Calculation of Ionization Amplitudes by the Complex-Energy Method

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It is shown that, as the complex energy approaches its real physical value, the dominant part of the amplitude for ionization derived from the Faddeev equations is a product of a known singular factor and the physical scattering amplitude. This information suggests a method of calculating ionization amplitudes from the Faddeev equations. Corrections to the dominant term for this and another amplitude are discussed. Some numerical tests of the method as applied to a simple model are given.

I. INTRODUCTION

The method of extrapolation from complex energies[1] appears to have considerable promise as a means of computing amplitudes for processes such as electron–hydrogen-atom elastic scattering above the ionization threshold. In this paper, we discuss the modifications required to apply this method to the calculation of ionization amplitudes.

The essential point of the method is that an amplitude $f(E)$ depending on the complex energy E can be defined that may be calculated in any one of several straightforward ways for $\mathrm{Im}E > 0$. The physical amplitude is then obtained by extrapolating $f(E)$ onto the real axis. At the present time a direct calculation with E held at its real physical value is often difficult or impossible.

In the case of elastic scattering from, or excitation of, neutral atoms, there is an obvious definition of $f(E)$. However, for processes in which two separated constituents of the final (or initial) state each has a net charge—for instance, in e-H ionization—complications arise. The natural choice of amplitude—that satisfying the Faddeev equations—becomes singular as E approaches the real physical value. An important result of this paper is that the most singular part of the Faddeev amplitude $f_F(E)$ may be written as a product of a known singular factor with the physical scattering amplitude $f_0(E)$. Thus we can solve the physical problem by extrapolating from complex E the product of $f_F(E)$ with the inverse of the singular factor. We also investigate the nature of the corrections to the most singular part of $f_F(E)$, a knowledge of which should be of assistance in carrying out the extrapolation accurately.

Peterkop[2,3] and Rudge and Seaton,[4] realizing that the analog of the short-range-potential formula for the breakup matrix element is undefined for physical energies, have given a well-defined integral formula for the ionization amplitude. It should be possible to calculate this amplitude, $f_P(E)$, at complex energies and to determine its physical value by extrapolating without first having to remove a singular factor. Again it should be helpful to know the form of the most important terms in an expansion of $f_P(E)$ about E_0.

The amplitude $f_P(E)$ is not related in a simple manner to the solution of the Faddeev equations. It should be possible, however, to calculate $f_P(E)$ for complex E by a variational method, although this may be more difficult to do than for $f_F(E)$. Which approach would lead to the most accurate value of the physical amplitude is difficult to determine.

In Sec. II we derive the behavior of the amplitudes $f_F(E)$ and $f_P(E)$ as E approaches its physical value from the known asymptotic form of the wave function for the problem. The most singular part of an amplitude is related to the leading term in the asymptotic expansion. Section III contains a discussion of the two-particle problem, where we have tested several possible methods of performing the extrapolation.

II. IONIZATION IN e-H SCATTERING

To illustrate our ideas, we study the case of e-H scattering, except that to avoid inessential complications, we disregard the identity of the electrons. Using units in which $h = 2m = \frac{1}{2}e^2 = 1$, we first define the Faddeev amplitude $f_F(E)$ for E complex as

$$f_F(E) = \langle \vec{p}_1, \vec{p}_2 | [V_0 + V_0(E - H)^{-1}V] | \vec{k}, \alpha \rangle , \qquad (1)$$

where $|\vec{k}, \alpha\rangle = e^{i\vec{k}\cdot\vec{r}_1}\phi_\alpha(\vec{r}_2)$ is a state in which the first electron has momentum $\vec{k}$ and the second is bound in level α, and $|\vec{p}_1, \vec{p}_2\rangle = (2\pi)^{-3}e^{i(\vec{p}_1\cdot\vec{r}_1 + \vec{p}_2\cdot\vec{r}_2)}$ is a plane-wave state for each electron. Also,

$$V=-\frac{2}{r_1}+\frac{2}{r_3}\,,\quad V_0=-\frac{2}{r_1}-\frac{2}{r_2}+\frac{2}{r_3} \tag{2}$$

($r_3=|\vec{r}_1-\vec{r}_2|$), and H is the complete Hamiltonian.

It is convenient to introduce a six-dimensional space in which the coordinates are given by the 6-vector $\hat{\rho}=(\vec{r}_1,\vec{r}_2)$ and momenta by $\hat{P}=(\vec{p}_1,\vec{p}_2)$. With this notation we have

$$V_0=-2K\eta(\hat{\rho}_\mu)/\rho\,, \tag{3}$$

where $\rho=|\hat{\rho}|$, $K^2=E$, $\hat{\rho}_\mu=\hat{\rho}/\rho$, and η is a function of $\hat{\rho}_\mu$ defined by (2) and (3).

The differential cross section for ionization may be written directly in terms of the amplitude $f_0(\hat{P}_\mu)$, which is defined by means of the asymptotic form of the scattering wave function $\Phi(\hat{\rho})$ when ρ is large and all three particles are well separated. This form, given by Peterkop,[3] is

$$\Phi(\hat{\rho})\underset{\rho\to\infty}{\sim}(e^{iK\rho}/\rho^{5/2})\rho^{i\eta(\hat{\rho}_\mu)}f_0(\hat{\rho}_\mu)\,. \tag{4}$$

We shall show below that, as E approaches $P^2=\vec{p}_1{}^2+\vec{p}_2{}^2$, $f_F(E)$ defined in (1) is singular with dominant behavior

$$f_F(E)\underset{E\to P^2}{\sim}\frac{2(2\pi)^{-5/2}P^{-3/2}e^{i\pi/4}}{(-i)^{i\eta}\Gamma(-i\eta)(e^{\pi\eta}-e^{-\pi\eta})}\,(K-P)^{-i\eta}f_0(\hat{P}_\mu)\,, \tag{5}$$

with $\eta=\eta(\hat{P}_\mu)$. This result is the basis for our method of calculating the ionization cross section from the Faddeev amplitude, for it enables us to determine f_0 by extrapolation of $(K-P)^{i\eta}f_F(E)$.

We relate $f_F(E)$ to the wave function Φ by writing

$$\begin{aligned}f_F(E)&=\langle\vec{p}_1,\vec{p}_2\,|\,V_0\,|\,\Phi\rangle\\&=(2\pi)^{-3}\int d\vec{r}_1\,d\vec{r}_2\,e^{-i(\vec{p}_1\cdot\vec{r}_1+\vec{p}_2\cdot\vec{r}_2)}\\&\quad\times\left(-\frac{2}{r_1}-\frac{2}{r_2}+\frac{2}{r_3}\right)\Phi(\vec{r}_1,\vec{r}_2)\,,\end{aligned} \tag{6}$$

with

$$|\,\Phi\rangle=[1+(E-H)^{-1}V]\,|\vec{k},\alpha\rangle\,. \tag{7}$$

As $E\to p_1{}^2+p_2{}^2$, Φ becomes the wave function describing the physical scattering process with initial state $|\vec{k},\alpha\rangle$.

It is only because of a lack of convergence at large distances that (6) can be singular. For $\mathrm{Im}E>0$, the phase of the integrand is not stationary for large ρ and $f_F(E)$ is nonsingular. However, when $K=P$, the phase of the integrand, which may be taken as $-\hat{P}\cdot\hat{\rho}+K\rho$ for these purposes, is stationary along the ray $\hat{\rho}_\mu=\hat{P}_\mu$. It is therefore possible that contributions from large values of ρ in this direction will give rise to a singularity of $f_F(E)$ when $K=P$. For other values of P, a contour distortion $\hat{\rho}\to\hat{\rho}+i\delta\hat{\rho}$ can be found that will give the phase a positive imaginary part, corresponding to a decreasing exponential behavior for large ρ.

To study this region, we change variables to $x=\hat{\rho}\cdot\hat{P}/P$, the component of $\hat{\rho}$ parallel to $\hat{P}$, and the 5-vector y defined in terms of the component of $\hat{\rho}$ perpendicular to $\hat{P}$, $\hat{\rho}_\perp$, by $y=\hat{\rho}_\perp/x$. We may use y in place of $\hat{\rho}_\mu$ in (4) to specify directions in the six-dimensional space. After substituting (3) into (6) we obtain

$$\begin{aligned}f_F(E)=&-2K(2\pi)^{-3}\eta(\hat{P}_\mu)f_0(\hat{P}_\mu)\\&\times\int dx\,x^5\,d^5y\,\rho^{-7/2+i\eta(\hat{\rho}_\mu)}e^{i(K\rho-Px)},\end{aligned} \tag{8}$$

where we have replaced the slowly varying factor $\eta(\hat{\rho}_\mu)f_0(\hat{\rho}_\mu)$ by its value in the stationary direction. The region of interest is x large, y small, so that we approximate $\rho=x(1+y^2)^{1/2}\approx x+\frac{1}{2}xy^2$ in the exponent and elsewhere replace ρ by x. The most important term for $K\approx P$ is found when $\eta(\hat{\rho}_\mu)$ inside the integral in (8) is replaced by $\eta(\hat{P}_\mu)$. With these approximations, the integrations over y may be carried out to give, for $K\approx P$,

$$\begin{aligned}f_F(E)\approx{}&2K^{-3/2}(2\pi)^{-1/2}e^{i\pi/4}\eta(\hat{P}_\mu)f_0(\hat{P}_\mu)\\&\times\int_A^\infty dx\,e^{i(K-P)x}x^{i\eta(\hat{P}_\mu)-1}\,.\end{aligned} \tag{9}$$

These approximations do violence to the contribution from finite ρ, so that we have begun the integral from a positive value A, and we should add an unknown constant to (9).

The above argument has led to the very reasonable conclusion that the part of coordinate space which gives rise to the singular part of $f_F(E)$ is that where the electrons would be if they traveled from the origin with momenta $\vec{p}_1,\vec{p}_2$. The additional terms in (4) corresponding to two-body channels with hydrogen in its various excited states do not affect the argument unless $\vec{p}_1=0$ or $\vec{p}_2=0$. For these values, and also for $\vec{p}_1=\vec{p}_2$, we expect $f_F(E)$ to be singular, and they are omitted from the discussion.

The behavior of the integral may be studied by change of variable $x=it/(K-P)$ to yield

$$\int_A^\infty dx\,e^{i(K-P)x}x^{i\eta-1}=[-i(K-P)]^{-i\eta}\int_{-iA(K-P)}dt\,e^{-t}t^{i\eta-1}. \tag{10}$$

A change of the lower limit to zero merely adds an analytic function of $K-P$, so that we have

$$\begin{aligned}\int_A^\infty dx\,e^{i(K-P)x}x^{i\eta-1}=\Gamma(i\eta)[-i(K-P)]^{-i\eta}\\+(\text{a function analytic at } K=P).\end{aligned} \tag{11}$$

Assembling these results, we obtain (5), with the possible addition of an unknown constant.

It can be shown that the constant is zero. One argument is to use an equation for Φ, derived from (7), that reads, with T the kinetic-energy operator,

$$|\phi\rangle = (E-T)^{-1}(E-k^2-E_\alpha)|\vec{k},\alpha\rangle + (E-T)^{-1}V_0|\phi\rangle \tag{12}$$

or

$$\Phi(\hat{\rho}) = \chi(\hat{\rho}) + (2\pi)^{-3}\int d\hat{P}e^{i\hat{P}\cdot\hat{\rho}}(E-P^2)^{-1}\langle\hat{P}|V_0|\Phi\rangle. \tag{13}$$

Here χ represents the inhomogeneous term, not important to our reasoning.

The asymptotic form (4) must follow from the integral in (13). An argument similar to that used above (see Nuttall[5]) shows that it is the region $\hat{P}=K\hat{\rho}_\mu$ that dominates, and the form (5) may be substituted for $\langle\hat{P}|V_0|\Phi\rangle$. The singular part of (5) leads to the required behavior (4), but a constant term in (5) gives a term $\Phi\sim e^{iK\rho}\rho^{-5/2}\times$const, which is unacceptable, and so the constant must be zero. There is no reason why a term of the form $(K-P)\times$(function analytic at $K=P$) cannot be present.

The nature of further terms in the expansion of $f_F(E)$ about $K=P$ may be deduced from the form of the complete expansion for $\Phi(\hat{\rho})$, of which (4) is the leading term. According to Peterkop,[3] we have

$$\Phi(\hat{\rho}) \underset{\rho\to\infty}{\sim} \frac{e^{iK\rho}}{\rho^{5/2}}\rho^{i\eta(\hat{\rho}_\mu)}\sum_{m=0}^{\infty}\sum_{p=0}^{2m}A_{mp}(\hat{\rho}_\mu)\frac{(\ln\rho)^p}{\rho^m}, \tag{14}$$

where

$$A_{00}(\hat{\rho}_\mu)=f_0(\hat{\rho}_\mu).$$

We expect from this to find that

$$f_F(E)\sim(K-P)^{i\eta(P_\mu)} \times\sum_{m=0}^{\infty}\sum_{p=0}^{2m}B_{mp}(\hat{P}_\mu)(K-P)^m[\ln(K-P)]^p, \tag{15}$$

where B_{00} is given by (5).

We shall now show that the coefficient of the first correction, B_{12}, is zero, so that after (5), the most important contribution to $f_F(E)$ has the form

$$B_{11}(\hat{P}_\mu)(K-P)^{-i\eta(\hat{P}_\mu)+1}\ln(K-P). \tag{16}$$

The coefficient $B_{11}(\hat{P}_\mu)$ can be evaluated in terms of derivatives of $f_0(\hat{P}_\mu)$, but this is not done here.

Contributions to B_{12} come from two sources: (a) expanding $\eta(\hat{\rho}_\mu)$ inside the integral in (8) and (b) including the A_{12} term in the expansion (14). To deal with source (a), we think of η as a function of y, $\eta(\hat{\rho}_\mu)\equiv n(y)$, and expand:

$$n(y)\approx\eta(\hat{P}_\mu)+y\cdot\nabla n. \tag{17}$$

The integral in (8) leads to

$$\int dx\, x^{3/2+i\eta(\hat{P}_\mu)}e^{i(K-P)x}\int d^5y\, e^{iKxy^2/2}\exp(iy\cdot\nabla n\ln x). \tag{18}$$

The exponential is expanded as

$$\exp(iy\cdot\nabla n\ln x)\approx 1+iy\cdot\nabla n\ln x-\tfrac{1}{2}(y\cdot\nabla n)^2(\ln x)^2. \tag{19}$$

The first term leads to (5), the second gives zero after the y integration, and the third results in

$$+e^{i\pi/4}(\nabla n)^2 2^{3/2}\pi^{5/2}K^{-7/2}\int dx\, x^{i\eta(\hat{P}_\mu)-2}e^{i(K-P)x}(\ln x)^2. \tag{20}$$

The most singular part of the integral here is $\Gamma(i\eta-1)[-i(K-P)]^{-i\eta+1}[\ln(K-P)]^2$, so that the contribution to B_{12} from source (a) is

$$e^{-i\pi/4}(2\pi)^{-1/2}K^{-5/2}(\nabla n)^2\eta f_0(\hat{P}_\mu)(-i)^{-i\eta+1}\Gamma(i\eta-1). \tag{21}$$

Substitution into Schrödinger's equation shows that

$$A_{12}(\hat{\rho}_\mu)=-[(\nabla n)^2+(y\cdot\nabla n)^2]f_0(\hat{\rho}_\mu)/2ik. \tag{22}$$

If the A_{12} part of Φ is inserted into (6), it is found that only the first term in (19) gives rise to a contribution of the required order, and that this contribution is the negative of (21).

The analysis of the amplitude $f_P(E)$ proceeds in a similar manner. A definition of $f_P(E)$ that is valid for both real and complex values of E is

$$f_P(E)=\int d\hat{\rho}\,\psi^*(\vec{p}_1,z_1,\vec{r}_1)\psi^*(\vec{p}_2,z_2,\vec{r}_2)[V_0-\overline{V}]\,\Phi(\hat{\rho}), \tag{23}$$

where

$$\overline{V}=-2z_1/r_1-2z_2/r_2 \tag{24}$$

and $\psi(\vec{p},z,\vec{r})$ is a Coulomb wave function for charge z with ingoing scattered waves. If $\mathrm{Im}E>0$, we may use the equations satisfied by ψ and Φ to rewrite (23) as

$$f_P(E)=(K^2-P^2)\int d\hat{\rho}\,\psi^*(\vec{p}_1,z_1,\vec{r}_1)\psi^*(\vec{p}_2,z_2,\vec{r}_2)\Phi(\hat{\rho}), \tag{25}$$

since the contribution of the surface term that appears when the kinetic-energy operator is switched is zero. Our previous techniques show that the integral in (25) has a pole at $K=P$ and that the leading correction term is again zero. As a resutl, we find

$$f_P(E)\underset{K\to P}{\sim}\left(\frac{2}{\pi}\right)^{1/2}P^{-3/2}e^{-i3\pi/4}\left(\frac{2p_1^2}{P}\right)^{-iz_1/p_1}\left(\frac{2p_2^2}{P}\right)^{-iz_2/p_2} \times f_0(\hat{P}_\mu)+C(\hat{P}_\mu)(K-P)[\ln(K-P)]+\cdots, \tag{26}$$

provided that z_1 and z_2 are chosen so that $z_1/p_1+z_2/p_2=\eta(\hat{P}_\mu)$. This result agrees with that given by Rudge[6] for the value of (23) when $K=P$, after

inserting an overlooked factor of i. The coefficient C of the leading correction term in (26) may be calculated in terms of known quantities.

It may be of interest to point out that (23) may be rewritten as

$$f_P(E)=\int d\hat{\rho}\,\{[H-P^2]\psi^*(\vec{p}_1,z_1,\vec{r}_1)\psi^*(\vec{p}_2,z_2,\vec{r}_2)\}\,\Phi(\hat{\rho})\,, \tag{27}$$

which compares with Rudge's formula (2.42). It is important to use P^2 in (27) rather than E, which would lead to $f_P(E)=0$ for $\mathrm{Im}E>0$.

III. TWO-PARTICLE COULOMB SCATTERING

A singularity such as that found in $f_F(E)$ is present whenever the final (or initial) state contains at least two charged constituents. The simplest example of this situation is the scattering of two particles interacting via the Coulomb potential. Since this problem can be solved in terms of easily calculated known functions, it provides a testing ground for methods of performing the extrapolation.

A suitable starting point is the work of Schwinger on the Coulomb Green's function in momentum space.[7] Let us define $f(E)$ by

$$\langle\vec{p}\,|\,[V+V(E-H)^{-1}V]\,|\vec{p}\,'\rangle\,, \tag{28}$$

where H is the Hamiltonian for the problem and V is the Coulomb potential. Using the definition $G(\vec{p},\vec{p}\,')=\langle\vec{p}\,|(E-H)^{-1}|\vec{p}\,'\rangle$, we can show that (with Schwinger's notation)

$$G(\vec{p},\vec{p}\,')=\delta(\vec{p}-\vec{p}\,')(E-T)^{-1}+(E-T)^{-1}f(E)(E-T')^{-1}. \tag{29}$$

From Eq. (1′) of Schwinger we deduce

$$f(E)=-\frac{Ze^2}{2\pi^2 t}-\frac{Ze^2 i\eta}{2\pi^2}\int_0^1 d\rho\,\rho^{-i\eta}\,[t\rho-y(1-\rho)^2]^{-1}\,, \tag{30}$$

where

$$t=(\vec{p}-\vec{p}\,')^2,\quad \eta=Ze^2/2k\,,$$

$$y=\frac{(E-T)(E-T')}{4E}\,,\quad E=k^2,\quad 2m=1\,.$$

Ford[8] has shown how to write this formula in terms of hypergeometric functions.

Physical scattering in a nonforward direction is characterized by

$$E=T=T'=\vec{p}^{\,2}/2m=\vec{p}\,'^2/2m\,,\quad t>0\,.$$

However, Schwinger shows that $T(E)$ is singular at this value. In fact, if we set $\vec{p}^{\,2}=\vec{p}\,'^2$, i.e., $T-T'$, we find for E near T, $t>0$, that

$$f(E)\sim(k-p)^{-2i\eta}f_c\,, \tag{31}$$

with

$$f_c=-\left(\frac{2\pi\eta_0}{e^{2\pi\eta_0}-1}\right)\frac{Ze^2}{2\pi^2 t}\,e^{i\eta_0\ln t},\quad \eta_0=Ze^2/2p\,. \tag{32}$$

The singular factor $(k-p)^{-2i\eta}$ is analogous to that in the three-particle case, except that since both initial and final states contain charged pairs, the exponent involves 2η rather than η. The nonsingular factor f_c differs from the normal Coulomb scattering amplitude by a factor independent of direction. We shall not discuss how this factor might be determined, for in e-H ionization, this difficulty, relating to the normalization of the initial state, disppears.

Corrections to (31) may be determined from the work of Ford, giving the result that

$$f(E)=(k-p)^{-2i\eta}f_c g_1(k)+(k-p)g_2(k)\,, \tag{33}$$

where $g_1(k)$ and $g_2(k)$ are analytic functions near $k=p$ that are nonzero at $k=p$, with $g_1(p)=1$.

In a realistic calculation of ionization, we would determine f at a number of complex values of k—say, $k=k_j$, $j=1,\ldots,N$—inevitably introducing numerical errors, and then attempt to extrapolate to $k=p$ to find f_c.

In the present example we are able to calculate the values of f at $k=k_j$ (call them f_j, $j=1,\ldots,N$) with very high precision, but we remember that this may not be possible in the three-body problem, and we must be concerned with the effect of errors in f_j on the extrapolation process.

In Fig. 1 we plot the function $d(k)=f(E)\times\exp[2i\eta\ln(k^2-p^2)]$ against $\mathrm{Im}k$, for $\mathrm{Re}k=p=3$, $Ze^2=6$, and $t=9$. As expected from (33), this function approaches f_c in a relatively smooth manner. Extrapolation by eye would be possible from a reasonable distance away from the real axis if results of high accuracy were not required.

It should be possible to utilize the information about the nature of the singularity at $k=p$ that is contained in (33) to improve the accuracy of the extrapolation procedure. A way of doing this is to try to represent $g_1(k)$ and $g_2(k)$ by rational fractions of the form

$$g_1(k)=\left(\sum_{i=0}^{l}a_i(k-p)^i\right)\Big/\left(\sum_{i=0}^{n}c_i(k-p)^i\right)\,,$$

$$g_2(k)=\left(\sum_{i=0}^{m-1}b_i(k-p)^i\right)\Big/\left(\sum_{i=0}^{n}c_i(k-p)^i\right)\,, \tag{34}$$

with $a_0=c_0=1$. If we choose $l+m+n=N$, then the coefficients $[a_i,b_i,c_i]$ may be determined from the f_j by inserting (34) into (33) and evaluating at $k=k_j$, $j=1,\ldots,N$. The results of such a procedure are shown in Table I. It is apparent that quite accurate estimates can be obtained. However, we find that the method is extremely sensitive to errors in the values of f_j used, and in realistic prob-

lems it may be difficult to obtain f_j with sufficient accuracy.

A more stable method, which we have studied briefly, is to modify the last approach by taking $l+m+n<N$. Suppose that for a given choice of $[a_i, b_i, c_i]$ the values of f_j and f_c given by (33) are $\bar{f}_j$ and $\bar{f}_c$. The quantities of interest that measure the errors in f_c and f_j are then

$$\delta = |\bar{f}_c - f_c|^2, \quad \Delta = \sum_{j=1}^{N} |\bar{f}_j - f_j|^2 .$$

If in a realistic calculation we believe that our calculations of f_j might be in error by up to a given amount, then there is little point in finding values of $[a_i, b_i, c_i]$ that make Δ significantly less than some corresponding value Δ_0. We must consider as equally possible all values of $\bar{f}_c$ that correspond to choices of $[a_i, b_i, c_i]$ that give $\Delta < \Delta_0$.

In the present test case, we have considered, for $p=3$, $Ze^2=6$, and $t=10$, two different choices of the points k_j. The two choices were

(a) $k_j = 3 + i0.2(0.025)0.55$ (15 points),

(b) $k_j = 3 + [0.3(0.025)0.475]\, e^{i\eta\pi/4}$, $\eta = 1, 2, 3$ (24 points).

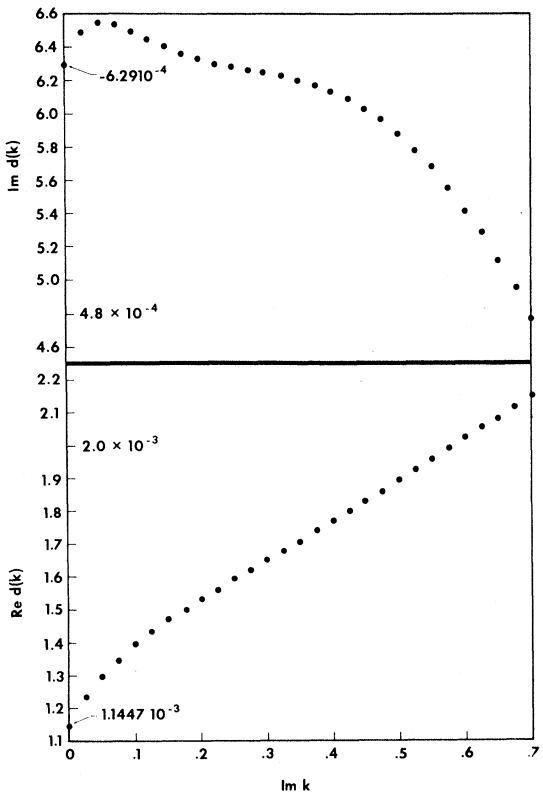

FIG. 1. Graphs of the real and imaginary parts of the function $d(k)$ plotted against Imk for the case Re$k=p=3$, $Ze^2=6$, and $T=9$.

TABLE I. Estimates of f_c obtained by the rational fraction fit described in the text for the case Re$k_j = p = 3$, $Ze^2=6$, and $t=10$, using Im$k_j = 0.3(0.025)0.525$. The integers l, m, and n relate to the type of rational fractions used. The correct answer is $f_c = (1.084 - 0.455i)\times 10^{-3}$.

Re$f_c\times10^3$	Im$f_c\times10^3$	l	m	n
0.988	−0.165	1	1	1
0.943	−0.403	1	1	2
0.824	−0.262	1	2	1
1.026	−0.498	1	1	3
0.864	−0.538	1	2	2
1.101	−0.401	2	2	1
1.091	−0.475	1	1	4
1.091	−0.600	1	2	3
1.073	−0.434	2	2	2
1.069	−0.416	2	3	1
1.099	−0.438	1	1	5
1.165	−0.469	1	2	4
1.092	−0.444	2	2	3
1.094	−0.459	2	3	2
1.100	−0.435	3	3	1
1.109	−0.396	1	1	6
1.174	−0.415	1	2	5
1.179	−0.402	2	2	4
1.065	−0.294	2	3	3
1.050	−0.419	3	3	2
1.077	−0.365	3	4	1
1.174	−0.238	1	1	7
1.240	−0.323	1	2	6
1.176	−0.441	2	2	5
1.065	−0.371	2	3	4
1.022	−0.471	3	3	3
1.032	−0.452	3	4	2
1.116	−0.428	4	4	1
1.413	0.175	1	1	8
1.307	−0.292	1	2	7
1.113	−0.423	2	2	6
1.081	−0.400	2	3	5
1.085	−0.500	3	3	4
1.139	−0.509	3	4	3
1.076	−0.451	4	4	2
1.089	−0.433	4	5	1

The smallest values of Imk_j are about the same in each case, so that we expect that the f_j could be calculated with comparable accuracy.

Our results show that, in each of these two cases, if f_j were known to $\frac{1}{10}\%$, then we could estimate f_c to about 5%, with choice (b) providing a marginally superior accuracy.

These studies on the two-particle problem cannot be used to estimate the accuracy of the results of an ionization calculation but should provide some guide as to the relative effectiveness of alternative extrapolation schemes.

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Resonant Interaction between Two Neutral Atoms*

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A standard formalism of quantum electrodynamics is used to investigate the interaction between two neutral atoms. The study is based on an approximate solution of the two-particle Green's function. The frequency distribution of the photon scattering is obtained. We also consider the self-stimulation effect when both atoms are in excited states.

I. INTRODUCTION

The two-atom problem has drawn considerable interest since the advent of lasers and masers. In fact, by using the Weisskopf-Wigner method, this problem has been solved exactly by Ernst and Stehle,[1] who deal with the atoms interacting with a common radiation field. The purpose of their work is partly directed toward constructing a rigorous description of the behavior of an ensemble of atoms and using some characteristics of the two-atom solution as a check for the approximate solution of the N-atom problem. In the present work, we shall use a different approach, based on the approximate solution of the Bethe-Salpeter equation,[2] to discuss the physical properties of the two-atom interaction. In particular, we shall pay some attention to the problem of the frequency shift of the emitted photons due to the resonant interaction; such a shift has been ignored in the Weisskopf-Wigner method of Ernst and Stehle. Several other features contained in our solution will be discussed in detail.

In Sec. II, we solve the Bethe-Salpeter equation in the ladder approximation. The approximate solution for the two-particle Green's function is then applied in Sec. III to discuss the interaction between two neutral atoms when no external field exists, and the results are compared with those obtained by others.[3-5] In Sec. IV, we consider low-intensity photon scattering, taking the two-atom interaction into account. We obtain an expression for the frequency distribution of the emitted photons. Our result is different from that derived by Fontana and Hearn[6] when the separation of the two atoms is not very small compared with the wavelength of the emitted light. Finally, in Sec. V, we study the decay of two excited atoms. Complete agreement with the work of Ernst and Stehle[1] on the two-atom problem is obtained. The extension of the present approach to the N-atom problem for a laser model is deferred to a future publication.

Appendixes A and B contain the necessary algebra to complete the derivations omitted in the text. Finally, a brief derivation of the natural line shape for a single isolated atom using the standard quantum-electrodynamical (QED) formalism is given in Appendix C; the result agrees with that of the Weisskopf-Wigner method.[7]

II. SOLUTION FOR THE TWO-PARTICLE GREEN'S FUNCTION IN THE LADDER APPROXIMATION

The two-atom problem has been considered extensively by Ernst and Stehle[1] using the method of Weisskopf and Wigner, and by Stephen[3] and many others using time-dependent perturbation methods. We now present a different method based on the Bethe-Salpeter equation and compare the results with the previous works. We solve the Bethe-Salpeter equation for the two-particle Green's function in the ladder approximation in this section, and apply the resulting two-particle Green's function to discuss the nature of interactions of the two neutral atoms in Sec. III. A further application of this Green's function to the photon scattering problem is given in Secs. IV and V.

Consider the integral form of the Bethe-Salpeter equation