Excited states as resonances in the photon-atom continuum and the natural-line-shape problem

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A variational Hamiltonian method for quantum field theory is applied to the problem of natural line shape. Within scalar quantum electrodynamics, coupled variational equations are derived for the scattering of photons from a scalar (pionic) atom. It is shown that the coupled equations have a continuous spectrum for all energies above the atomic ground state. Excited states of the atom appear as resonances in particular partial-wave cross sections. The line center and shape are derived from the behavior of the photon-atom scattering phase shifts.

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I. INTRODUCTION

In the elementary treatment of atomic bound states, the energy levels of isolated atoms are obtained as discrete eigenvalues of the Schrödinger equation. However, an atom does not have a true discrete spectrum of bound-state energy levels, since an excited state will naturally decay via photon emission. This means that an excited atom such as hydrogen should not be viewed as an isolated two-body problem (nucleus plus electron with a static potential interaction). Rather, the explicit presence of the radiation field (photons) must be taken into account. Excited states, then, do not correspond to infinitely sharp energy eigenvalues, and so the spectral lines of the emitted or absorbed radiation that arise in the excitation or decay process are themselves not infinitely sharp, but have a broadening referred to as the natural line shape.

The first correct calculation of the shape of atomic lines was made by Weisskopf and Wigner [1] in 1930, using an approximation to the two-state emitter model. In the lowest approximation, any line shape turns out to be symmetric, but the effects of higher-order and nonresonant terms distort the symmetry. An extensive study of the line-shape problem was made by Arnous and coworkers [2] around 1950. They mainly focused on the radiative corrections of the resonant term to the line center and shape, and the effects of nonresonant terms were not considered. To study the distorting effects on the line shape of a closely lying level near the upper level of a transition pair, Morozov and Shorygin [3] and Bali and Higgins [4] have respectively developed different approaches to the multistate emitter problem. From the viewpoint of photon-atom scattering, Low [5] has presented a completely different approach to the natural-line-shape problem by using Feynman diagrams. This so-called S-matrix approach provides more physical insight and understanding of the higher-order corrections. However, it is not easy in this approach to incorporate the background effects of nonresonant terms to the line shape.

In this paper, we present another approach for the treatment of the natural-line-shape problem: an excited state is viewed as a resonance in the photon-atom continuum. This idea itself is not new. The connection between the lifetime of (compound) excited states that decay by particle emission and the resonating behavior of appropriate particle-bound system scattering phase shifts is discussed in detail by Goldberger and Watson [6]. What we do obtain is the fact that the photon-atom scattering equations are derived directly from quantum electrodynamics (QED). To illustrate the method, we consider a hydrogenlike atom consisting of two scalar particles coupled to a photon field. We use the Hamiltonian formalism of scalar QED (SQED) and apply the variational method to derive the coupled wave equations for the relevant channels. Within this method wave equations were derived recently for positronium [7,8], scalar positronium [9], and photon-photon scattering [10,11]. It is the latter work in which the positronium states appear as resonances in the γ-γ scattering channel that motivated the present study. In the γ-γ scattering calculation it was shown how the positronium wave equation derived from QED, which initially represents a discrete eigenvalue problem below the continuum threshold, becomes modified due to the coupling to the photon-photon sector. This coupling turns the bound-state equation into an inhomogeneous problem with solutions at all energies. Similarly, in the present work we show how the coupling of the atomic wave equation to the one-photon sector modifies the Schrödinger equation in such a way that the excited states become simply resonances in the photon-atom scattering channel.

The scattering of atoms by light and the role played by virtually populated excited states have been investigated long ago by Kramers and Heisenberg [12]. For our problem of elastic scattering of a photon by an atom there are two lowest-order Feynman diagrams of equal importance (cf. Fig. 1). In the equal-time Hamiltonian approach that

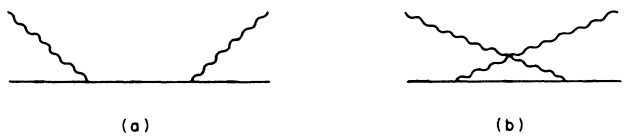

FIG. 1. Lowest-order Feynman diagrams for elastic resonant photon-atom scattering.

we use, one obtains process (1a) through an ansatz that couples the one-photon sector with the atomic bound state. Incorporation of process (1b) requires an expanded Fock-space ansatz, which includes two photons coupled to the atom.

In order to keep the presentation as simple as possible we derive first the equations for process (1a) in Sec. II. Two coupled integral equations are obtained using a variational ansatz, which includes Fock-space states for a pair of two scalars (spinless hydrogen) and two scalars plus a photon. In Sec. III we show how to obtain an approximate solution of these equations and the cross section for photon-atom scattering. In Sec. IV the expanded Fock-space results are presented. Numerical calculations of the scattering partial-wave cross sections are presented in Sec. V. These results show that resonances in partial-wave cross sections correspond to atomic unstable excited states, and that the lines are symmetric in the first approximation. Effects of nonresonant terms can be incorporated naturally in our approach. Concluding remarks are given in Sec. VI.

II. VARIATIONAL EQUATIONS FOR TWO SCALARS AND ONE PHOTON

In order to treat the particles and the radiation field (photons) on an equal footing, we resort to a quantum-field-theoretic description. The use of quantum field theory to describe relativistic bound (and continuum) states has been described by many authors. The work of Blankenbecler and Sugar [13], Sucher and co-workers [14,15], and Fulton [16] can be cited as representative examples of such an approach.

In the present work we use a variational method within the Hamiltonian formalism of SQED to derive wave equations for the amplitudes of the included Fock-space states. This formalism has the advantage that it is straightforward (though sometimes tedious) to apply, and is very close to ordinary Schrödinger quantum mechanics, which it contains as a nonrelativistic limit. The Hamiltonian is constructed by the canonical prescription from a covariant Lagrangian. In radiation gauge, the Hamiltonian for the system of photons and distinct scalars of masses m and M and charges e_1 and e_2 takes the form ($\hbar=c=1$)

$$H=\int d^3x[\mathcal{H}_\phi(x)+\mathcal{H}_\psi(x)+\lambda_c'\phi^*\phi\psi^*\psi+\mathcal{H}_\gamma(x)+\mathcal{H}_C(x)] , \tag{2.1}$$

where λ_c' is the coupling constant for the direct interaction between scalars. The various parts of this Hamiltonian are, explicitly,

$$\mathcal{H}_\phi(x)=\pi_\phi\pi_{\phi^*}+\left[\nabla-ie_1\mathbf{A}\right]\phi^*\cdot\left[\nabla+ie_1\mathbf{A}\right]\phi+m^2\phi^*\phi ,$$

$$\mathcal{H}_\gamma(x)=\tfrac{1}{2}[\dot{\mathbf{A}}^2+(\nabla\times\mathbf{A})^2] ,$$

$$\mathcal{H}_C(x)=\frac{1}{8\pi}\int d^3y\frac{\rho(x)\rho(y)}{|\mathbf{x}-\mathbf{y}|} ,$$

with

$$\rho(x)=ie_1(\phi^*\pi_{\phi^*}-\phi\pi_\phi)+ie_2(\psi^*\pi_{\psi^*}-\psi\pi_\psi) ,$$

and $\mathcal{H}_\psi(x)$ takes the same form as $\mathcal{H}_\phi(x)$, but with e_1 and m replaced by e_2 and M. In the above π_ϕ and π_{ϕ^*} are the conjugate momenta of ϕ and ϕ^*, respectively.

We make the usual Fourier expansion of the field operators at equal time $t=0$ [17]. For the scalar fields we have

$$\phi(\mathbf{x})=\int d^3q\left[(2\pi)^3 2\omega(\mathbf{q})\right]^{-1/2}\times\left[A_m(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}+B_m^\dagger(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{x}}\right] , \tag{2.2a}$$

$$\phi^*(\mathbf{x})=\int d^3q\left[(2\pi)^3 2\omega(\mathbf{q})\right]^{-1/2}\times\left[A_m^\dagger(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{x}}+B_m(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}\right] , \tag{2.2b}$$

$$\pi_\phi(\mathbf{x})=i\int d^3q\left[\frac{\omega(\mathbf{q})}{2(2\pi)^3}\right]^{1/2}\times\left[A_m^\dagger(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{x}}-B_m(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}\right] , \tag{2.2c}$$

$$\pi_{\phi^*}(\mathbf{x})=-i\int d^3q\left[\frac{\omega(\mathbf{q})}{2(2\pi)^3}\right]^{1/2}\times\left[A_m(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}-B_m^\dagger(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{x}}\right] , \tag{2.2d}$$

where $\omega(\mathbf{p})=(\mathbf{p}^2+m^2)^{1/2}$. Similar expressions hold for $\psi(\mathbf{x})$, $\pi_\psi(\mathbf{x})$, etc., but with m and $\omega(\mathbf{p})$ replaced by M and $\Omega(\mathbf{p})=(\mathbf{p}^2+M^2)^{1/2}$. For the electromagnetic field we have

$$\mathbf{A}(\mathbf{x})=\sum_{\lambda=1}^{2}\int d^3k\,\boldsymbol{\epsilon}_\lambda(\mathbf{k})\left[(2\pi)^3 2|\mathbf{k}|\right]^{-1/2}\times\left[a_\lambda(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}+a_\lambda^\dagger(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\right] , \tag{2.3a}$$

$$\dot{\mathbf{A}}(\mathbf{x})=-i\sum_{\lambda=1}^{2}\int d^3k\,\boldsymbol{\epsilon}_\lambda(\mathbf{k})\left[\frac{|\mathbf{k}|}{2(2\pi)^3}\right]^{1/2}\times\left[a_\lambda(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}-a_\lambda^\dagger(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\right] , \tag{2.3b}$$

where the transverse polarization vectors $\boldsymbol{\epsilon}_\lambda(\mathbf{k})$ satisfy $\boldsymbol{\epsilon}_\lambda(\mathbf{k})\cdot\mathbf{k}=0$. The momentum-space operators A, B, a_λ, etc., obey the usual commutation relations. The nonvanishing ones are

$$\left[A(\mathbf{p}),A^\dagger(\mathbf{q})\right]=\left[B(\mathbf{p}),B^\dagger(\mathbf{q})\right]=\delta^3(\mathbf{p}-\mathbf{q}) , \tag{2.4}$$

$$\left[a_\lambda(\mathbf{k}),a_{\lambda'}^\dagger(\mathbf{k}')\right]=\delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'} , \tag{2.5}$$

while all the other commutators vanish. We are not interested in the vacuum energy problem and so we use the normal-ordered Hamiltonian after expressing it in terms of momentum-space operators A, B, a_λ, etc. The operators $A^\dagger(\mathbf{p})$ and $A(\mathbf{p})$ [$B^\dagger(\mathbf{p})$ and $B(\mathbf{p})$] are identified with creation and annihilation operators of positively (negatively) charged free scalars of momentum $\mathbf{p}$, and $a_\lambda^\dagger(\mathbf{k})$ and $a_\lambda(\mathbf{k})$ with those of transverse photons of momentum $\mathbf{k}$ and linear polarization index λ.

To take account of the processes shown schematically in Fig. 1(a) the variational ansatz is chosen as

$$|\Psi\rangle = \int d^3p F(\mathbf{p}) B_m^\dagger(-\mathbf{p}) A_M^\dagger(\mathbf{p})|0\rangle + \sum_{\lambda=1}^{2} \int d^3q\, d^3p\, G(\mathbf{q},\mathbf{p}\lambda) B_m^\dagger(\mathbf{p}_2) A_M^\dagger(\mathbf{p}_1) a_\lambda^\dagger(\mathbf{p})|0\rangle , \tag{2.6}$$

with $\mathbf{p}_1=\mathbf{q}-\mathbf{p}M/(m+M)$ and $\mathbf{p}_2=-\mathbf{q}-\mathbf{p}m/(m+M)$. Here $|0\rangle$ stands for the trial vacuum state, which has the defining property $a_\lambda(\mathbf{p})|0\rangle=0$ and similarly for the A and B annihilation operators. The functions F and G are two variational coefficients to be determined from the variational principle

$$\delta\langle\Psi|:H:-E|\Psi\rangle=0 , \tag{2.7}$$

where $:H:$ stands for the normal-ordered Hamiltonian operator. F and G are identified with the momentum-space wave functions that describe the channel of two scalars of opposite charges and the channel of two scalars plus one photon, respectively.

Taking the functional derivatives with respect to F and G in Eq. (2.7), we obtain the following two coupled integral equations:

$$\begin{aligned}\left[\omega(\mathbf{p})+\Omega(\mathbf{p})-E\right]F(\mathbf{p}) &= \frac{e_1e_2}{(2\pi)^3}\int d^3p' \frac{F(\mathbf{p}')}{|\mathbf{p}'-\mathbf{p}|^2}K(\mathbf{p},\mathbf{p}') \\ &\quad -\frac{e_1}{(4\pi)^{3/2}}\sum_{\lambda=1}^{2}\int d^3p' G\left(\mathbf{p}+\frac{M}{m+M}\mathbf{p}',\mathbf{p}'\lambda\right)\frac{2\mathbf{p}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p}')}{[\omega(\mathbf{p})\omega(\mathbf{p}+\mathbf{p}')|\mathbf{p}'|]^{1/2}} \\ &\quad -\frac{e_2}{(4\pi)^{3/2}}\sum_{\lambda=1}^{2}\int d^3p' G\left(\mathbf{p}-\frac{m}{m+M}\mathbf{p}',\mathbf{p}'\lambda\right)\frac{2\mathbf{p}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p}')}{[\Omega(\mathbf{p})\Omega(\mathbf{p}-\mathbf{p}')|\mathbf{p}'|]^{1/2}}\end{aligned} \tag{2.8}$$

with

$$K(\mathbf{p},\mathbf{p}')=\frac{[\omega(\mathbf{p})+\omega(\mathbf{p}')][\Omega(\mathbf{p})+\Omega(\mathbf{p}')]-\lambda_c'(\mathbf{p}'-\mathbf{p})^2/e_1e_2}{4[\omega(\mathbf{p})\omega(\mathbf{p}')\Omega(\mathbf{p})\Omega(\mathbf{p}')]^{1/2}} ,$$

and

$$\begin{aligned}&[\omega(\mathbf{q}+\mathbf{p}_m)+\Omega(\mathbf{q}-\mathbf{p}_M)+|\mathbf{p}|-E]G(\mathbf{q},\mathbf{p}\lambda) \\ &= \frac{e_1e_2}{(2\pi)^3}\int d^3q' \frac{G(\mathbf{q}',\mathbf{p}\lambda)}{|\mathbf{q}-\mathbf{q}'|^2}\frac{[\omega(\mathbf{q}+\mathbf{p}_m)+\omega(\mathbf{q}'+\mathbf{p}_M)][\Omega(\mathbf{q}-\mathbf{p}_M)+\Omega(\mathbf{q}'-\mathbf{p}_M)]-\lambda_c'(\mathbf{q}-\mathbf{q}')^2/e_1e_2}{4[\omega(\mathbf{q}+\mathbf{p}_m)\omega(\mathbf{q}'+\mathbf{p}_m)\Omega(\mathbf{q}-\mathbf{p}_M)\Omega(\mathbf{q}'-\mathbf{p}_M)]^{1/2}} \\ &\quad -\frac{e_1}{(4\pi)^{3/2}}F(\mathbf{q}-\mathbf{p}_M)\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p})}{[\omega(\mathbf{q}-\mathbf{p}_M)\omega(\mathbf{q}+\mathbf{p}_m)|\mathbf{p}|]^{1/2}} -\frac{e_2}{(4\pi)^{3/2}}F(\mathbf{q}+\mathbf{p}_m)\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p})}{[\Omega(\mathbf{q}+\mathbf{p}_m)\Omega(\mathbf{q}-\mathbf{p}_M)|\mathbf{p}|]^{1/2}} \\ &\quad -\frac{e_1^2}{(2\pi)^3}\sum_{\lambda'=1}^{2}\int d^3p'd^3q'\delta^3\left(\mathbf{q}'-\mathbf{q}+\frac{M}{m+M}(\mathbf{p}-\mathbf{p}')\right)\frac{G(\mathbf{q}',\mathbf{p}'\lambda')\boldsymbol{\epsilon}_\lambda(\mathbf{p})\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p}')}{\left[4\omega(\mathbf{q}+\mathbf{p}_m)\omega\left(\mathbf{q}'+\frac{m}{m+M}\mathbf{p}'\right)|\mathbf{p}|\,|\mathbf{p}'|\right]^{1/2}} \\ &\quad -\frac{e_2^2}{(2\pi)^3}\sum_{\lambda'=1}^{2}\int d^3p'd^3q'\delta^3\left(\mathbf{q}'-\mathbf{q}-\frac{m}{m+M}(\mathbf{p}-\mathbf{p}')\right)\frac{G(\mathbf{q}',\mathbf{p}'\lambda')\boldsymbol{\epsilon}_\lambda(\mathbf{p})\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p}')}{\left[4\Omega(\mathbf{q}-\mathbf{p}_M)\Omega\left(\mathbf{q}'-\frac{M}{m+M}\mathbf{p}'\right)|\mathbf{p}|\,|\mathbf{p}'|\right]^{1/2}} ,\end{aligned} \tag{2.9}$$

where $\mathbf{p}_m=[m/(m+M)]\mathbf{p}$ and $\mathbf{p}_M=[M/(m+M)]\mathbf{p}$. These two equations determine the momentum-space wave functions describing the two-scalar and two-scalar plus one-photon channels, and the coupling between them. Equation (2.8) with G set equal to zero describes the two-scalar bound state as an eigenvalue problem. With $G\neq0$ this equation, together with (2.9), turns into a nonhomogeneous problem with solutions at any energy E. Near the eigenvalues of the $G=0$ equation, the nonhomogeneous wave equation resonates, i.e., $F(\mathbf{p})$ acquires a very large amplitude. Equation (2.9) describes, similarly, a $(Mm\gamma)$ state. It contains on the left-hand side the free energies of these particles and on the right-hand side their interactions and coupling to the (mM) channel.

As it stands Eq. (2.9) is difficult to solve. In order to make the problem tractable a simpler version is derived in the next section, in which the (Mm) degrees of freedom are factored away and a simple photon scattering equation emerges. This equation, when solved together with (2.8), describes how the photon scatters from the atom with the temporary formation of an excited $(Mm)^*$ state. We study these solutions for the limiting case where the mass of the scalar particle with positive charge tends to infinity.

III. APPROXIMATE SCATTERING SOLUTIONS

In the limit where the mass of the positively charged scalar tends to infinity, i.e., $M \to \infty$, Eq. (2.8) reduces to

$$[\omega(\mathbf{p})-E']F(\mathbf{p})=\frac{e_1e_2}{(2\pi)^3}\int d^3p'\frac{F(\mathbf{p}')}{|\mathbf{p}-\mathbf{p}'|^2}\frac{\omega(\mathbf{p})+\omega(\mathbf{p}')}{2[\omega(\mathbf{p})\omega(\mathbf{p}')]^{1/2}} - \frac{e_1}{(4\pi)^{3/2}}\sum_{\lambda=1}^{2}\int d^3p'G(\mathbf{p}+\mathbf{p}',\mathbf{p}'\lambda)\frac{2\mathbf{p}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p}')}{[\omega(\mathbf{p})\omega(\mathbf{p}+\mathbf{p}')|\mathbf{p}'|]^{1/2}}\ , \tag{3.1}$$

where $E'=E-M$. Similarly Eq. (2.9) reduces to

$$[\omega(\mathbf{q})+|\mathbf{p}|-E']G(\mathbf{q},\mathbf{p}\lambda)=-\frac{e_1}{(4\pi)^{3/2}}F(\mathbf{q}-\mathbf{p})\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p})}{[\omega(\mathbf{q}-\mathbf{p})\omega(\mathbf{q})|\mathbf{p}|]^{1/2}}+\frac{e_1e_2}{(2\pi)^3}\int d^3q'G(\mathbf{q}',\mathbf{p}\lambda)\frac{1}{|\mathbf{q}-\mathbf{q}'|^2}\frac{\omega(\mathbf{q})+\omega(\mathbf{q}')}{2[\omega(\mathbf{q})\omega(\mathbf{q}')]^{1/2}} - \frac{e_1^2}{(2\pi)^3}\sum_{\lambda'=1}^{2}\int d^3p'd^3q'\delta^3(\mathbf{q}'-\mathbf{q}+\mathbf{p}-\mathbf{p}')\frac{G(\mathbf{q}',\mathbf{p}'\lambda')\boldsymbol{\epsilon}_\lambda(\mathbf{p})\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p}')}{[4\omega(\mathbf{q})\omega(\mathbf{q}')|\mathbf{p}||\mathbf{p}'|]^{1/2}}\ . \tag{3.2}$$

Now suppose that the function G can be separated into two factors: one describing the two-scalar atom, which is in a stable state, say ground state, and the other part describing one photon. That is, we factorize G as

$$G(\mathbf{q},\mathbf{p}\lambda)=F_0(\mathbf{q})g_\lambda(\mathbf{p})\ , \tag{3.3}$$

and perform a restricted variation on $g_\lambda(\mathbf{p})$ only. In Eq. (3.3) $F_0(\mathbf{q})$ is the wave function describing the ground state of the atom. In practice we represent $F_0(\mathbf{q})$ by the following analytic form:

$$F_0(\mathbf{q})=\frac{2(2\gamma^5)^{1/2}}{\pi}\frac{1}{(\mathbf{q}^2+\gamma^2)^2}\ , \tag{3.4}$$

where $\gamma=mZ\alpha$, $\alpha=e_1^2/4\pi$, and Z represents the atomic number. With unrestricted γ this function has been used as a variational approximation to the lowest eigenstate of the bound-state equation [9]:

$$[\omega(\mathbf{q})-E_0']F_0(\mathbf{q})=\frac{e_1e_2}{(2\pi)^3}\int d^3p'\frac{F_0(\mathbf{p}')}{|\mathbf{p}'-\mathbf{q}|^2}\frac{\omega(\mathbf{q})+\omega(\mathbf{p}')}{2[\omega(\mathbf{q})\omega(\mathbf{p}')]^{1/2}}\ , \tag{3.5}$$

which is just the homogeneous part of Eq. (3.1) with $G=0$. Note that in the nonrelativistic limit $\omega(\mathbf{q})\approx m+\mathbf{p}^2/2m$, and so Eq. (3.5) reduces to the momentum-space Schrödinger equation for a one-electron atom, as one would expect. The eigenenergies of Eq. (3.5), when expanded to order $(Z\alpha)^4$, are

$$E_0'=m-\frac{m\alpha^2Z^2}{2n^2}+\frac{m\alpha^4Z^4}{8n^4}\left[3-\frac{8n}{2l+1}\right]\ , \tag{3.6}$$

where n and l are the principal and angular quantum numbers, respectively. The approximate form of $F_0(\mathbf{q})$, Eq. (3.4), which we employ in practice, is the exact solution of Eq. (3.5) in the nonrelativistic (Schrödinger) limit, i.e., $p/m \ll 1$.

Using Eqs. (3.3) and (3.5), we obtain from Eq. (3.2) the following formal scattering solution:

$$g_{\lambda'}(\mathbf{p})=\delta^3(\mathbf{p}-\mathbf{k}_i)\delta_{\lambda'\lambda}+\frac{1}{E'-E_0'-|\mathbf{p}|}\left\{\frac{e_1}{(4\pi)^{3/2}}\int d^3qF_0^*(\mathbf{q})F(\mathbf{q}-\mathbf{p})\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p})}{[\omega(\mathbf{q}-\mathbf{p})\omega(\mathbf{q})|\mathbf{p}|]^{1/2}} + \frac{e_1^2}{2(2\pi)^3}\sum_{\lambda''=1}^{2}\int d^3qd^3q'F_0^*(\mathbf{q})F_0(\mathbf{q}') \times\frac{g_{\lambda''}(\mathbf{q}'+\mathbf{p}-\mathbf{q})\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p})\cdot\boldsymbol{\epsilon}_{\lambda''}(\mathbf{q}'+\mathbf{p}-\mathbf{q})}{[\omega(\mathbf{q})\omega(\mathbf{q}')|\mathbf{p}|\,|\mathbf{q}'+\mathbf{p}-\mathbf{q}|]^{1/2}}\right\}\ , \tag{3.7}$$

where we take the normalization condition $\int d^3qF_0^*(\mathbf{q})F_0(\mathbf{q})=1$, and require that the energy E' satisfy the restriction

$$E'=E_0'+|\mathbf{k}_i|\ . \tag{3.8}$$

This formal solution (3.7) contains two parts: a free photon wave function describing the incident flux plus a scattered standing wave that can be identified as the free real Green's function times the K matrix.

Correspondingly Eq. (3.1) is replaced by

$$[\omega(\mathbf{p})-E']F(\mathbf{p}) = \frac{e_1 e_2}{(2\pi)^3}\int d^3p' \frac{F(\mathbf{p}')}{|\mathbf{p}'-\mathbf{p}|^2}\frac{\omega(\mathbf{p})+\omega(\mathbf{p}')}{2[\omega(\mathbf{p})\omega(\mathbf{p}')]^{1/2}} - \frac{e_1}{(4\pi)^{3/2}}\sum_{\lambda=1}^{2}\int d^3p' F_0(\mathbf{p}+\mathbf{p}')g_\lambda(\mathbf{p}') \times \frac{2\mathbf{p}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{p}')}{[\omega(\mathbf{p})\omega(\mathbf{p}+\mathbf{p}')|\mathbf{p}'|]^{1/2}} . \quad (3.9)$$

It is of interest to note the difference between Eq. (3.9), which represents the coupling of the scalar-atom channel to the scalar-atom plus one-photon channel, and the isolated-atom equation (3.5). Equation (3.9) is no longer a homogeneous eigenvalue equation, and so has a continuous spectrum of solutions. The information about the scattering of the photon and scalar atom is provided by the terms in the curly brackets in Eq. (3.7).

The second term in the curly brackets of Eq. (3.7) is of higher order in $\alpha=e_1^2/4\pi$ than the first one. Evaluation of this term in lowest order $[g_\lambda(\mathbf{p})=\delta^3(\mathbf{p}-\mathbf{k}_i)\delta_{\lambda\lambda_i}]$ shows that it describes Waller scattering [18]. This is evident from the appearance of the term $F_0^*(\mathbf{q})F_0(\mathbf{q}')$ under the integral. In the case where the photon energy is very large compared to the binding energies of atomic electrons, but very small compared to the electron rest energy, it reduces to Thomson scattering. When a resonance occurs in photon-atom scattering this contribution is negligible and is ignored. In this approximation we identify the K-matrix elements for the linearly polarized photon scattering to be

$$K_{\lambda'\lambda}(\mathbf{k}_f,\mathbf{k}_i)=\frac{\sqrt{\alpha}}{4\pi}\int d^3q F_0^*(\mathbf{q}+\mathbf{k}_f)F(\mathbf{q}) \times \frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{k}_f)}{[\omega(\mathbf{q})\omega(\mathbf{q}+\mathbf{k}_f)|\mathbf{k}_f|]^{1/2}} . \quad (3.10)$$

This reactance matrix describes how photons are deflected due to the fact that the atom makes a transition from F_0 to F and back. Here $\mathbf{k}_i$ and λ ($\mathbf{k}_f$ and λ') stand for the initial (final) momentum vector and linear polarization index. The F function is determined by Eq.. (3.9), which in lowest-order approximation reduces to

$$[\omega(\mathbf{q})+|\mathbf{p}_1|+|\mathbf{p}_2|-E'][I(\mathbf{q},\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)+I(\mathbf{q},\mathbf{p}_2\lambda_2,\mathbf{p}_1\lambda_1)] = -\frac{e_1}{(4\pi)^{3/2}}\frac{1}{\sqrt{\omega(\mathbf{q})}}\left[G(\mathbf{q}-\mathbf{p}_2,\mathbf{p}_1\lambda_1)\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_{\lambda_2}(\mathbf{p}_2)}{\sqrt{\omega(\mathbf{q}-\mathbf{p}_2)|\mathbf{p}_2|}}+G(\mathbf{q}-\mathbf{p}_1,\mathbf{p}_2\lambda_2)\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_{\lambda_1}(\mathbf{p}_1)}{\sqrt{\omega(\mathbf{q}-\mathbf{p}_1)|\mathbf{p}_1|}}\right] + \frac{e_1 e_2}{2(2\pi)^3}\int d^3q' \frac{I(\mathbf{q}',\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)+I(\mathbf{q}',\mathbf{p}_2\lambda_2,\mathbf{p}_1\lambda_1)}{|\mathbf{q}'-\mathbf{q}|^2}\frac{\omega(\mathbf{q})+\omega(\mathbf{q}')}{[\omega(\mathbf{q})\omega(\mathbf{q}')]^{1/2}} - \frac{e_1^2}{2(2\pi)^3}F(\mathbf{q}-\mathbf{p}_1-\mathbf{p}_2)\frac{\boldsymbol{\epsilon}_{\lambda_1}(\mathbf{p}_1)\cdot\boldsymbol{\epsilon}_{\lambda_2}(\mathbf{p}_2)}{\sqrt{\omega(\mathbf{q}-\mathbf{p}_1-\mathbf{p}_2)\omega(\mathbf{q})|\mathbf{p}_1||\mathbf{p}_2|}} - \frac{e_1^2}{2(2\pi)^3}\sum_{\lambda'}\int\frac{d^3p'}{[\omega(\mathbf{q})|\mathbf{p}'|]^{1/2}}\left\{\frac{\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p}')\cdot\boldsymbol{\epsilon}_{\lambda_1}(\mathbf{p}_1)}{[\omega(\mathbf{q}+\mathbf{p}'-\mathbf{p}_1)|\mathbf{p}_1|]^{1/2}}[I(\mathbf{q}+\mathbf{p}'-\mathbf{p}_1,\mathbf{p}'\lambda',\mathbf{p}_2\lambda_2)+I(\mathbf{q}+\mathbf{p}'-\mathbf{p}_1,\mathbf{p}_2\lambda_2,\mathbf{p}'\lambda')] + \frac{\boldsymbol{\epsilon}_{\lambda'}(\mathbf{p}')\cdot\boldsymbol{\epsilon}_{\lambda_2}(\mathbf{p}_2)}{[\omega(\mathbf{q}+\mathbf{p}'-\mathbf{p}_2)|\mathbf{p}_2|]^{1/2}}[I(\mathbf{q}+\mathbf{p}'-\mathbf{p}_2,\mathbf{p}'\lambda',\mathbf{p}_1\lambda_1)+I(\mathbf{q}+\mathbf{p}'-\mathbf{p}_2,\mathbf{p}_1\lambda_1,\mathbf{p}'\lambda')]\right\} . \quad (4.2)$$

$$[\omega(\mathbf{p})-E']F(\mathbf{p}) = \frac{Z\alpha}{2\pi^2}\int d^3p' \frac{F(\mathbf{p}')}{|\mathbf{p}'-\mathbf{p}|^2}\frac{\omega(\mathbf{p})+\omega(\mathbf{p}')}{2[\omega(\mathbf{p})\omega(\mathbf{p}')]^{1/2}} - \frac{\sqrt{\alpha}}{4\pi}F_0(\mathbf{p}+\mathbf{k}_i)\frac{2\mathbf{p}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k}_i)}{[\omega(\mathbf{p})\omega(\mathbf{p}+\mathbf{k}_i)|\mathbf{k}_i|]^{1/2}} , \quad (3.11)$$

where we have set $e_2=Ze_1$.

The unpolarized total cross section for the scattering of the photon with the two-scalar atom is given by [19]

$$\sigma=\int d\Omega_{k_f}\frac{1}{2}\sum_{\lambda=1}^{2}\sum_{\lambda'=1}^{2}(2\pi)^4\mathbf{k}_f^2|T_{\lambda'\lambda}(\mathbf{k}_f,\mathbf{k}_i)|^2 , \quad (3.12)$$

where $T_{\lambda'\lambda}$ are the elements of the transition matrix. They are related to the K-matrix elements (3.10) through the Heitler equation

$$T_{\lambda'\lambda}(\mathbf{k}_f,\mathbf{k}_i)=K_{\lambda'\lambda}(\mathbf{k}_f,\mathbf{k}_i)-i\pi k_i^2 \times\sum_{\lambda_1=1}^{2}\int d\Omega_{k_1}T_{\lambda'\lambda_1}(\mathbf{k}_f,\mathbf{k}_1)K_{\lambda_1\lambda}(\mathbf{k}_1,\mathbf{k}_i) , \quad (3.13)$$

where $k_1=k_f=k_i$, as given by the energy-conservation law.

IV. TWO-SCALAR AND TWO-PHOTON FOCK-SPACE TREATMENT

In order to incorporate the process corresponding to the diagram of Fig. 1(b), which also contributes to the resonance in lowest order, we have to expand the Fock space to allow for the simultaneous presence of the scalars and two photons. The variational ansatz in addition to (2.6) now contains the term

$$|\Psi\rangle_{\gamma\gamma}=\sum_{\lambda_1=1}^{2}\sum_{\lambda_2=1}^{2}\int d^3q\, d^3p_1 d^3p_2 I(\mathbf{q},\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)B_m^\dagger(\mathbf{p}_4) \times A_M^\dagger(\mathbf{p}_3)a_{\lambda_2}^\dagger(\mathbf{p}_2)a_{\lambda_1}^\dagger(\mathbf{p}_1)|0\rangle , \quad (4.1)$$

with $\mathbf{p}_3=\mathbf{q}-[M/(m+M)](\mathbf{p}_1+\mathbf{p}_2)$ and $\mathbf{p}_4=-\mathbf{q}-[m/(m+M)](\mathbf{p}_1+\mathbf{p}_2)$.

After taking the variation (2.7) and the limit $M\to\infty$, additional terms are obtained on the right-hand side of Eqs. (3.1) and (3.2) as well as an equation for the $(Mm\gamma\gamma)$ amplitude:

The additional term on the right-hand side of Eq. (3.1) is given by

$$-\frac{e_1^2}{(4\pi)^3}\sum_{\lambda_1'\lambda_2'}\int d^3p_1'd^3p_2' I(\mathbf{p}+\mathbf{p}_1'+\mathbf{p}_2',\mathbf{p}_1'\lambda_1',\mathbf{p}_2'\lambda_2') \times\frac{\boldsymbol{\epsilon}_{\lambda_1'}(\mathbf{p}_1')\cdot\boldsymbol{\epsilon}_{\lambda_2'}(\mathbf{p}_2')}{[\omega(\mathbf{p})\omega(\mathbf{p}_1+\mathbf{p}_1'+\mathbf{p}_2')|\mathbf{p}_1'|\,|\mathbf{p}_2'|]^{1/2}}\ , \tag{4.3}$$

and on the right-hand side of Eq. (3.2) by

$$-\frac{e_1}{(4\pi)^{3/2}}\sum_{\lambda'}\int d^3q'[I(\mathbf{q}',\mathbf{p}\lambda,(\mathbf{q}'-\mathbf{q})\lambda') +I(\mathbf{q}',(\mathbf{q}'-\mathbf{q})\lambda',\mathbf{p}\lambda)] \times\frac{2\mathbf{q}\cdot\boldsymbol{\epsilon}_{\lambda'}(\mathbf{q}'-\mathbf{q})}{[\omega(\mathbf{q}')\omega(\mathbf{q})|\mathbf{q}'-\mathbf{q}|]^{1/2}}\ . \tag{4.4}$$

The two-photon plus bound-scalar amplitude I appears in a symmetric way with respect to the photon variables, and therefore we introduce

$$I'(\mathbf{q},\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)=I(\mathbf{q},\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)+I(\mathbf{q},\mathbf{p}_2\lambda_2,\mathbf{p}_1\lambda_1)\ . \tag{4.5}$$

Again, we shall not attempt to solve the three coupled equations (3.1) [with (4.3)], (3.2) [with (4.4)], and (4.2) for the variational coefficients F, G, and I. Rather, we shall proceed as in Sec. III and, in addition, we shall choose I' to take on the particular factorized form

$$I'(\mathbf{q},\mathbf{p}_1\lambda_1,\mathbf{p}_2\lambda_2)=F(\mathbf{q})\delta^3(\mathbf{p}_1+\mathbf{p}_2)\delta_{\lambda_1\lambda_2}(-1)^{\lambda_1}\ , \tag{4.6}$$

where, as previously, $F(\mathbf{q})$ describes the intermediate state of the atom during the collision. This form is the simplest possible choice that is symmetric in the photon variables and links this channel properly to the scalar particle's degrees of freedom. The incident and outgoing photon flux is still described by the amplitude G. Equation (4.2) could be used, in principle, to describe the collision of two photons with a ground-state atom, but this is not our interest for the present paper.

This restriction of the two-photon plus scalar atom amplitude to the form (4.6) results in an additional mass renormalization term in Eq. (3.1), which can be absorbed in the usual way [9], as well as an additional scattering term in Eq. (3.2), namely, that shown in Eq. (4.4). This term is identical in form to the first term on the right-hand side of Eq. (3.2) and in effect replaces e_1 by $2e_1$ in that term. Thus on resonance the results from the previous section are only modified by the fact that the K matrix [Eq. (3.10)] is multiplied by a factor of 2.

V. RESULTS

For a numerical study of the scattering cross section, we need to make Eqs. (3.10)–(3.13) numerically treatable. To this end, we make a partial-wave electromagnetic multipole expansion of the K matrix as follows [20]:

$$K(\mathbf{k}_2,\mathbf{k}_1)=\sum_{J=1}^{\infty}\sum_{M_J=-J}^{J}\sum_{\mu_1\mu_2}Y_{JM_J}^{(\mu_2)}(\mathbf{k}_2)R^J_{\mu_2\mu_1}(k)Y_{JM_J}^{(\mu_1)*}(\mathbf{k}_1)\ , \tag{5.1}$$

where the indices μ_2 and μ_1 run over e and m, and $Y^{(e)}_{JM_J}$ and $Y^{(m)}_{JM_J}$ are, respectively, the electric and magnetic vector spherical harmonics. In addition, the momenta k_1 and k_2 are equal ($k_2=k_1=k$) by energy conservation. For a spherically symmetric scatterer under parity conservation, we have

$$R^J_{em}=R^J_{me}=0\ , \tag{5.2}$$

$$R^J_{ee}=-R^J_{mm}\ . \tag{5.3}$$

We expand the T matrix in the same way as Eq. (5.1), denoting the multipole expansion coefficients by $T^J_{\mu_1\mu_2}$. If we parametrize the expansion coefficients of the diagonal K matrix in terms of eigenphases

$$R^J_{\mu\mu}(k)=\frac{1}{\pi k^2}\tan\delta^\mu_J(k)\ ,\quad \mu=e,m\ , \tag{5.4}$$

then from Eq. (3.13) it follows that

$$T^J_{\mu\mu}(k)=\frac{R^J_{\mu\mu}}{1+i\pi k^2R^J_{\mu\mu}}=\frac{1}{\pi k^2}\sin\delta^\mu_J(k)e^{-i\delta^\mu_J(k)}\ . \tag{5.5}$$

Here δ^e_J and δ^m_J are the electric and magnetic eigenphase shifts, respectively. The total scattering cross section Eq. (3.12) can then be written in the form

$$\sigma=\sum_{\mu=e,m}\sum_{J=1}^{\infty}\sigma^\mu_J(k)\ , \tag{5.6}$$

with the partial-wave cross sections given by the expression

$$\sigma^\mu_J(k)=\frac{2\pi}{k^2}(2J+1)\sin^2\delta^\mu_J(k)\ , \tag{5.7}$$

where we recall that $k_i=k_f=k$.

In order to evaluate the partial-wave cross sections, we make the partial-wave decomposition of Eq. (3.11) with

$$F(\mathbf{q})=F^{(\lambda)}(\mathbf{q})=\sum_{l=0}^{\infty}\sum_{m_l=-l}^{l}f^{(\lambda)}_{nlm_l}(q)Y_{lm_l}(\theta,\phi)\ , \tag{5.8}$$

where Y_{lm_l} are the usual spherical harmonics. Therefore, Eq. (3.11) is replaced by the radial equation

$$[\omega(p)-E']f^{(\lambda)}_{nlm_l}(p) =\frac{\alpha Z}{\pi}\int_0^\infty dq\, f^{(\lambda)}_{nlm_l}(q)\frac{q}{p}K_l(p,q)+S^{(\lambda)}_{lm_l}(p,k_i)\ , \tag{5.9}$$

where the kernel K_l and inhomogeneous term $S^{(\lambda)}_{lm_l}$ are given in the Appendix for the $l=1,2$ cases. Numerically this equation is solved by expanding $f^{(\lambda)}_{nlm_l}(q)$ in a sine basis using the variable $x=2\tan^{-1}q$, and the expansion is truncated, typically, after 80 terms. Performing these partial-wave expansions we evaluate the phase shift δ^μ_J from the partial-wave form of Eq. (3.10):

$$\frac{1}{\pi k^2}\tan\delta_J^{\mu}(k)=2(-1)^{\mu-1}\frac{1}{\pi^2 J(J+1)}\left[\frac{8\alpha\gamma^5}{\pi k}\right]^{1/2}$$
$$\times\sum_{l=1}^{\infty}\left[\frac{2l+1}{l(l+1)}\right]^{1/2}\int_0^{\infty}dq\frac{q^3 f_{nl1}^{(1)}(q)}{(m^2+q^2)^{1/4}}\int_0^{\pi}d\theta_f\left[P_J^1(\cos\theta_f)-\sin\theta_f\frac{d}{d\theta_f}P_J^1(\cos\theta_f)\right]$$
$$\times\int_0^{2\pi}d\phi_f\cos\phi_f\int_0^{\pi}d\theta\sin\theta P_l^1(\cos\theta)\int_0^{2\pi}d\phi\frac{\cos\phi}{(q^2+k^2+\gamma^2+2\mathbf{q}\cdot\mathbf{k}_f)^2}$$
$$\times\frac{\sin\theta\cos\theta_f\cos(\phi-\phi_f)-\cos\theta\sin\theta_f}{(q^2+k^2+m^2+2\mathbf{q}\cdot\mathbf{k}_f)^{1/4}}\ , \tag{5.10}$$

where $\mu=1$ means $\mu=e$, $\mu=2$ means $\mu=m$, and P_J^1 are the associated Legendre polynomials. This equation is obtained from Eq. (3.10) with F_0 replaced by Eq. (3.4), i.e., the ground-state wave function. The factor 2 to the right of the equal sign arises from the Fock-space states of Eq. (4.1), that is, the additional term given in Eq. (4.4). The partial-wave cross sections are then calculated from Eq. (5.7). Obviously, because of Eq. (5.3), $\sigma_J^e=\sigma_J^m$, and so we need to study only one of them.

We have calculated the $J=1$ partial-wave cross section σ_J^{μ} as a function of the photon energy $k=E'-E_0'$, where the atomic ground-state energy E_0' is given by Eq. (3.6). For a given fixed atomic number Z, the resonance structure of the cross section is obvious: These resonances occur near the energies $k_0=E_{np}-E_{1s}$, which are calculated by using Eq. (3.6), and the spectral lines correspond to the atomic transitions from the np states to the ground state. Comparing the centers of the resonances with the energies k_0, we find that they are decreased from k_0 by an amount of the order of the resonance widths. This shift is due to the coupling of the bound state to the photon-continuum channel. When n increases, the nu-

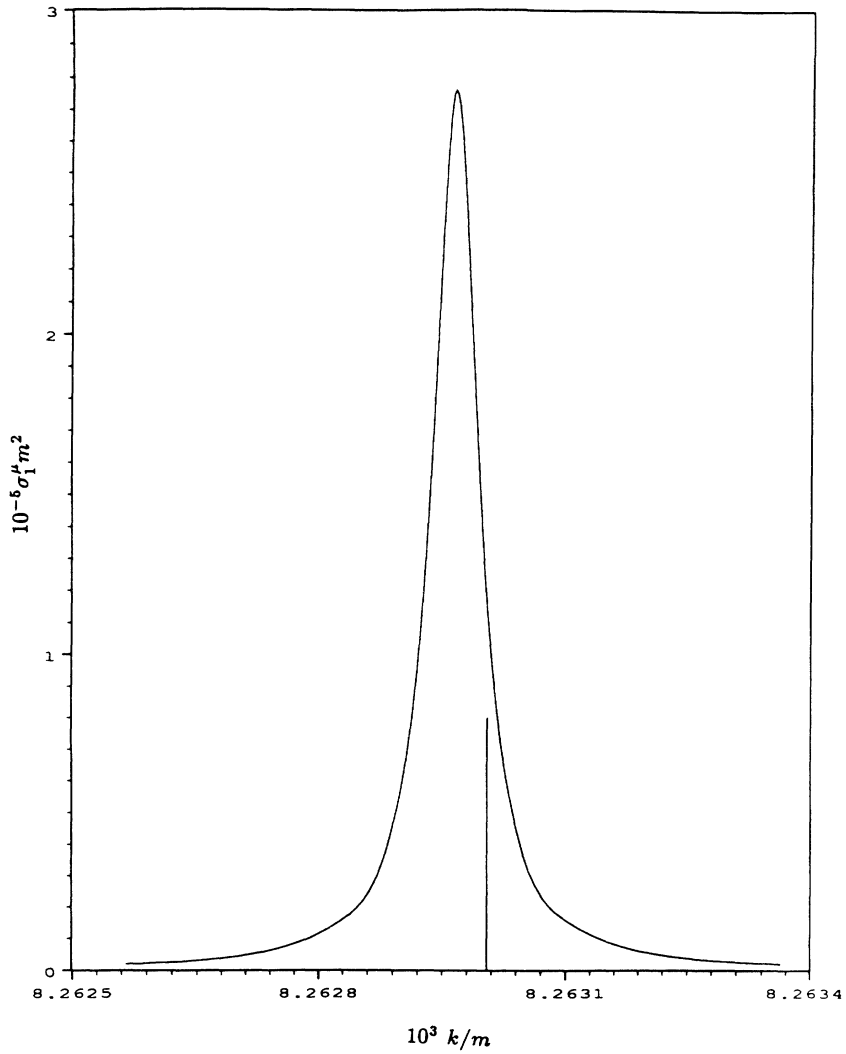

FIG. 2. The behavior of the electric or magnetic p-wave cross section in the vicinity of the first resonance for an atom with $Z=20$. The vertical line indicates the position of $k_0=E_{2p}-E_{1s}$.

merical calculations become less accurate and more expansion terms in the numerical solution are needed.

In Figs. 2 and 3, we show the behaviors of $\sigma^{\mu}_{J=1}$ for $Z=20$ in the vicinities of the first and second resonances. The two lines respectively correspond to the $2p$-$1s$ and $3p$-$1s$ transitions. Detailed analysis shows that the lines have the Lorentzian shape, i.e., they are well fitted by the Breit-Wigner formula. For example, for the results in Fig. 2, we obtain an excellent fit of our calculated curve to the Breit-Wigner form $A\Gamma_{\mu}^2/[(k-k_c)^2+(\Gamma_{\mu}/2)^2]$ with $k_c=8.262\,964\times10^{-3}$ m, $\Gamma_{\mu}=6.649\times10^{-8}$ m, and $A=6.902\times10^{4}$. Indeed, the Breit-Wigner fit is indiscernible from the calculated curve on the scale of the figure. It agrees with the numerical value to three significant figures over the domain of k shown in the figure. Similarly, for Fig. 3 the corresponding results are $k_c=9.746\,962\times10^{-3}$ m, $\Gamma_{\mu}=1.758\times10^{-8}$ m, and $A=4.960\times10^{4}$.

We retain only the contribution from the $l=1$ term in the calculation of $\sigma^{\mu}_{J=1}$, using a two-state atom model. The numerical results indicate, as one would expect, that the contribution from the $l=1$ term is dominant near the maxima of the resonances and the shape of the lines is symmetric. The contributions from the nonresonant l terms have less effect on the $2p$-$1s$ line than on the np-$1s$ lines with $n\geq3$, as there are other closely lying levels near the higher-n, levels. It is difficult to include the effects of many nonresonant terms in the numerical calculation. As an example, we have calculated the effects of the $p=2$ term and find that they can hardly be demonstrated in a diagram, like Fig. 2 or 3.

For a fixed spectral line, for example, the $2p$-$1s$ line, when changing the atomic number Z, we find that the widths of the resonances are proportional to Z^4 for small Z, which is in agreement with perturbation theory [5,21]. For large Z the results deviate from this behavior, and the larger Z is, the larger the deviation. This can be clearly seen in Fig. 4. The reciprocal of $\Gamma=\Gamma_e+\Gamma_m$ of these resonances yields the lifetime of the excited states.

We have also calculated the $J=2$ partial-wave cross section σ^{μ}_{J} as a function of the photon energy k. The d-wave cross section $\sigma^{\mu}_{J=2}$ has a similar resonance structure as the p-wave cross section, but the resonances occur near the energies $k_0=E_{nd}-E_{1s}$. These spectral lines correspond to the atomic transition from the nd state to the ground state. Figure 5 shows the first resonance of the

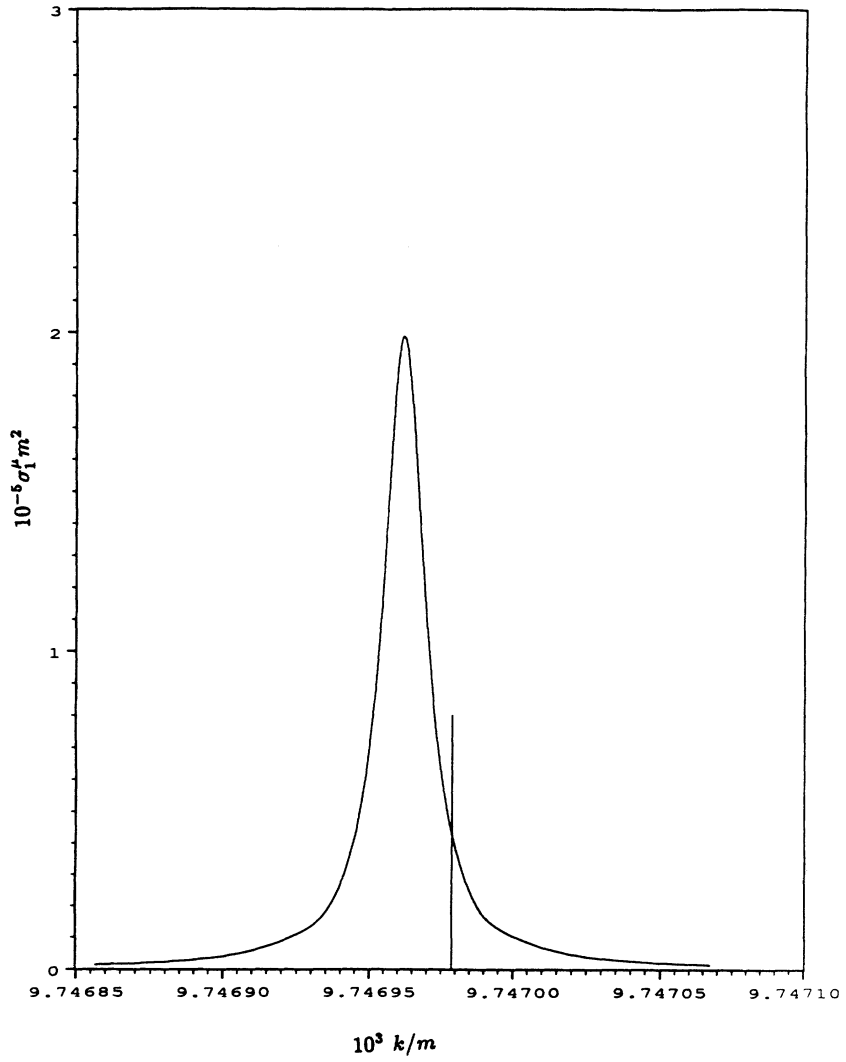

FIG. 3. The behavior of the electric or magnetic p-wave cross section in the vicinity of the second resonance for an atom with $Z=20$. The vertical line indicates the position of $k_0=E_{3p}-E_{1s}$.

d-wave cross section for $Z=20$, which corresponds to the $3d$-$1s$ line. This line has the same Lorentzian line shape as the ones in Fig. 2 and Fig. 3, and is well fitted by the Breit-Wigner formula with $k_c=9.749\,217\times10^{-3}$ m, $\Gamma_\mu=6.071\times10^{-8}$ m, and $A=8.263\times10^4$. The calculation shows that near the resonance the contribution of the resonant term, i.e., the $l=2$ term, is dominant and the effects of the nonresonant terms are small (indiscernible on the scale of Fig. 5). The line center is also decreased from k_0 but by an amount of about one order less than the resonance width, as one would expect for a radiative shift in a higher l state.

VI. CONCLUDING REMARKS

We have used the Hamiltonian formalism of scalar quantum electrodynamics to describe unstable (excited) states of atoms as resonances in the photon-atom continuum. The Hamiltonian formalism is particularly convenient for the description of such unstable states, since the variational method can be used to derive relativistic wave equations that couple the discrete-energy ground state to the excited atomic state and its decay to the stable ground state is naturally described as a coupled-channel problem in this approach. Moreover, the Hamiltonian formalism has the advantage that it is closely related to the familiar Schrödinger description of atoms, which it contains as a nonrelativistic limit. Thus we have applied the variational method, within the Hamiltonian formalism of SQED, to the problem of the natural line shape of atoms from the scattering viewpoint. In this approach, the unstable excited states of atoms appear naturally as resonances in the photon-atom scattering cross section. The widths of these resonances yield the transition rate from the atomic excited state to the ground state. In contrast to the usual descriptions, we do not need to introduce the concept of complex energy, and effects of nonresonance terms can be incorporated naturally.

An unappealing aspect of the equal-time Hamiltonian variational method also becomes apparent in the present work. Within covariant perturbation theory, photon-atom scattering is described, in lowest order, by the two Kramers-Heisenberg terms depicted in Figs. 1(a) and 1(b). These are easily seen to be of equal importance as they contribute at the same order of perturbation theory. In the presently used formalism these two terms corre-

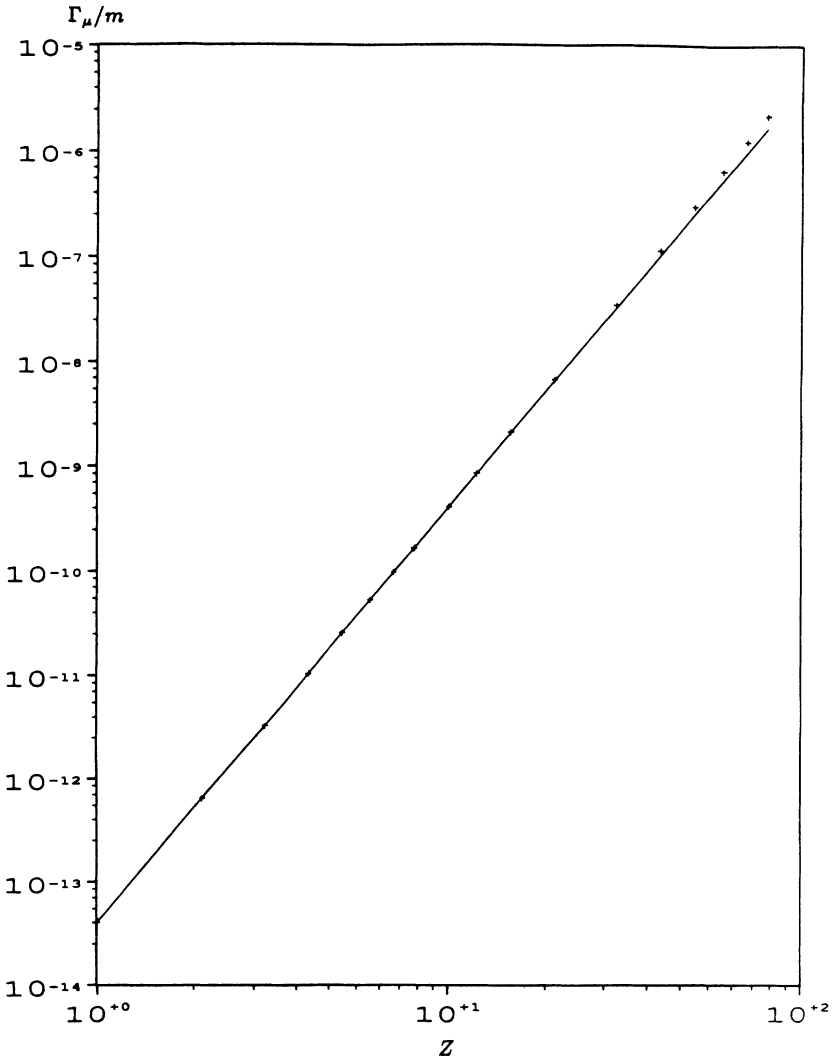

FIG. 4. The electric or magnetic width Γ_μ as a function of Z for the $2p$-$1s$ resonances. Solid line, perturbative result; crosses, present numerical results.

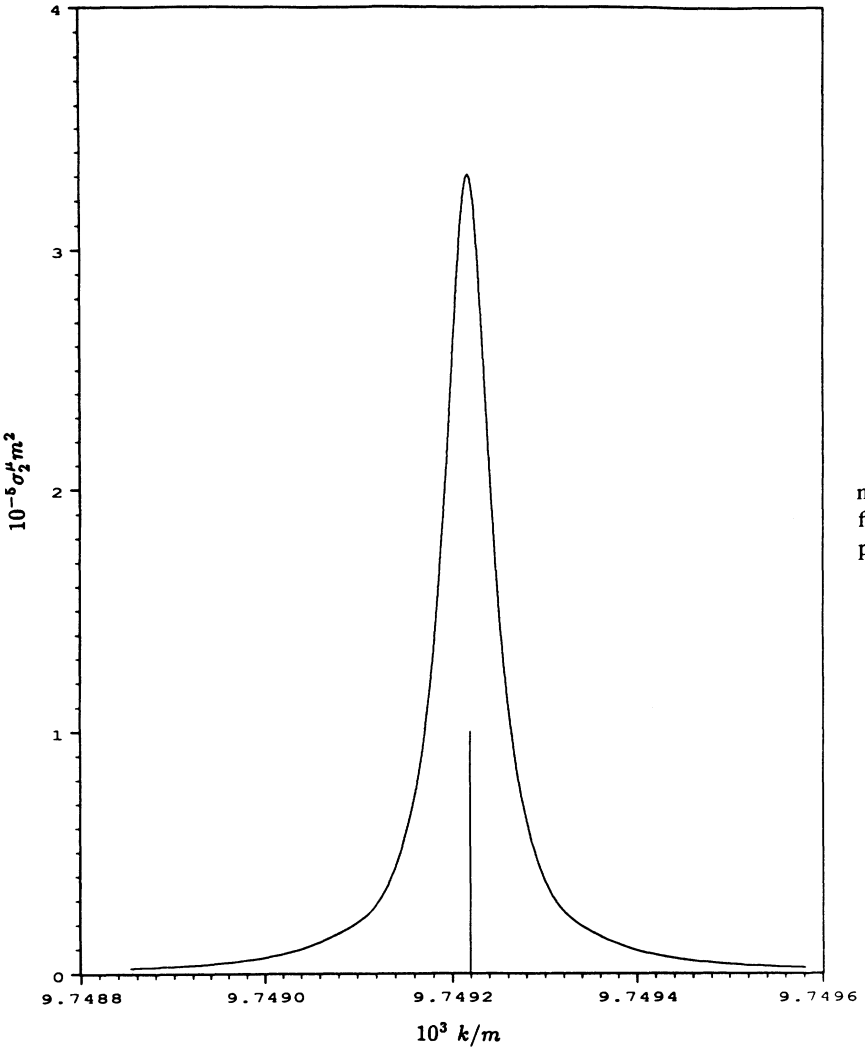

FIG. 5. The behavior of the electric or magnetic d-wave cross section in the vicinity of the first resonance. The vertical line indicates the position of $k_0=E_{3d}-E_{1s}$.

spond to Fock-space trial states with different photon number [Eqs. (2.6) and (4.1)], which leads to equations [(4.2) in the present case] that involve more than two momentum coordinates. Such equations can be handled, in practice, only in some approximate way, such as the separable approximation Eq. (4.6) used in the present work. On the other hand, as we have stressed previously, the Hamiltonian formalism provides equations that are easily interpreted in terms of ordinary quantum mechanics. In particular it is transparent how the quantum-mechanical eigenvalue problem becomes modified so that the excited states appear as continuum resonances without any *ad hoc* assumptions.

More work is required to exploit fully the possibilities of the present approach, and in particular, to exploit the relativistic treatment of the bound-state problem. In particular, an extension to the case of fermionic QED would be of interest for the study of transitions in high-Z atoms, which are currently being investigated in heavy-ion storage rings.

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APPENDIX

For the $l=1,2$ cases, the kernel $K_l(p,q)$ and inhomogeneous term $S_{lm_l}^{(\lambda)}$ in Eq. (5.9) take the following forms:

$$K_1(p,q)=\frac{\omega(p)+\omega(q)}{4\sqrt{\omega(p)\omega(q)}}\left[\frac{p^2+q^2}{pq}\ln\left|\frac{p+q}{p-q}\right|-2\right], \quad \text{(A1)}$$

$$K_2(p,q)=\frac{3}{4}\frac{\omega(p)+\omega(q)}{\sqrt{\omega(p)\omega(q)}}\left\{\left[\left[\frac{p^2+q^2}{pq}\right]^2-\frac{1}{3}\right]\times\ln\left|\frac{p+q}{p-q}\right|-\frac{p^2+q^2}{2pq}\right\}. \quad \text{(A2)}$$

In the coordinate system formed by $\epsilon_1(\mathbf{k}_i)$, $\epsilon_2(\mathbf{k}_i)$, and $\mathbf{k}_i$, for $\lambda=1$ we get

$$S^{(1)}_{1m_1}(p,k_i)=\pm\frac{1}{2\pi}\left[\frac{3\alpha^6Z^5m^5}{\pi k_i}\right]^{1/2}\frac{p}{(p^2+m^2)^{1/4}}\times[W_0(p,k_i)-W_2(p,k_i)]\delta_{\pm 1m_1}\,,\quad m_1=0,\pm1\,, \tag{A3}$$

$$S^{(1)}_{2m_2}(p,k_i)=\pm\frac{1}{2\pi}\left[\frac{15\alpha^6Z^5m^5}{\pi k_i}\right]^{1/2}\frac{p}{(p^2+m^2)^{1/4}}\times[W_1(p,k_i)-W_3(p,k_i)]\delta_{\pm 1m_2}\,,\quad m_2=0,\pm1,\pm2\,, \tag{A4}$$

and for $\lambda=2$,

$$S^{(2)}_{lm_l}(p,k_i)=\mp iS^{(1)}_{lm_l}(p,k_i)\,, \tag{A5}$$

where the minus $(-)$ is for $m_l>0$ and plus $(+)$ for $m_l\le 0$. In the above W_i $(i=0,1,2,3)$ are given as follows:

$$W_0(p,k_i)=\frac{1}{2pk_i(m^2-\gamma^2)}\times\left[\frac{t_1^3}{(p-k_i)^2+\gamma^2}-\frac{t_2^3}{(p+k_i)^2+\gamma^2}-W(p,k_i)\right], \tag{A6}$$

where here and hereafter $\gamma=Z\alpha m$, and

$$t_1=[(p-k_i)^2+m^2]^{1/4}\,, \tag{A7}$$

$$t_2=[(p+k_i)^2+m^2]^{1/4}\,, \tag{A8}$$

$$W(p,k_i)=\frac{1}{4(m^2-\gamma^2)^{1/4}}\left[\ln\left|\frac{t_2-(m^2-\gamma^2)^{1/4}}{t_2+(m^2-\gamma^2)^{1/4}}\right|-\ln\left|\frac{t_1-(m^2-\gamma^2)^{1/4}}{t_1+(m^2-\gamma^2)^{1/4}}\right|+2\arctan\frac{t_2}{(m^2-\gamma^2)^{1/4}}-2\arctan\frac{t_1}{(m^2-\gamma^2)^{1/4}}\right], \tag{A9}$$

$$W_1(p,k_i)=\frac{1}{p^2k_i^2}\left[W(p,k_i)-(\gamma^2+p^2+k_i^2)\frac{pk_i}{2}W_0(p,k_i)\right], \tag{A10}$$

$$W_2(p,k_i)=\frac{1}{2p^3k_i^3}\left[\frac{t_2^3-t_1^3}{3}-2(\gamma^2+p^2+k_i^2)W(p,k_i)+(\gamma^2+p^2+k_i^2)^2\frac{pk_i}{2}W_0(p,k_i)\right], \tag{A11}$$

$$W_3(p,k_i)=\frac{1}{4p^4k_i^4}\left\{\frac{t_2^7-t_1^7}{7}-(t_2^3-t_1^3)\left[\frac{m^2-\gamma^2}{3}+\gamma^2+p^2+k_i^2\right]+(\gamma^2+p^2+k_i^2)^2\left[3W(p,k_i)-\frac{(\gamma^2+p^2+k_i^2)pk_i}{(\gamma^2+p^2+k_i^2)^2-(2pk_i)^2}\right]\right\}. \tag{A12}$$

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