)=\sigma_b\frac{[(\epsilon+q)\Gamma/\Omega]^2+(q^2+1)\Gamma/\Omega+1}{[(\Gamma/\Omega)\epsilon]^2+(1+\Gamma/\Omega)^2}, \qquad \text{(A2)}$$

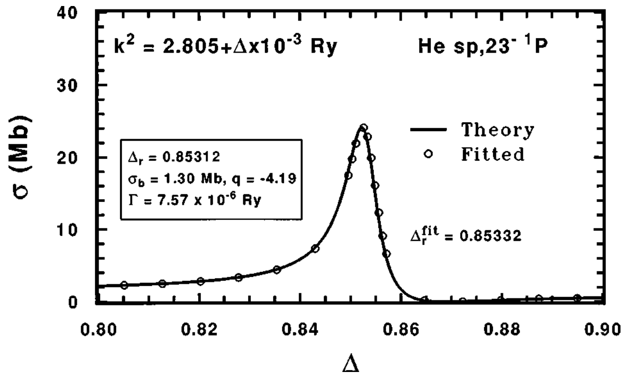

FIG. 8. Comparison between the theoretical He ground-state photoionization spectrum near the $sp,23^{-}\ ^1P$ resonance [8] and the fitted result using the present procedure. The photoelectron energy is expressed in terms of Δ by $E=2.805+\Delta\times10^{-3}$ Ry.

where $\epsilon=(E-E_r)/(\frac{1}{2}\Gamma)$. The second term that corresponds to the Gaussian distribution is far more complicated and can be expressed analytically by

$$\sigma_g^c(E;\Omega)=\sigma_b[1+\sqrt{\beta\pi}e^{\beta(1-\epsilon^2)}\Xi(\beta,\epsilon)], \qquad \text{(A3)}$$

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

$$\Xi(\beta,\epsilon)=(q^2-1)\Lambda(\beta,\epsilon)-2q\Phi(\beta,\epsilon). \qquad \text{(A4)}$$

Λ and Φ are expressed in terms of a complex variable η, i.e.,

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

and

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

where

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

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

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

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