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Theory of K-shell ionization during nuclear resonance scattering

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Recently the measured proton-induced C K-shell ionization probability was found to vary significantly near the 0.461-MeV $j=\frac{1}{2}+$ elastic resonance in ^{12}C. Since the resonance was so wide that time-delay effects on K-shell ionization should be very small, it was hypothesized that this effect was due to the exchange of angular momentum between the projectile motion and electron. Assuming a potential description of the nuclear scattering, we make a completely quantum-mechanical calculation of the ionization probability in the distorted-wave Born approximation and show that angular momentum effects do not account for these results. We also show how the amplitude for monopole excitation is augmented by the "shake-off" or "sticking" term found in the semiclassical theory of Ciocchetti and Molinari, and display the formal correspondence between the semiclassical and quantum-mechanical theories. Numerical calculations of the ionization probability show only a slight dip at the minimum in the p-C elastic cross section, opposite in sign and of much smaller magnitude than the reported variation.

I. INTRODUCTION

In most atomic-collision studies, nuclear physics plays no role. Some years ago, however, Ciocchetti and Molinari[1] pointed out that a semiclassical description of K-shell ionization leads to a modified ionization probability P_K when there is a nonnegligible nuclear reaction time or time delay t_0. A similar modification[2] results when a completely quantum-mechanical description of the ionization is made; from this point of view, for there to be an appreciable variation in $P_K(\theta, E)$, it is necessary that the reaction amplitude vary sufficiently rapidly with incident center-of-mass energy E.

To test these predictions, one naturally thinks of measuring the ionization probability in the vicinity of a nuclear resonance. For P_K to vary significantly across a resonance, the width Γ of the resonance should be of the order of or smaller than the K-shell binding energy U_K, or equivalently, the time delay $t_0(\sim h/\Gamma)$ should be of the order of or greater than the K-shell orbiting period. Significant variations in the K-shell ionization probability have been observed in the elastic scattering of protons from ^{58}Ni across the $s_{1/2}$ resonance at E_p (lab)$=3.15$ MeV (Ref. 2) and from ^{88}Sr near the $d_{5/2}$ isobaric analog resonance at 5.06 MeV (Ref. 3), reactions for which Γ and U_K are of comparable magnitude.

In the light of the above, the recent measurements of Duinker *et al.*[4] who found a strongly varying $P_K(\theta, E)$ in p-^{12}C scattering near the 0.461-MeV $s_{1/2}$ resonance, whose width $\Gamma(=38$ keV) was much greater than $U_K(=0.284$ keV), are very surprising. Duinker *et al.*[4] hypothesized that this variation was due to the angular-momentum exchange between the projectile and the electron. Conceivably this enters in because when K elec- are excited into p-wave continuum states, the projectile must lose one unit of orbital angular momentum. Therefore, to excite an $l=0$ nuclear resonance and to excite the electron on the way into the collision, the incoming projectile wave must be an $l=1$ wave; to excite the electron on the way out, the incoming projectile wave must be an s wave.

The effect of the exchange of angular momentum on the K-shell ionization probability near a nuclear resonance is a leading concern of this paper. We calculate the K-shell ionization probability in the

distorted-wave Born approximation (DWBA), making a partial-wave expansion of the incoming and outgoing projectile waves, and taking explicit account of the coupling between the electronic and projectile angular momenta. A slightly corrected version of Eq. (1) in Ref. 2 is derived. We shall find that when $\Gamma >> U_K$, $P_K(\theta, E)$ should be almost independent of E, in disagreement with Duinker's hypothesis.

In Sec. II the ingredients of the DWBA calculation are described. The relative projectile space is separated into an exterior and an interior region and an approximate evaluation of the exterior contribution to the ionization amplitude is made in Sec. III. The corrections to this coming from the interior region are considered in Sec. IV; only the inner contribution of monopole excitation is found to be important. Our present expressions are compared to those of previous quantum-mechanical and semiclassical descriptions in Sec. V. The formulas are specialized to sub-Coulomb resonant scattering and numerical calculations are described for the case of p-^{12}C scattering in Sec. VI. Details concerning the various semiclassical theories are given in the Appendix.

II. DWBA AMPLITUDE

As a model of the ionization process, we consider the three-body system comprised of an incident nuclear projectile with charge Z_1e, a spin-zero target nucleus of mass M_2 and charge Z_2e from which the projectile scatters elastically, and an electron initially bound to the target nucleus in the K-shell orbit. We assume that the nuclear scattering is described by a spherically symmetric potential $V_N(R)$ which is the sum of the Coulomb and a specifically nuclear term (which may be complex). Such a potential description does not suffice to describe most nuclear resonances; however, for $p+^{12}$C scattering it is a rather good approximation to consider the 461-keV $s_{1/2}$ resonance as a slightly unbound $2s$ single-particle state. The virtues of the potential model are: (1) the familiar procedures of the distorted-wave Born approximation may be used to calculate the amplitudes for ionization during a nuclear scattering and (2) the wave function of the nuclear system, even when the projectile is in the interior of the target nucleus, is then only a function of the internuclear coordinate $\vec{R}$ and is calculable. This permits us to examine explicitly the contributions to the ionization when the projectile and target nuclei overlap.

In the distorted-wave Born approximation, the differential cross section for the ionization of a K-shell electron by projectiles of center-of-mass energy E scattering to the angle θ is given by[5]

$$\frac{d\sigma_K}{d\Omega}=\sum_{\lambda\mu}\int_0^\infty d\epsilon_f \,|A_{\epsilon_f\lambda\mu}(E,\theta)|^2 , \tag{1}$$

where ϵ_f, λ, and μ are the energy and orbital quantum numbers for the ionized electron and $\vec{R}$, respectively. Assuming that there is a long-range convergence factor in the R coordinate and using the Ehrenfest theorem, one finds that the matrix elements of H_R above are equivalent to those of the form

$$A_{\epsilon_f\lambda\mu}=\frac{\sqrt{KK'}}{2\pi\hbar v}\langle\chi^-(\vec{K}',\vec{R})\phi_{\epsilon_f\lambda\mu}(\vec{r})\,|\,H'\,|\,\chi^+(\vec{K},\vec{R})\phi_{1s}(\vec{r})\rangle \tag{2}$$

and

$$H'=\frac{-Z_1e^2}{|\vec{r}-\vec{R}|}+H_R \ . \tag{3}$$

Here $\vec{K}$ and $\vec{K}'$ are the initial and final center-of-mass momenta, v is the initial velocity of the projectile relative to the target nucleus, $\vec{r}$ is the electron coordinate relative to the target and $\phi_{\epsilon_f\lambda\mu}$ and ϕ_{1s} are the final and initial electronic wave functions.

It follows from a straightforward calculation that the recoil Hamiltonian H_R for the present choice of coordinates has the form[1]

$$H_R=\frac{\vec{p}\cdot\vec{P}}{M_2} , \tag{4a}$$

where $\vec{p}$ and $\vec{P}$ are the momenta conjugate to $\vec{r}$

$$H_R=\frac{mM\omega^2}{M_2}\vec{R}\cdot\vec{r} \tag{4b}$$

or[6,7]

$$H_R=\frac{m}{M_2}\vec{\nabla}_R V_N(R)\cdot\vec{r} , \tag{4c}$$

where

$$\hbar\omega\equiv\Delta E\equiv U_K+\epsilon_f$$

is the energy transferred to the electron, M is the reduced mass of the projectile and target nuclei,

and m is the reduced mass of the electron-target nucleus system.

The nuclear distorted wave χ^+ may be given by the partial-wave expansion[5]

$$\chi^+(\vec{K},\vec{R})=4\pi\sum_{lm} i^l Y^*_{lm}(\hat{K})Y_{lm}(\hat{R})(KR)^{-1} \times e^{i\delta_l}\mathcal{F}_l(KR) , \quad (5)$$

where $\mathcal{F}_l$ is the exact radial wave function for the nuclear Hamiltonian $H_N=T_N+V_N$, subject to the boundary condition

$$\lim_{R\to 0}\mathcal{F}_l(KR)\sim R^{l+1} \quad (6a)$$

and the normalization condition

$$\lim_{R\to\infty}\mathcal{F}_l(KR)=\sin\left[KR-\eta\ln(2KR)-\frac{l\pi}{2}+\delta_l(E)\right] . \quad (6b)$$

Here $\eta\equiv Z_1Z_2e^2/\hbar v$ and $\delta_l(E)$ is the sum of the Coulomb and specifically nuclear (possibly complex) phase shifts for the lth partial wave. The logarithmic term in the argument in Eq. (6b) is a ubiquitous consequence of the long-range nature of Coulomb distortion. Except for obvious changes in notation, the final-state distorted-wave function corresponding to energy $E'=E-\Delta E$, $\chi^-(\vec{K}',\vec{R})^*$, is also given by Eq. (5) when use is made of the property

$$\chi^-(\vec{K}',\vec{R})^*=\chi^+(-\vec{K}',\vec{R}) . \quad (7)$$

The matrix elements of the electronic wave functions can readily be evaluated.[7,8] Their dependence on $\vec{R}$ is conveniently written as

$$\frac{1}{\hbar v}\langle\phi_{\epsilon_f\lambda\mu}|H'|\phi_{1s}\rangle=G_\lambda(R)\left[\frac{4\pi}{2\lambda+1}\right]^{1/2}Y^*_{\lambda\mu}(\hat{R}) , \quad (8)$$

with $G_\lambda\equiv C_\lambda+W_\lambda$. Here, C_λ is the matrix element originating from the Coulomb potential part of H' in Eq. (3), and W_λ originates from the recoil contribution Eq. (4). Explicitly we have

$$C_\lambda(R)=\frac{-Z_1e^2}{\hbar v}(2\lambda+1)^{-1/2}\int_0^\infty r^2dr\,\mathcal{R}_{\epsilon_f\lambda}\mathcal{R}_{1s}\frac{r_<^\lambda}{r_>^{\lambda+1}} \quad (9)$$

and

$$W_\lambda(R)=\delta_{\lambda1}\frac{m}{\hbar vM_2\sqrt{3}}(M\omega^2R)\int_0^\infty dr\,r^3\mathcal{R}_{\epsilon_f\lambda}\mathcal{R}_{1s} , \quad (10)$$

where $\mathcal{R}_{\epsilon_f\lambda}$ and $\mathcal{R}_{1s}$ are the radial electronic wave functions. As mentioned earlier, an equivalent matrix element for $W_\lambda(R)$ is obtained by replacing $(M\omega^2R)$ with $(\partial V_N/\partial R)$.

We take the quantization axis to be along $\hat{K}$ so that

$$Y^*_{lm}(\hat{K})=\delta_{m0}\left[\frac{2l+1}{4\pi}\right]^{1/2} . \quad (11)$$

Inserting Eqs. (5) and (8) into Eq. (2) and carrying out the integration over $\hat{R}$, we obtain the following basic formula for the ionization amplitude in the distorted-wave Born approximation:

$$A_{\epsilon_f\lambda\mu}=\frac{8\pi}{(KK')^{1/2}}\sum_{ll'}(i)^{l-l'}e^{i(\delta_l+\delta'_{l'})}\left[\frac{(2l+1)^2}{4\pi(2l'+1)}\right]^{1/2}Y^*_{l'\mu}(\hat{K}')C(l\lambda l'000)C(l\lambda l'0\mu\mu) \times\int dR\,\mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)G_\lambda(R) . \quad (12)$$

III. ASYMPTOTIC EVALUATION

As a preliminary to the evaluation of the radial integrals in Eq. (12) let us consider the various lengths which characterize the electronic-nuclear system.[9] The most important parameters governing the electronic ionization are the K-shell radius for the target

$$a(Z_2)=(\hbar^2/Z_2e^2m)$$

and the inverse of the minimum momentum transfer

$$(1/q)\equiv 1/(K-K')\cong(v/\omega) .$$

The nuclear scattering is characterized by three distances: $D\equiv Z_1Z_2e^2/E$, the distance of closest

approach for a head-on Coulomb internuclear collision; $(1/K)$, the wavelength for relative nuclear motion; and R_N, a radius parameter for the specifically nuclear potential. The ratio of $(D/2)$ to $(1/q)$ is the familiar[10] dimensionless parameter ξ, which here is a measure of the importance of nuclear Coulomb distortion.

It is crucial to our approximate evaluation of the radial matrix elements that there exist a "matching radius" R_m between the electronic and nuclear distances, such that

$$(1/q), a(Z_2) >> R_m >> D, \ (1/K), \text{ and } R_N \ . \tag{13}$$

For K-shell ionization of ^{12}C by 0.461-MeV protons, the length parameters have the approximate values $(1/q)\sim 2(10^{-9})$ cm, $a(Z_2)\sim 0.9(10^{-9})$ cm, while $D\sim 2.0(10^{-12})$ cm, $(1/K)\sim 0.7(10^{-12})$ cm, and $R_N\sim 0.4(10^{-12})$ cm. Thus a choice $R_m \sim 40(10^{-12})$ cm amply satisfies these inequalities.

Our evaluation of the radial integrals proceeds by splitting the radial integral into two contributions, one exterior to R_m, the other interior to R_m. The virtue of this procedure is that, provided the inequalities above are satisfied, the asymptotic expression for the radial wave functions, Eq. (6b), can be used in the exterior integral.

With the asymptotic approximation, the exterior radial integral in Eq. (12) is the sum of four terms. Two of these, however contain the rapidly oscillating factors $e^{\pm i(K+K')R}$, so that their integrals may be neglected. (This neglect corresponds to the intuitively obvious observation that electron ionization will not reverse the direction of relative nuclear motion.) The remaining two terms give

$$4\int_{R_m}^{\infty} dR\, \mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)G_\lambda(R) \cong b_\lambda e^{i(\delta_l-\delta'_{l'})}(i)^{l'-l}+b^*_\lambda e^{i(\delta'_{l'}-\delta_l)}(i)^{l-l'} \ , \tag{14}$$

where

$$b_\lambda = \int_{R_m}^{\infty} dR\, G_\lambda(R)\exp(i\bar{q}R) \tag{15}$$

and

$$\bar{q}R \equiv qR - \eta \ln 2KR + \eta' \ln 2K'R \approx qR - \xi \ln 2KR. \tag{16}$$

It is important to note that the "exterior atomic amplitude" b_λ is independent of l and l'.

Equation (12) can now be written as the sum of two terms A_1 and A_2, where

$$A_1 = \frac{4\pi}{2K}\sum_{ll'} e^{2i\delta_l}\left[\frac{(2l+1)^2}{(2l'+1)4\pi}\right]^{1/2} Y^*_{l'\mu}(\hat{K}') \times C(l\lambda l'000)C(l\lambda l'0\mu\mu)b_\lambda \ , \tag{17}$$

and

$$A_2 = \frac{4\pi}{2K}\sum_{ll'} (-1)^{l-l'} e^{2i\delta'_{l'}}\left[\frac{(2l+1)^2}{(2l'+1)4\pi}\right]^{1/2} Y^*_{l'\mu}(\hat{K}') \times C(l\lambda l'000)C(l\lambda l'0\mu\mu)b^*_\lambda \ . \tag{18}$$

At first glance these expressions still appear fairly cumbersome, in spite of the elimination of the radial integral. Exploiting some lore[11] concerning angular momentum, however, we shall see that these expressions collapse to simple formulas which have direct physical interpretation.

For A_1 it is convenient first to make the rearrangement

$$A_1 = \frac{4\pi}{2K}\sum_{ll'} e^{2i\delta_l}\left[\frac{4\pi}{2\lambda+1}\right]^{1/2}\left[\frac{2l+1}{4\pi}\right]^{1/2} b_\lambda \left[\left[\frac{(2l+1)(2\lambda+1)}{(2l'+1)4\pi}\right]^{1/2} C(l\lambda l'000)C(l\lambda l'0\mu\mu)Y^*_{l'\mu}(\hat{K}')\right] . \tag{19}$$

The index l' occurs only in the last bracket. When summed over l', this bracket is just the coupling rule for spherical harmonics.[11] We thus obtain

$$A_1 = \frac{4\pi}{2K}\sum_{l} e^{2i\delta_l}\left[\frac{4\pi}{2\lambda+1}\right]^{1/2}\left[\frac{2l+1}{4\pi}\right]^{1/2} \times Y_{l0}(\hat{K}')Y^*_{\lambda\mu}(\hat{K}')b_\lambda = if(\theta,E)D^\lambda_{\mu 0}(\hat{K}')b_\lambda \ , \tag{20}$$

where[11]

$$D^\lambda_{\mu 0}(0,\theta,0) = \left[\frac{4\pi}{2\lambda+1}\right]^{1/2} Y^*_{\lambda\mu}(\hat{K}') \ , \tag{21}$$

and

$$f(\theta,E) = (2iK)^{-1}\sum_l (2l+1)P_l(\cos\theta)e^{2i\delta_l(E)} \ . \tag{22}$$

The sum $f(\theta, E)$ is the nuclear scattering amplitude for spinless projectiles[12] provided the scattering angle does not equal zero. Here, the scattering is assumed to lie in the xz plane so that the direction $\hat{K}'$ is specified solely by the scattering angle θ.

For the A_2 term, we note first that by conservation of parity the factor $(-1)^{l-l'}$ may be written as $(-1)^{\lambda}$, independent of the nuclear angular-momentum quantum numbers. Inverting the order in the Clebsch-Gordan coefficients,[11]

$$C(l\lambda l'000)C(l\lambda l'0\mu\mu)=\left[\frac{2l'+1}{2l+1}\right](-1)^{2\lambda-\mu}C(l'\lambda l000)C(l'\lambda l-\mu\mu 0)\,, \tag{23}$$

we have

$$A_2=\frac{4\pi}{2K}\sum_{ll'}(-1)^{\lambda-\mu}e^{2i\delta'_{l'}}\left[\frac{2l'+1}{4\pi}\right]^{1/2}Y^*_{l'\mu}(\hat{K}')b^*_{\lambda}[C(l'\lambda l000)C(l'\lambda l-\mu\mu 0)]\,. \tag{24}$$

The index l occurs only in the last bracket; this latter quantity, when summed over l, is one of the orthogonality relations[11] for Clebsch-Gordan coefficients

$$\sum_{l}C(l'\lambda l000)C(l'\lambda l-\mu\mu 0)=\delta_{-\mu 0}\,. \tag{25}$$

We therefore find

$$\begin{aligned}A_2&=\delta_{\mu 0}\frac{1}{2K}\sum_{l'}(-1)^{\lambda-\mu}e^{2i\delta'_{l'}(E')}[4\pi(2l'+1)]^{1/2}\\&\quad\times Y^*_{l'\mu}(\hat{K}')b^*_{\lambda}\\&=if(\theta,E')(-1)^{\lambda}\delta_{\mu 0}b^*_{\lambda}\,.\end{aligned} \tag{26}$$

The complete expression for the exterior contribution to the K-shell ionization amplitude is therefore given by

$$A_{\epsilon_f\lambda\mu}=i[f(\theta,E)D^{\lambda}_{\mu 0}(0,\theta,0)b_{\lambda}+(-1)^{\lambda}\delta_{\mu 0}f(\theta,E-\Delta E)b^*_{\lambda}]\,. \tag{27}$$

This equation has a simple interpretation. If ionization occurs on the way into the nuclear collision with an atomic amplitude b^*_{λ}, only $\mu=0$ electronic states can be populated and the projectile loses an energy ΔE before encountering the nuclear potential; hence the nuclear scattering amplitude is to be evaluated at the reduced energy $E-\Delta E$. If ionization occurs on the way out with an amplitude b_{λ}, the scattering has already occured at the incoming projectile energy and so f must be evaluated at the initial energy E. The D function takes account of the direction of the projectile on its way out.

The ionization probability is defined by

$$P_K(\theta,E)=\frac{d\sigma_K}{d\Omega}\Big/|f(\theta,E)|^2\,. \tag{28}$$

Using the exterior ionization amplitude of Eq. (27) we have

$$P_K(\theta,E)\cong\int_0^{\infty}d\epsilon_f\sum_{\lambda\mu}|D^{\lambda}_{\mu 0}(\theta)b_{\lambda}+(-1)^{\lambda}\delta_{\mu 0}[f(\theta,E-\Delta E)/f(\theta,E)]b^*_{\lambda}|^2\,. \tag{29}$$

When the variation in in $f(\theta, E)$ is such that $f(\theta,E)\approx f(\theta, E-\Delta E)$, the ionization probability collapses to

$$P_K(\theta,E)=\int d\epsilon_f\sum_{\lambda\mu}|D^{\lambda}_{\mu 0}(\theta)b_{\lambda}+(-1)^{\lambda}\delta_{\mu 0}b^*_{\lambda}|^2\,. \tag{30}$$

which is the semiclassical prediction[1] for a "fast" nuclear collision.

Without further elaboration, Eqs. (29) and (30) suffice to demonstrate a leading contention of this paper: Angular-momentum transfer (i.e., $\lambda\geq 1$) does not alter the structure of the ionization probability from that indicated in Ref. 2; as a special case, when the reduction in effective bombarding energy ΔE makes a negligible change in the nuclear scattering amplitude, one anticipates that there will be little variation in the ionization probability with changing incident energy.

It remains to ask whether consideration of the interior contributions to the radial integrals will alter these conclusions. These correction terms are

examined in the next section but we state here the main conclusions. We will find that there is an important correction to the monopole ($\lambda=0$) Coulomb ionization probability but this will only append the so-called "sticking" or shake-off term[1,13] to the monopole atomic amplitude b_0 and will not change the structure of Eq. (27). Further, the interior contributions for $\lambda \geq 1$ will be found to be of the order (qR_m) or less and are thus negligible under our stated assumptions.

The evaluation of the recoil contribution to b_λ deserves special attention since the result obtained will be needed later in discussing corrections and alternative calculations for the recoil contribution. Using Eqs. (10) and (15), and neglecting the logarithmic contribution to $\bar{q}R$ in Eq. (16), we have

$$b_\lambda^W \cong \delta_{\lambda 1}\frac{mM\omega^2}{\hbar v M_2\sqrt{3}}\int_0^\infty dr\, r^3 \mathscr{R}_{\epsilon_f \lambda}\mathscr{R}_{1s}\int_{R_m}^\infty dR\, R\, e^{iqR}\,. \tag{31}$$

Clearly, the last integral is not well behaved, but with a long-range convergence factor, it becomes

$$\int_{R_m}^\infty dR\, R\, e^{iqR} = -\frac{e^{iqR_m}}{q^2}(1-iqR_m)\,. \tag{32}$$

For $(qR_m) << 1$, this may be expanded

$$\int_{R_m}^\infty dR\, R\, e^{iqR} = -\frac{1}{q^2}\left[1+\left[\frac{q^2R_m^2}{2}\right]\right]. \tag{33}$$

Thus dropping terms of order $(qR_m)^2$, we have

$$\int_{R_m}^\infty dR\, R\, e^{iqR} \cong \int_0^\infty dR\, R\, e^{iqR} = -\frac{1}{q^2} = -\frac{v^2}{\omega^2}\,, \tag{34}$$

so that

$$b_\lambda^W \cong -\delta_{\lambda 1}\frac{2mE}{\hbar v M_2\sqrt{3}}\int_0^\infty dr\, r^3 \mathscr{R}_{\epsilon_f}\mathscr{R}_{1s}\,, \tag{35}$$

or equivalently,

$$\int_{R_m}^\infty dR \mathscr{F}_{l'}(K'R)\mathscr{F}_l(KR)W_\lambda(R) \cong -\delta_{\lambda 1}\frac{mE}{\hbar v M_2\sqrt{3}}\left[\int_0^\infty dr\, r^3 \mathscr{R}_{\epsilon_f 1}\mathscr{R}_{1s}\right]\cos\left[\delta_l-\delta_{l'}'-(l-l')\frac{\pi}{2}\right]. \tag{36}$$

IV. INTERIOR CORRECTIONS

A. Monopole Coulomb

Of the various terms correcting the asymptotic results, we consider first the contribution to the monopole Coulomb term from the interior region, $R < R_m$, since this will prove to be the only term for which the correction is important.

For small values of R, the electronic matrix element of the monopole Coulomb potential is conveniently rewritten

$$C_0(R) = \frac{-Z_1e^2}{\hbar v}\left[\int_0^\infty dr\, r\mathscr{R}_{\epsilon_f 0}\mathscr{R}_{1s} + \left[\frac{1}{R}\int_0^R dr\, r^2\mathscr{R}_{\epsilon_f 0}\mathscr{R}_{1s} - \int_0^R dr\, r\mathscr{R}_{\epsilon_f 0}\mathscr{R}_{1s}\right]\right]. \tag{37}$$

When $R << a(Z_2)$, the last two terms will be less than the first by a factor $[R/a(Z_2)]^2$; since it has been our assumption that $R_m << a(Z_2)$ and we are here considering only values of $R \leq R_m$, it is thus a good approximation to take

$$C_0(R) \cong C_0(R=0) = \frac{-Z_1e^2}{\hbar v}\int_0^\infty dr\, r\mathscr{R}_{\epsilon_f 0}\mathscr{R}_{1s}\,. \tag{38}$$

With this, the interior contribution to the monopole raidal matrix element is

$$4\int_0^{R_m} dR\, \mathscr{F}_l(K'R)\mathscr{F}_l(KR)C_0(R) \cong 4C_0(0)\int_0^{R_m} dR\, \mathscr{F}_l(K'R)\mathscr{F}_l(KR)\,. \tag{39}$$

At first glance, it appears that this term will be sensitive to details of the interior wave function but closer

examination shows this is not so; rather, we shall find that nuclear physics enters only through a difference in scattering phase shifts.

Since the radial functions $\mathcal{F}_l$ satisfy the radial wave equation

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dR^2}+V_N(R)+\frac{\hbar^2}{2M}\frac{l(l+1)}{R^2}\right]\mathcal{F}_l(KR)=E\mathcal{F}_l(KR)\ , \tag{40}$$

we may rewrite the radial integral

$$\int_0^{R_m}dR\,\mathcal{F}_l(K'R)\mathcal{F}_l(KR)=-\frac{\hbar^2}{2M\Delta E}\int_0^{R_m}dR\left[\mathcal{F}_l(K'R)\frac{d^2}{dR^2}\mathcal{F}_l(KR)-\left[\frac{d^2}{dR^2}\mathcal{F}_l(K'R)\right]\mathcal{F}_l(KR)\right]\ . \tag{41}$$

Integrating by parts, we have

$$-\frac{\hbar^2}{2M\Delta E}\left[\mathcal{F}_l(K'R)\frac{d}{dR}\mathcal{F}_l(KR)-\left[\frac{d}{dR}\mathcal{F}_l(K'R)\right]\mathcal{F}_l(KR)\right]_{R_m}\ . \tag{42}$$

By assumption, the radial functions are well approximated by their asymptotic form at R_m; further, the difference $(K-K')R_m\equiv qR_m$ is assumed to be much less than unity. Consequently,

$$4C_0(0)\int_0^{R_m}dR\,\mathcal{F}_l(K'R)\mathcal{F}_l(KR)\cong 4C_0(0)\frac{\hbar^2K}{2M\Delta E}\sin[\delta_l(E)-\delta_l(E')]\ . \tag{43}$$

Thus, the interior monopole integral may be written in the form of Eq. (14),

$$4\int_0^{R_m}dR\,\mathcal{F}_l(K'R)\mathcal{F}_l(KR)C_0(R)\cong b_0(\text{int})e^{i[\delta_l(E)-\delta_l(E')]}+b_0^*(\text{int})e^{i[\delta_l(E')-\delta_l(E)]}\ , \tag{44}$$

where

$$b_0(\text{int})=\frac{v}{i\omega}C_0(0)=-\frac{i}{q}C_0(0)\ . \tag{45}$$

Since the interior monopole integral has the same structure as the exterior integral, we may append $b_0(\text{int})$ to the b_0 already obtained for the exterior region to form the total monopole atomic amplitude

$$b_0(\text{tot})\equiv b_0+b_0(\text{int})\ . \tag{46}$$

Clearly, Eqs. (27) and (29) still result provided we replace b_0 with $b_0(\text{tot})$.

It should be noted that, because it is purely imaginary, $b_0(\text{int})$ will not contribute to the ionization amplitude, Eq. (27), in a fast nuclear elastic scattering where fast is defined by the requirement that $f(\theta, E-\Delta E)=f(\theta, E)$. This result is consistent with the designation of $b_0(\text{int})$ as the sticking or shake-off term.[1,13]

B. Dipole Coulomb and recoil

The electronic matrix element of the dipole Coulomb potential is conveniently regrouped

$$C_1(R)=-\frac{Z_1e^2}{\hbar v\sqrt{3}}\left[R\int_0^{\infty}dr\,\mathcal{R}_{\epsilon_f1}\mathcal{R}_{1s}+\left[R^{-2}\int_0^R dr\,r^3\mathcal{R}_{\epsilon_f1}\mathcal{R}_{1s}-R\int_0^R dr\,\mathcal{R}_{\epsilon_f1}\mathcal{R}_{1s}\right]\right]\ . \tag{47}$$

When $R<<a(Z_2)$, as it is for the interior region $R<R_m$, the products of the radial functions (here assumed to be nonrelativistic) occurring in the last two integrals may be approximated, $\mathcal{R}_{\epsilon_f1}\mathcal{R}_{1s}\cong c_{\epsilon_f1}R$ so that the quantity in parentheses in Eq. (47) becomes $[(\frac{3}{10})c_{\epsilon_f1}R^3]$. In contrast, the first integral in Eq. (47) will be of the order $\{c_{\epsilon_f1}R[a(Z_2)]^2\}$. Consequently, it is permissible to drop the last two terms of Eq. (47) in evaluating the interior contribution for the dipole Coulomb term, and thus obtain the approximate dipole radial matrix element

$$\int_0^{R_m} dR\, \mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)C_1(R) \cong -\frac{Z_1 e^2}{\hbar v\sqrt{3}} \left[\int_0^{\infty} dr\, \mathcal{R}_{\epsilon_f 1}\mathcal{R}_{1s}\right] \int_0^{R_m} dR\, R\mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)\ . \tag{48}$$

We now observe that the last integral over R in Eq. (48) is identical to that encountered in the evaluation of the interior contribution of the recoil term $W_{\lambda=1}(R)$. The parallel between these two interior radial matrix elements of the dipole Coulomb and recoil terms is heightened when we apply the Ehrenfest theorem to the electronic matrix element occurring in Eq. (48):

$$e^2 \int_0^{\infty} dr\, \mathcal{R}_{\epsilon_f 1}\mathcal{R}_{1s} = \frac{1}{Z_2} \int_0^{\infty} dr\, r^2 \left[\frac{Z_2 e^2}{r^2}\right] \mathcal{R}_{\epsilon_f 1}\mathcal{R}_{1s} = \frac{m\omega^2}{Z_2} \int_0^{\infty} dr\, r^3 \mathcal{R}_{\epsilon_f 1}\mathcal{R}_{1s}\ . \tag{49}$$

With this, these two interior radial matrix elements may be combined[14] to give

$$\int_0^{R_m} dR\, \mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)[W_1(R)+C_1(R)]$$

$$\cong \frac{m\omega^2}{\hbar v\sqrt{3}} \left[\frac{M}{M_2} - \frac{Z_1}{Z_2}\right] \left[\int_0^{\infty} dr\, r^3 \mathcal{R}_{\epsilon_f 1}\mathcal{R}_{1s}\right] \int_0^{R_m} dR\, R\mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)\ . \tag{50}$$

An immediate corollary[14] worth noting is that this sum of the interior contributions vanishes when the charge-mass ratios of target and (relative) projectile are the same. Further, even when these ratios are not equal, as is the case for proton scattering, the magnitude of this combined term will be less than that of the recoil term by itself.

We have found that the most expeditious way for estimating the importance of this interior matrix element proceeds from the Ehrenfest theorem and the following identities:

$$M\omega^2 \int_0^{\infty} dR\, R\mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR) \equiv I = M\omega^2 \left[\int_0^{R_m} + \int_{R_m}^{\infty}\right]$$

$$\equiv I_{\text{int}} + I_{\text{ext}} = \int_0^{\infty} dR\, \mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)\frac{\partial V}{\partial R} \equiv J\ . \tag{51}$$

Here, I_{int} is the integral in question while the approximate evaluation of I_{ext}, using Eqs. (10) and (36) gives

$$I_{\text{ext}} \cong -E\cos\left[\delta_l - \delta'_{l'} - (l-l')\frac{\pi}{2}\right]\ , \tag{52}$$

apart from terms of order qR_m.

Since the integral J is yet unkown, it is not obvious that anything has been gained by this rearrangement; indeed, it appears at first sight that J will depend on details of nuclear physics, since V is the sum of the nuclear and Coulomb potentials and the integral includes the nuclear interior. To see that this is not the case, we appeal to a little known theorem due to Gerjuoy[15] which, in our notation, may be written

$$\lim_{R_{\max}\to\infty} \int_0^{R_{\max}} dR\, \mathcal{F}_{l'}(KR)\mathcal{F}_l(KR)\frac{\partial V}{\partial R} = -E\cos\left[\delta_l - \delta'_{l'} - (l-l')\frac{\pi}{2}\right]\ . \tag{53}$$

In other words, in the limit $K'\to K$ the integral over all space equals the approximate evaluation of the exterior integral I_{ext}, Eq. (52).

Since the wave numbers occurring in the Gerjouy theorem are equal, this integral is not quite the same as our integral J. Apart from terms of order (qR_m) and (D/R_m), however, it is equivalent to our interior integral

$$J_{\text{int}} = \int_0^{R_m} dR\, \mathcal{F}_{l'}(K'R)\mathcal{F}_l(KR)\frac{\partial V}{\partial R}\ .$$

Further, an approximate evaluation of J_{ext}, which involves only asymptotic wave functions and the $(1/R^2)$ term of the Coulomb force, shows that J_{ext} is negligible in comparison to J_{int}. (We note

parenthetically that the Ehrenfest theorem interchanges the roles of the exterior and interior regions.)

Consequently, we have that the terms in $I_{\rm int}$ are of order (qR_m) and (D/R_m), or less, times E. In view of our assumed inequalities, Eq. (13), $I_{\rm int}$ may therefore be neglected.

The result, that the interior $\lambda=1$ term may be dropped while the interior monopole contribution is significant, is not unexpected since the integrands of the $\lambda=1$ matrix elements bear an additional factor of R, suppressing the interior, which is not present in the monopole integrand.

C. Higher Coulomb mulitpoles

In the analysis of most experiments, only monopole and dipole excitations need be considered. Further, if the higher multipoles are considered at all, only the exterior contributions will be significant, since additional powers of R suppress the interior.

For example, an analysis similar to that given at the beginning of Sec. IV B shows that the leading term in the electronic matrix element of the quadrupole Coulomb potential for small values of R is

$$C_2(R)=-\frac{Z_1e^2}{\hbar v\sqrt{5}}R^2\int_0^\infty dr\, r^{-1}\mathscr{R}_{\epsilon_f 2}\mathscr{R}_{1s}\ . \tag{54}$$

Consequently, the interior radial matrix element will be reduced, relative to the exterior, by additional factors of (qR_m) or $[R_m/a(Z_2)]$ over what was just found for dipole excitation.

V. RELATION TO PREVOUS RESULTS AND TO SEMICLASSICAL THEORY

The conclusion to be drawn from Sec. IV is that the ionization probability is still well approximated by Eq. (29) with the amendment that the monopole atomic amplitude to be used is the b_0(tot) of Eq. (46), which is a sum of exterior and interior contributions.

An expression nearly equivalent to the amended Eq. (29) was given by Blair *et al.*[2] in their analysis of K-shell ionization in proton scattering from ^{58}Ni, their (ϵ,l,m) corresponding to the present (ϵ_f,λ,μ). Their formula was based on a derivation which overlapped the present treatment in several respects but which used an S-matrix description to match the interior to the exterior nuclear wave functions at R_m. The notation of Ref. 2 was deficient in not indicating that the coefficient $B(\epsilon,l,m)$ [which equaled $(b_\lambda D^\lambda_{\mu 0})$ of the present paper] was also to be considered a function of θ. In addition, an error was made in their numerical computations in that the sign factor $(-1)^\lambda$ was omitted in the coefficient $A(\epsilon,l,m)$ $(=[b^*_\lambda(-1)^\lambda\delta_{\mu 0}]$ of the present paper). This omission had little effect on the results of Ref. 2, however, since the ^{58}Ni experiment was peformed at $\theta=90°$; consequently, there was negligible interference for the dipole $(\lambda=l=1)$ contributions.

Further, it should be noted that the monopole atomic amplitude of Ref. 2 included the internal contribution to b_0 given by Eq. (45). In that S-matrix formulation the interior contribution b_0(int) emerged as a consequence of the matching conditions at R_m.

There is a close correspondence between the quantum-mechanical expression for P_K, i.e., the amended Eq. (29), and that given by the semiclassical theory of Ciocchetti and Molinari,[1] P_K(CM). In Appendix A we show that for scattering of the projectile to substantial angles and for cases where $qD<<1$, the latter ionization probability can be written as

$$P_K(\mathrm{CM})=\int d\epsilon_f\sum_{\lambda\mu}|\,D^\lambda_{\mu 0}(\theta)b_\lambda(\mathrm{tot}) +(-1)^\lambda\delta_{\mu 0}e^{-i\omega t_0}b^*_\lambda(\mathrm{tot})\,|^2\ . \tag{55}$$

Here the real parameter t_0 is the classical nuclear time delay while b_λ(tot) is the sum of the previous external and interior atomic amplitudes, Eqs. (14) and (45), respectively, evaluated in the limit that $\bar{q}R$ is approximated by qR and the lower limit of the integral in Eq. (15), R_m, is extended in to 0. [In obtaining this expression, we have divided the amplitude of Eq. (A7) by the phase factor $e^{i\omega t_0}$ so that $e^{-i\omega t_0}$ multiplies the "incoming" ionization amplitude b^*_λ.]

Comparing Eq. (55) to the amended Eq. (29), we see that the semiclassical and quantum-mechanical theories differ only in that the phase factor of the semiclassical theory $\exp(-i\omega t_0)$, is replaced by the ratio of scattering amplitudes $f(\theta,E-\Delta E)/f(\theta,E)$ in a completely quantum-mechanical formulation.[2]

The correspondence between the two formulations may be pursued further when t_0 is so small

that a linear expansion suffices for the phase factor

$$e^{-i\omega t_0} \cong 1-\omega t_0 \tag{56}$$

and, similarly, the energy variation of the scattering is sufficiently small so that

$$f(\theta,E-\Delta E)/f(\theta,E) \cong 1-\hbar\omega \frac{\frac{\partial}{\partial E} f(\theta,E)}{f(\theta,E)} . \tag{57}$$

Recalling the quantum-mechanical definition of time delay[16]

$$\tau_{QM}(E,\theta) = -i\hbar \frac{\partial}{\partial E} \ln f(\theta,E) , \tag{58}$$

we see that the latter ratio may be written as

$$f(\theta,E-\Delta E)/f(\theta,E) \cong 1-i\omega\tau_{QM}(E,\theta) . \tag{59}$$

Yet while there is now a precise formal correspondence between the two expressions Eqs. (56) and (59) and, consequently, between the CM and QM formulas for P_K to first order in ω, we note that τ_{QM} is, in general, a complex function of E and θ, in contrast to the implied real constant t_0 of the semiclassical theory. Thus, evaluations of the semiclassical formulas for the ionization probability will not resemble even qualitatively the quantum-mechanical predicitons, even when the linear approximations are justified. While it is fair to speak figuratively of the role of nuclear "time delay" in modifying the atomic ionization probability, any precise discussion of time delay must be cast in terms of the energy dependence of the nuclear reaction amplitudes.

After carrying out the derivation of Eq. (29) we became aware of an older paper which bears on this subject. Pursuing the concern of Breit,[17,18] that atomic excitations might possibly alter the low-energy p-p cross section, de Wit *et al.*[19] obtained expressions for the nuclear scattering amplitude when simultaneously there is atomic dipole excitation. The detailed distorted-wave calculation was carried out only for the special case of nuclear Coulomb scattering plus S-wave potential scattering, where the further loss of energy to the atomic excitation was assumed not to alter the nuclear amplitudes. Inspection indicates that the amplitudes they obtained may be cast in the form of Eq. (27), i.e., there is a factorization of nuclear and atomic amplitudes, with no alteration in form due to angular-momentum exchange. We have also been recently informed of two independent derivations[20,21] of the exterior DWBA ionization amplitudes, which reach conclusions similar to our own.

VI. SUB-COULOMB RESONANT SCATTERING

In the time-delay experiments which have so far been performed, the incident proton energies have been below or near the Coulomb barrier. Thus the nuclear scattering amplitudes entering Eqs. (27) and (29) are well approximated as the sum of pure Coulomb plus Breit-Wigner resonance amplitudes. For the s-wave resonances of Refs. 2 and 4, we need consider only the single spin-independent amplitude

$$f(\theta,E) = f_C + f^0_{\rm res} , \tag{60}$$

where

$$f_C = -(D/4)\csc^2\left[\frac{\theta}{2}\right] \times \exp\{ i\eta \ln[\csc^2(\theta/2)] + 2i\sigma_0 \} \tag{61}$$

and

$$f^0_{\rm res} = (2K)^{-1}\exp(2i\sigma_0 + i\delta_0^{\rm res})\sin\delta_0^{\rm res} = (2K)^{-1}\exp(2i\sigma_0)\frac{\Gamma_p}{(E_R-E)-i\Gamma/2} . \tag{62}$$

Here σ_l is the Coulomb phase shift for partial wave l, $\delta_0^{\rm res} = \delta_0 - \sigma_0$ is the resonance phase shift, Γ_p is the partial width for the elastic channel, Γ is the total width, and E_R is the resonance energy.

When a proton scattering resonance occurs in a state of total angular momentum J with orbital angular momentum L different from zero, it is necessary to take the proton spin into account. In general, the nuclear waves are labeled by the spin projection along the incident direction ν and are expanded in partial waves[22] of total angular momentum j as well as orbital angular momentum l. Retracing the steps of Secs. II and III with spin-orbit distorted waves, we find that the joint cross section for K-shell ionization and nuclear scattering when there is a J, $L \neq 0$ resonance becomes

$$\frac{d\sigma_K}{d\Omega}=\int_0^\infty d\epsilon_f \sum_{\lambda,\mu}\sum_{\nu'} |f_{\nu'\nu}(\theta,E)D^{\lambda}_{\mu 0}b_\lambda + f_{\nu'\nu}(\theta,E-\Delta E)(-1)^{\lambda}\delta_{\mu 0}b^*_\lambda|^2 , \tag{63}$$

where

$$f_{\nu'\nu}=f_C\delta_{\nu\nu'}+f^{J,L}_{\text{res},\nu'\nu} \tag{64}$$

with a resonant nonspin-flip amplitude

$$f^{J,L}_{\text{res},\nu\nu}=(2K)^{-1}\exp(2i\sigma_L)(J+\tfrac{1}{2}) \times\frac{\Gamma_p}{(E_R-E)-i\Gamma/2}P_L(\cos\theta) \tag{65}$$

and a resonant spin-flip amplitude

$$f_{\nu'\neq\nu}=\pm(2K)^{-1}\exp(2i\sigma_L)(-1)^{J+L+1/2} \times\frac{\Gamma_p}{(E_R-E)-i\Gamma/2}P^1_L(\cos\theta) . \tag{66}$$

When $\Delta << /2$, which is the case for ionization in p-^{12}C scattering near the 0.461-MeV resonance, there will be little difference in the resonance amplitudes at the two energies E and $E-\Delta E$. Consequently, we anticipate that there will be only a small variation in the ionization probability as one varies the incident energy through the resonance. In Fig. 1 we show the calculated cross section and ionization probability, relative to that obtained in the absence of a resonance, as a function of incident energy for p-^{12}C scattering near the $s_{1/2}$ resonance.

In this calculation the atomic amplitudes b_λ and b^*_λ have been evaluated using one-electron Dirac wave functions. Only monopole and dipole contributions were included; excitation into $\lambda=2$ continuum states contributes less than 1% to the total ionization probability. It should be emphasized that the monopole amplitudes of this calculation include both the exterior and interior contributions. The atomic amplitudes were calculated for $E_p=460$ keV, and were assumed to be independent of E_p between 380 and 530 keV. We verified that the monopole amplitude varies by less than 2% over this energy range. The dipole ionization probability increases roughly linearly with E_p, and thus varies by $\sim 30\%$ over this energy span. This variation is not included in the present calculations.

The scattering amplitude entering this calculation is the sum of the background and resonance terms given by Duinker *et al.*,[4] which provide a best fit to the differential cross section. The calculation of P_K and $d\sigma/d\Omega_p$ was done at $\theta_p=125°$; no average over the particle detector angular aperture was made.

We see in Fig. 1 that P_K is practically independent of E_p. There is a slight dip near 450 keV, amounting to about 3%. The dip is due to the interference between the incoming and outgoing inelastic scattering amplitudes for monopole and dipole $\mu=0$ ionization. For monopole ionization alone the ionization at the dip is 0.96 and for dipole ionization it is 0.975. Since dipole ionization is dominant, the total ionization probability is ~ 0.97 at the minimum.

VII. SUMMARY

Assuming that a potential model suffices to describe the nuclear scattering, we have made a DWBA calculation of the probability for ionizing the K shell while the projectile undergoes nuclear scattering. Crucial in our development is the separation of the relative projectile space into an exterior and interior region; the boundary between these lies at a radius R_m which is assumed to be large compared to nuclear distances and small compared to the two atomic lengths, the target K-

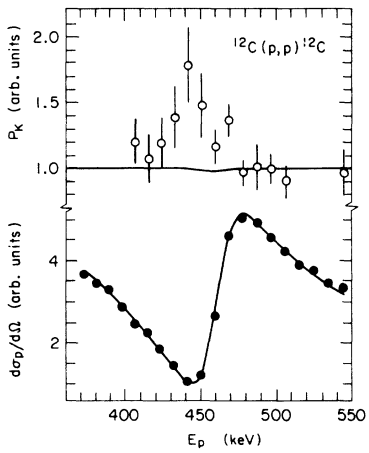

FIG. 1. Calculated and measured (Ref. 4) differential cross section $d\sigma/d\Omega_p$ and ionization probability P_K relative to that obtained in the absence of a resonance, as a function of incident energy for p-^{12}C scattering near the $s_{1/2}$ resonance at 0.461 MeV. The scattering amplitudes use the parametrization of Duinker *et al.* (Ref. 4).

shell radius, $a(Z_2)$, and the inverse of the minimum momentum transfer $(1/q)$.

The exterior contribution to the K-shell ionization amplitude is found to have the simple form reported previously,[2] which resulted from an alternative S-matrix theory. In view of the suggestion of Duinker *et al.*[4] that angular-momentum exchange would alter that form, it is of particular interest that the factorization of this amplitude, as given in Eq. (27), holds for atomic excitations of arbitrary multipolarity. Of the interior contributions, only the monopole term is found to be significant and this merely appends the sticking term of Ciocchetti and Molinari[1] to the exterior monopole atomic amplitude. Computations of the ionization probability predicted by our theory for p-^{12}C scattering at $\theta=125°$ yield only a slight dip at the minimum of the cross section, in contrast to the large increase reported in Ref. 4.

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APPENDIX A: RELATION BETWEEN OUR QUANTUM-MECHANICAL THEORY AND VARIOUS SEMICLASSICAL THEORIES

In the semiclassical approximation (SCA), one typically writes the amplitude for exciting K-shell electrons into continuum states with energy ϵ_f and orbital quantum numbers λ and μ as[1,7–9]

$$a_{\lambda\mu}=-iv\int_{-\infty}^{\infty}dt\,e^{i\omega t}G_\lambda(R)D^\lambda_{\mu0}(\theta(R))\ , \tag{A1}$$

where $D^\lambda_{\mu0}(\theta(R))=D^\lambda_{\mu0}(0,\theta(R),0)$, and $\theta(R(t))$ is the time-dependent angle between the internuclear axis and the z axis. The integral over t in this equation is normally done along a Coulomb trajectory with an impact parameter b, classically related to the center-of-mass scattering angle θ and the distance to closest approach for a head-on collision D by the equation $b=(D/2)\cot(\theta/2)$.

When a compound nucleus is formed at $R=0$ for a time t_0, the integral over t can be written as

$$\begin{aligned}(ia_{\lambda\mu}/v)=&\int_{-\infty}^{0}dt\,e^{i\omega t}G_\lambda(R)D^\lambda_{\mu0}(\theta(R))\\&+\int_0^{t_0}dt\,e^{i\omega t}G_0(0)\delta_{\lambda0}\\&+\int_{t_0}^{\infty}dt\,e^{i\omega t}G_\lambda(R)D^\lambda_{\mu0}(\theta(R))\ ,\end{aligned} \tag{A2}$$

where we have used the fact that only the monopole matrix element $G_0(0)$ is nonzero at $R=0$.

If one calculates $a_{\lambda\mu}$ in coordinate system A, as shown in Fig. 2, takes $b\approx0$, and approximates the Coulomb trajectory by two straight lines, as indicated by coordinate system A' of Fig. 2, one has

$$D^\lambda_{\mu0}(\theta(R))=\begin{cases}D^\lambda_{\mu0}(\theta) & t>t_0\\(-1)^\lambda\delta_{\mu0} & t<0\end{cases}. \tag{A3}$$

Performing the elementary integral from $t=0$ to $t=t_0$, we may then rewrite Eq. (A2) as

$$(ia_{\lambda\mu}/v)=D^\lambda_{\mu0}(\theta)\left[\int_{t_0}^{\infty}dt\,G_\lambda(R)e^{i\omega t}+\delta_{\lambda0}\frac{G_0(0)}{i\omega}e^{i\omega t_0}\right]+(-1)^\lambda\delta_{\mu0}\left[\int_{-\infty}^{0}dt\,G_\lambda(R)e^{i\omega t}-\delta_{\lambda0}\frac{G_0(0)}{i\omega}\right]. \tag{A4}$$

Consistent with taking $b\approx0$, and neglecting Coulomb deflection effects (valid if $qD\ll1$), we can write

$$\begin{aligned}v\int_{-\infty}^{0}dt\,e^{i\omega t}G_\lambda(R)&=\int_0^{\infty}dR\,e^{-iqR}G_\lambda(R)\\&\cong\int_{R_m}^{\infty}dR\,e^{-i\bar qR}G_\lambda(R)=b^*_\lambda\ ,\end{aligned} \tag{A5}$$

since $R=-vt$ for negative values of t and, by our assumptions, $qD\ll qR_m\ll1$. Similarly for $t>t_0$, for which $R=v(t-t_0)$, we can put

$$\begin{aligned}v\int_{t_0}^{\infty}dt\,e^{i\omega t}G_\lambda(R)&=e^{i\omega t_0}\int_0^{\infty}dR\,e^{iqR}G_\lambda(R)\\&\cong e^{i\omega t_0}b_\lambda\ .\end{aligned} \tag{A6}$$

Thus we obtain the result, equivalent to that of Ciocchetti and Molinari,[1]

$$\begin{aligned}a_{\lambda\mu}\cong-i[&D^\lambda_{\mu0}(\theta)b_\lambda(\text{tot})e^{i\omega t_0}\\&+(-1)^\lambda b^*_\lambda(\text{tot})],\end{aligned} \tag{A7}$$

where $b_\lambda(\text{tot})$ is given by

$$b_\lambda(\text{tot})=b_\lambda+\delta_{\lambda0}b_0(\text{int})\ , \tag{A8}$$

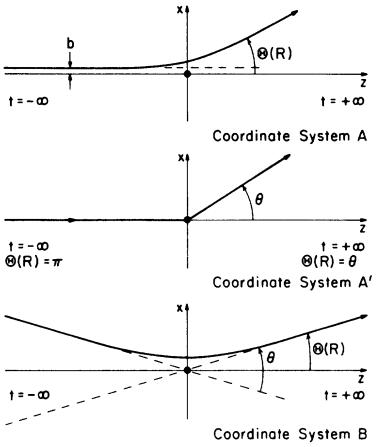

FIG. 2. Relative coordinate systems used in various semiclassical theories. In coordinate system A the projectile enters at an impact parameter b, parallel to the z axis, then scatters to an angle θ. In coordinate system A' we approximate the ion trajectory by two straight lines so that $\theta(R)=\pi$ for $t<0$ and $\theta(R)=\theta$ for $t>0$. In coordinate system B the trajectory is assumed to be symmetric about the x axis, in the xz plane.

which is the same as Eq. (46). In this derivation, the internal contribution to b_0 comes about from considering the contribution to $a_{\lambda\mu}$ during the lifetime of the compound nucleus ($0<t<t_0$). The K-shell ionization probability is given by the absolute square of $a_{\lambda\mu}$, which is the same as Eq. (55).

Several semiclassical calculations for $\omega t_0=0$ appear in the literature which use different coordinate systems. Amundsen[7] uses coordinate system B shown in Fig. 2 for which the Coulomb trajectory is assumed to be in the xz plane and to be symmetric about the x axis. He parametrizes the Coulomb trajectory using[10]

$$R=\frac{D}{2}(\epsilon\cosh w+1)$$

and

$$t=\frac{D}{2v}(\epsilon\sinh w+w)\ , \tag{A9}$$

where $\epsilon^{-1}=\sin(\theta/2)$. In this coordinate system

$$\cos\theta(R)=(\epsilon^2-1)^{1/2}\frac{\sinh w}{(\epsilon\cosh w+1)}$$

and

$$\sin\theta(R)=\frac{\cosh w+\epsilon}{\epsilon\cosh w+1)}\ . \tag{A10}$$

Various other coordinate systems are defined by Alder *et al.*,[10] which are similar to our system B but the x, y, and z axes are interchanged, and thus the definition of $\cos\theta(R)$ and $\sin\theta(R)$ are interchanged. It is clear that with type-B coordinate systems, $\theta(R)\neq\pi$ at $t=-\infty$ ($w=-\infty$). Hence although

$$P_K=\sum_{\lambda\mu}|a_{\lambda\mu}|^2$$

is the same in coordinate systems A and B, the amplitudes $a_{\lambda\mu}$ are different.

One can still use the Coulomb trajectory parametrization of Eq. (A6) in coordinate system A if one defines

$$\cos\theta(R)=\frac{(\epsilon^2-1)\sinh w-\epsilon-\cosh w}{\epsilon(\epsilon\cosh w+1)}\ ,$$
$$\sin\theta(R)=\frac{(\epsilon^2-1)^{1/2}}{\epsilon}\frac{\epsilon+e^w}{\epsilon\cosh w+1}\ . \tag{A11}$$

It is straightforward to show that here $\theta(R)\to\pi$ for $w=-\infty$ and $\theta(R)=\theta$ for $w=+\infty$.

Finally, we note the connection to the calculations of Pauli and Trautman[23] based on the stationary-phase approximation to the QM ionization amplitudes. In terms of our notation, their expression for the ionization amplitude has the form

$$a_{\lambda\mu}\propto\sum_m D^{\lambda}_{-m0}(0,\pi/2,0)\times D^{\lambda*}_{-m-\mu}\left[\frac{\pi+\theta}{2},\pi/2,\pi/2\right]I_{\lambda m}\ , \tag{A12}$$

where

$$I_{\lambda m}\propto\int_{-\infty}^{\infty}dt\,e^{i\omega t}G_\lambda(R)\times\left[\frac{\cosh w+\epsilon+i(\epsilon^2-1)^{1/2}\sinh w}{1+\epsilon\cosh w}\right]^m\ . \tag{A13}$$

Consistent with the neglect of Coulomb deflection we can put

$$\frac{\cosh w+\epsilon+i(\epsilon^2-1)^{1/2}\sinh w}{1+\epsilon\cosh w}\approx\frac{1}{\epsilon}\pm\frac{i(\epsilon^2-1)^{1/2}}{\epsilon}\ , \tag{A14}$$

where one uses the plus sign for $t>0$ and the minus sign for $t<0$. Using Eqs. (A5) and (A6) for the time integral and inserting the values of the rotation matrix elements, one finds that Eq. (A12) reduces to Eq. (A7) with t_0 set equal to 0. Hence we conclude that for $b\approx 0$, and $qD\ll 1$, the Pauli SCA gives the same result as our QM evaluation in the absence of time delay.

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