Mechanisms for charge transfer (or for the capture of any light particle) at asymptotically high impact velocities

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Within the nonrelativistic approximation the authors discuss three different mechanisms for the capture of a light particle from a bare heavy nucleus by another bare heavy nucleus which is incident with a very high relative velocity. The emphasis is on physical interpretation. For each mechanism a "physical" (i.e., more readily comprehensible) derivation is given of the asymptotic form of the total cross section, and a comparison is made of the relative importance of the different mechanisms in the case of electron capture from hydrogenlike "atoms." (Electron capture is normally referred to as charge transfer). The first mechanism is knock-on capture, where the two nuclei have equal masses and simply switch places. The second mechanism is radiative capture, which occurs with the emission of a photon. The third mechanism, which is perhaps the most interesting one, is double scattering, first suggested within the framework of classical mechanics by Thomas in 1927. In this mechanism the light particle undergoes two collisions, the first with the incident nucleus, and the second with the target nucleus; the light particle finally has almost the same velocity as the incident nucleus and therefore has a reasonable probability of being captured. The capture process in the asymptotic domain is a fascinating one theoretically since radiative capture can dominate over nonradiative capture; what is perhaps more remarkable is that for nonradiative capture integrated over the forward direction the second Born contribution dominates over the first in the asymptotic limit. For the capture of an electron bound in a high Rydberg state, capture via the knock-on the double scattering mechanisms are describable classically (Thomas' result becomes exact!) and (near the forward direction) the second Born(Born again) term dominates over the first at much lower energy. (Changing only the notation and the kinematics, the results can be used to study mass transfer processes in which one of a massive gravitationally bound pair of astrophysical objects is captured by a third massive object). A number of results for capture into a true bound state can be readily carried over to "capture to the continuum," with the electron emerging with a small positive energy relative to the incident nucleus. An understanding of the asymptotic form of the capture cross section is of considerable interest in its own right; it may also be helpful in understanding the dynamics of the capture process in the medium velocity range where applications are important. At medium velocities electron capture is of interest in many areas of physics such as astrophysics, chemical physics, plasma physics, and atomic physics; it is also of practical interest, having applications in laser and fusion research.

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I. INTRODUCTION

Atomic collisions that involve the capture of an electron (i.e., charge transfer collisions) are of interest in many areas of physics. Cross sections for various electron capture processes are needed to understand, for example, some astrophysical processes, the "paths" of certain chemical reactions, and the properties of plasmas. In atomic physics renewed interest in the theory of electron capture has been stimulated by the realization that electron capture can play a competitive role to direct Coulomb ionization in the production of inner shell vacancies by swift highly stripped ions (Halpern and Law, 1973; McGuire, 1973). The subject may also be of practical interest owing to potential applications in technological areas such as the development of x-ray lasers and the heating of fusion plasmas by the injection of neutral beams. Unfortunately the dynamics of electron capture is still not well understood. The present article is devoted to a discussion of an old problem—one which has not yet been totally resolved—namely, the determination, within the context of nonrelativistic theory, of the velocity dependence of the cross section for electron capture from a one-electron ion or atom by a bare nucleus that is incident with an asymptotically high velocity. This problem continues to be of great interest since a proper understanding of the nonrelativistic asymptotic form of the cross section may be helpful in developing a reliable method for treating electron capture at intermediate velocities, the domain relevant to the applications mentioned above.

In discussing electron capture at asymptotically high velocities kinematical considerations are of paramount importance. This becomes apparent when one recognizes that in order for the electron to be captured the two-particle subsystem consisting of the electron and projectile nucleus (hereafter referred to in quotation marks simply as "the subsystem") must lose the very large *internal* kinetic energy (i.e., the kinetic energy of "the subsystem" relative to its center of mass) that it has initially. One of the very first problems is to determine the dominant mechanisms for ridding "the subsystem" of this large amount of internal energy. From the theoretical point of view, the nature of the electron capture mechanisms which dominate at high impact velocity is extraordinarily interesting. The mechanism which might be expected to dominate—a "single scattering" mechanism—corresponds to the first Born approximation with the perturbation taken to be the interaction between the projectile nucleus and the electron. Now this mechanism does *not* in fact dominate. The physics behind this remark has its origin in the simple fact that a bare nucleus incident on a *free* electron cannot capture the electron in a nonradiative process. In this mechanism, therefore, the electron can be captured only if one takes into account the high-momentum component of the wave function of the target "atom," a component which decreases very rapidly with the magnitude of the incident velocity. Mechanisms which do not require the high-momentum component of the target wave function must therefore be considered, even if these mechanisms are of "greater complexity" than the single scattering mechanism. There appear to be three such mechanisms which contribute significantly to the electron capture cross section at high impact velocities.

In the first mechanism the incident nucleus and the target nucleus simply exchange places without appreciably disturbing the electron. However, this can only occur if the two nuclei have equal or nearly equal masses. This mechanism, first analyzed in detail by Mapleton (1964), is often referred to as the "knock-on" process since in the lab frame (in which the target nucleus is initially at rest) the incident nucleus gives up all of its kinetic energy to the target nucleus, which is therefore knocked forward, but the electron remains behind and becomes bound to the incident nucleus, which has come to rest. Hence in the lab frame the internal energy of "the subsystem" is absorbed by the target nucleus. Note that the knock-on process is a single scattering mechanism, described by the first Born term; the perturbation is the interaction between the two nuclei.

The second mechanism is radiative capture. (The emission of radiation can be ignored in the first and third mechanisms.) This mechanism was first analyzed by Oppenheimer (1928). In radiative capture the target nucleus plays almost no role; the process is essentially radiative recombination, and the internal energy of "the subsystem" is transferred to the photon. Thus, for example, for protons incident on hydrogen atoms, the process $p+\mathrm{H}\to\mathrm{H}+p+\gamma$ is effectively the process $p+e\to\mathrm{H}+\gamma$. Remarkably, radiative capture can dominate over nonradiative capture. The importance of radiative capture as a mechanism for charge transfer at high velocities has often been overlooked by atomic physicists, possibly because the cross section is so small when radiative capture dominates. The first experiment indicating the onset of radiative capture seems to have been that of Raisbeck and Yiou (1971). Definitive evidence for radiative capture in fast heavy-ion collisions was first observed by Schnopper *et al.* (1972), and has since been observed in a large number of experiments. The literature can be traced through the proceedings of the tenth International Conference on the Physics of Electronic and Atomic Collisions (published by Centre d'Etudes Nucléaires, Saclay, 1977).

The third mechanism, first pointed out and analyzed by Thomas (1927) within the framework of classical mechanics, and by Drisko (1955) within the framework of quantum mechanics, is, astonishingly for a high-energy limit, not a one-step but a *two*-step process. The electron is scattered first by the projectile nucleus and then by the target nucleus in such a manner that the electron finally has almost the same velocity as the projectile nucleus, the velocity of the latter not having changed appreciably during the collision. After this double scattering has occurred "the subsystem" has lost most of its internal energy and the electron and projectile nucleus can become bound by their mutual attraction. Since, in this mechanism, the target nucleus interacts with the electron but not with the projectile nucleus, and since the electron-nucleus mass ratio is very small, the energy transferred between "the subsystem" and the target nucleus is negligibly small in the lab frame. In this frame the role of the target nucleus is to convert the internal kinetic energy of "the subsystem" into the form of *external* kinetic energy, that is, into additional kinetic energy of the center of mass of "the subsystem."

Each of the mechanisms just described is a different means of ridding "the subsystem" of its initially large internal kinetic energy, and each mechanism leads to a different asymptotic velocity dependence for the cross section. The asymptotic form of the radiative capture cross section was generalized by Briggs and Dettmann (1974) to arbitrary initial and final s states, and to a wide class of interactions which includes the Coulomb interaction as a special case. The asymptotic forms of the cross sections for the two nonradiative mechanisms were generalized by Dettmann and Leibfried (1969), again to a wide class of interactions, and with the initial and final states restricted to being isotropic; no restriction was placed on the masses of the three interacting particles.

Although the analyses of Briggs and Dettmann and of Dettmann and Leibfried are fairly rigorous, the physics of each mechanism is unfortunately, if necessarily, obscured to a large extent by the complexity of the calculation. The purpose of this article is to give a full discussion of the physics of each mechanism. We shall largely restrict our discussion to the nonrelativistic capture of a *light* particle from a bare heavy nucleus by another bare heavy nucleus which is incident with a very high velocity. For each mechanism we give a nonrigorous but "physical," that is, more readily comprehensible, derivation of the asymptotic form of the cross section. No restriction will be placed on the initial and final states, and the interactions will be almost unrestricted. This heuristic treatment not only has merit in its own right; the insight it provides may enable one to comprehend the difficulties, if any, that would arise in an extension to more general cases such as particles of arbitrary masses, and atoms with many electrons. Furthermore, one might gain some feeling as to when relativistic corrections become important. Of course, the validity of this heuristic approach can only be fully borne out by the more rigorous approaches mentioned above. However, we expect to and do obtain the correct dependence of the different cross sections on their various parameters; two of the cross sections are exact and the third is correct to within a multiplicative constant of order unity.

In the subsequent discussion we assume that if a particle undergoes a large change of momentum in a double scattering or backward scattering process, it does so via a binary collision which is close and essentially instantaneous. (A binary collision can be regarded as close and essentially instantaneous only if the interaction between the two particles participating in the collision is sufficiently singular at zero separation. Coulomb potentials, for example, are sufficiently singular. A potential of the form $\exp[-(x^2+y^2+z^2)^{1/2}]$, where x, y, and z are Cartesian coordinates, is also acceptable; this potential has a branch cut, or, speaking physically, a cusp at $r=0$. The entire class of interactions considered by Dettmann and Leibfried (1969) is acceptable; these potentials have Fourier transforms that can be expanded in powers of $1/k$ for large argument k.) The assumption that the collision is instantaneous allows us to use the sudden approximation of perturbation theory (Schiff, 1968). We assume that the relative speed v of the nuclei is large compared to the initial and final orbital speeds of the light particle, but we assume that $(v/c)^2$, where c is the speed of light, is small compared to unity so that relativistic effects are unimportant.

Within the context of atomic physics, the binary collisions referred to in the previous paragraph can be (i) a close nuclear collision (in backward scattering) or, (ii) two close nuclear–electron collisions in double scattering. There are also close encounters of the third kind, true three-body collisions of the two nuclei and the electron which do not allow a decomposition into binary collisions. True three-body collisions occur in the Brinkman–Kramers approximation, which is the first Born approximation with the nuclear interaction omitted.

The outline of this article is as follows. In Sec. III we discuss the knock-on process, and in Sec. IV we discuss radiative capture. In Sec. V we discuss the double-scattering process; this is perhaps the most interesting, though most complicated, mechanism, and Sec. V is a relatively long one. These three sections, concerned with capture from an arbitrary state, can be read more or less independently. In Sec. VI we discuss the relative importance of the different mechanisms, in various energy domains, for electron capture from a hydrogenlike "atom" in its ground state. Those interested primarily in the numerical values of the different cross sections can skip much of the theoretical discussion and proceed to Sec. VI. In Sec. VII we consider situations for which the transfer mechanism can be described classically. Mass transfer processes for the capture by a massive object of one of a pair of massive gravitationally bound astrophysical objects are clearly classical; charge transfer from a high Rydberg state via knock-on and double scattering is another instance. Much of the classical material; especially that on knock-on capture, can be read independently of the earlier sections. Section VIII contains some concluding remarks, and also a table illustrating some of the salient differences between the various mechanisms for electron capture from a hydrogenlike atom by a bare ion. The reader may wish to glance at this table from time to time as he works his way through the article.

Specialized material which may be skipped without breaking continuity is indicated by a mark (•) at the beginning of the paragraph.

We first establish a notation.

II. NOTATION

Let m, M_A, and M_B denote the masses of the light particle and the heavy nuclei, respectively. We refer

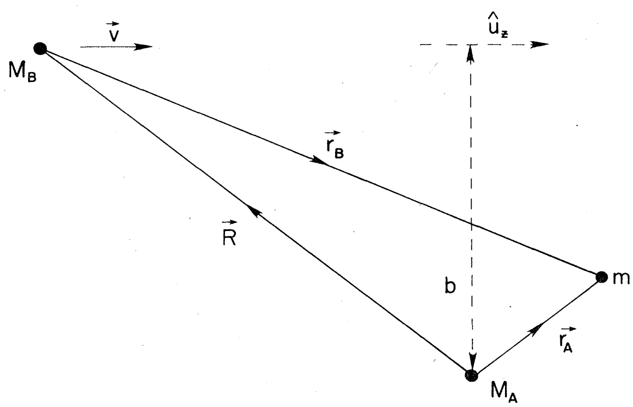

FIG. 1. Diagram showing the relative coordinates. In the laboratory frame M_B has an initial velocity $\mathbf{v}=v\hat{u}_z$ and M_A is initially at rest.

to the particles by their masses. When considering Coulomb interactions, we let e denote the charge of m, an electron, and we let $Z_A|e|$ and $Z_B|e|$ denote the charges of M_A and M_B, respectively. We assume that initially m is bound to M_A, and that M_B is incident with an impact parameter $\mathbf{b}$ and a high velocity $\mathbf{v}$ relative to M_A. Let $\mathbf{r}_A$ and $\mathbf{r}_B$, respectively, be the position vectors of m relative to M_A and to M_B, and let $\mathbf{R}$ be the position vector of M_B relative to M_A; when no confusion might arise, we omit the subscript A or B from the position vector of m. We define a coordinate frame (xyz) fixed in space, with unit vectors $\hat{u}_x$, $\hat{u}_y$, and $\hat{u}_z$, oriented so that the z axis is parallel to the beam axis (see Fig. 1). Let $\psi_i(\mathbf{r}_A)$ and $\psi_f(\mathbf{r}_B)$, respectively, be the normalized wave functions which represent the initial and final states, i and f, of m. Let $W_{AB}(R)$, $W_A(r_A)$, and $W_B(r_B)$ denote the interactions of M_A with M_B, m with M_A, and m with M_B, respectively; all interactions are assumed to be spherically symmetric. We denote the Fourier transform of any function $f(\mathbf{r})$ by $\tilde{f}(\mathbf{p})$, where

$$\tilde{f}(\mathbf{p})=(2\pi\hbar)^{-3/2}\int d^3r e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}f(\mathbf{r})\,; \tag{2.1}$$

when $f(\mathbf{r})=f(r)$, we can write $\tilde{f}(p)$ for $\tilde{f}(\mathbf{p})$. The words "center of mass" will frequently be abbreviated by c.m. The *k*nock-*o*n, *r*adiative *c*apture, and *d*ouble *s*cattering cross sections are denoted by $\sigma_{\rm ko}$, $\sigma_{\rm rc}$, and $\sigma_{\rm ds}$, respectively. The Brinkman–Kramers cross section, which will also be considered, is denoted by $\sigma_{\rm BR}$. The coordinate frame S is that in which the c.m. of M_A and M_B is at rest, while the coordinate frame F is that in which M_B is at rest. The polar axes of all coordinate frames are defined by $\mathbf{v}$; θ and ϕ will always represent polar and azimuthal angles, respectively, while l and μ are quantum numbers of the angular momentum and its projection, and n is a principle quantum number for a hydrogenlike system. The normalized hydrogenlike wave function for an electron with quantum numbers n, l, and μ in the field of a nucleus of charge $Z|e|$ is denoted by

$$\psi_{nl\mu}(\mathbf{r},Z)=R_{nl}(r,Z)Y_{l\mu}(\theta,\phi);$$

the parametric dependence upon Z will sometimes be dropped. With the appropriate subscript, a cross section for capture from a state characterized by n, l, and μ to a state characterized by n', l', and μ' will be denoted by $\sigma(nl\mu\to n'l'\mu')$. (Primed quantum numbers always characterize a final state.) The omission of a final-state quantum number in any σ denotes the sum over that quantum number, while the omission of an initial-state quantum number denotes an average over that quantum number. Thus, for example, we have

$$\sigma(nl\mu\to n')=\sum_{l'}\sigma(nl\mu\to n'l')=\sum_{l'\mu'}\sigma(nl\mu\to n'l'\mu')\,,$$

while

$$\sigma(n\to n')=(n)^{-1}\sum_{l}\sigma(nl\to n')=(n)^{-1}\sum_{l\mu}(2l+1)^{-1}\sigma(nl\mu\to n')\,.$$

We use the abbreviation "bd" to represent the sum over all bound states, and we use "cont" to represent the sum over all low-lying continuum states. Thus, for example, we have

$$\sigma(n\to \mathrm{bd})=\sum_{n'}\sigma(n\to n')\,.$$

For future reference we note that if $W(r)$ is the pure Coulomb potential Ze^2/r, we have

$$\tilde{W}(p)=(2\hbar/\pi)^{1/2}(Ze^2/p^2)\,. \tag{2.2}$$

A caret denotes a unit vector. For any argument and for any index, P denotes a probability. The initial and final internal atomic velocities of m are denoted by $\mathbf{v}_{mi}$ and $\mathbf{v}_{mf}$, respectively; the subscripts i and f will sometimes be dropped, however.

III. KNOCK-ON CAPTURE

In the knock-on process, M_A emerges with almost the same velocity which M_B had initially, and vice versa, but m is not significantly disturbed. (Knock-on is the only mechanism under which m can emerge with a velocity close to the final velocity of M_B without itself undergoing a collision.) This can occur only if the masses M_A and M_B are equal or nearly equal. We assume these masses to be equal throughout this section. For the present we also assume M_A and M_B to be distinguishable. For convenience we discuss the knock-on process in the frame S in which the c.m. of M_A and M_B is at rest, with M_A and M_B having incident velocities $-\frac{1}{2}\mathbf{v}$ and $\frac{1}{2}\mathbf{v}$, respectively. In this frame M_A and M_B backscatter from one another through almost identical angles, as shown in Fig. 2. The crux of the argument is to show that $\sigma_{\rm ko}$ can be factored into a cross section for M_A and M_B to backscatter, with m playing no role, and a conditional probability for capture of m by M_B if backscattering has occurred.

Although radiation may be emitted due to the sudden accelerations of M_A and M_B, the radiation reaction can be ignored for $(v/c)^2\ll 1$. If M_B scatters through an angle $\pi-\theta$, the momentum transferred to M_B is

$$\mathbf{q}(\theta)=-\tfrac{1}{2}Mv[(1+\cos\theta)\hat{u}_z-\sin\theta\hat{u}_\perp]\,, \tag{3.1}$$

where $M\equiv M_A=M_B$ and where $\hat{u}_\perp$ is a unit vector in the xy plane. The differential *b*ack*s*cattering cross section

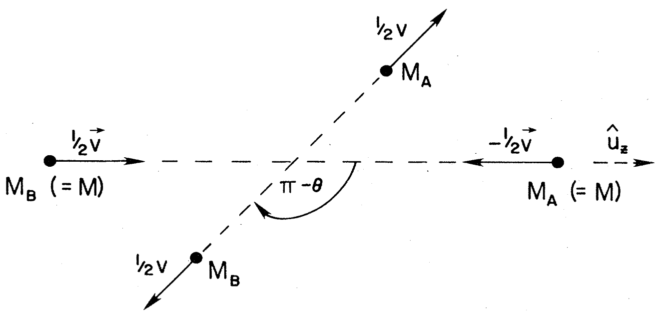

FIG. 2. Backscattering in the center-of-mass frame of M_A and M_B.

$d\sigma_{bs}$ for M_B to scatter from M_A through an angle of $\pi-\theta$ into the differential solid angle $d\Omega$, whether or not it captures the light particle m, is, in the Born approximation, which is adequate for potential scattering at the high relative velocity under consideration,

$$d\sigma_{bs}=[2(\tfrac{1}{2}M)/4\pi\hbar^2]^2(2\pi\hbar)^3\,|\tilde{W}_{AB}(\mathbf{q}(\theta))|^2 d\Omega\,. \tag{3.2}$$

Let $\mathbf{v}_{mi}$ be some characteristic velocity of m relative to the c.m. of the "atom" $(m+M_A)$ when this atom is in the initial state i. Neglecting a correction of order m/M, the initial (and to a good approximation the final) velocity of m in the frame S is of order $\mathbf{v}_{mi}-\frac{1}{2}\mathbf{v}$. After the collision of M_A and M_B, the velocity of m relative to the c.m. of m and M_B is therefore (again neglecting a correction of order m/M) of order

$$\mathbf{v}'_{mf}(\theta)=\mathbf{v}_{mi}-\mathbf{V}(\theta)\,, \tag{3.3}$$

where $\mathbf{V}(\theta)$ is the difference in the velocity of M_B after the collision and the velocity of M_A before the collision, that is,

$$\mathbf{V}(\theta)\equiv\tfrac{1}{2}v[(1-\cos\theta)\hat{u}_z+\sin\theta\hat{u}_\perp]\,. \tag{3.4}$$

For capture to occur, $|\mathbf{v}'_{mf}(\theta)|$ must not greatly exceed some characteristic speed $|\mathbf{v}_{mf}|$ of m relative to the c.m. of the "atom" $(m+M_B)$ when this atom is in the final state f. Since $v\gg|\mathbf{v}_{mi}|$ or $|\mathbf{v}_{mf}|$, we must therefore have θ very small. Roughly speaking, the requirement that $|\mathbf{v}'_{mf}(\theta)|\approx|\mathbf{v}_{mi}-(v\theta/2)\hat{u}_\perp|$ not greatly exceed $|\mathbf{v}_{mf}|$ gives $v\theta/2\lesssim v_{m>}$ where $v_{m>}$ is of the order of the larger of $|\mathbf{v}_{mi}|$ and $|\mathbf{v}_{mf}|$. We therefore have $0\leq\theta\lesssim\theta_{max}$, where

$$\theta_{max}=2(v_{m>}/v)\,.$$

Within this angular range $\mathbf{q}(\theta)$, $d\Omega$ and $\mathbf{V}(\theta)$ can be approximated by $-M\mathbf{v}$, $2\pi\theta d\theta$, and $(v\theta/2)\hat{u}_\perp$, respectively.

Assuming backscattering has taken place, we determine the *relative* (that is, conditional) probability for capture as follows. Since the collision is sudden, and since m is not appreciably disturbed, the nucleus to which m is attached is suddenly switched from M_A to M_B. The sudden approximation of perturbation theory therefore applies, and the relative probability for capture is simply the overlap of the initial and final wave functions multiplied by a factor which takes proper account of the translational motion of the "atoms." Therefore, if M_B is scattered through an angle $\pi-\theta$, the relative probability $P(\theta)$ for capture is, assuming that the nuclei are at the same point when capture occurs, so that $\mathbf{r}\equiv\mathbf{r}_A=\mathbf{r}_B$,

$$P(\theta)=\left|\int d^3r[e^{iX_f}\psi_f(\mathbf{r})]^*e^{iX_i}\psi_i(\mathbf{r})\right|^2. \tag{3.5}$$

The phases X_i and X_f account for the fact that M_A has a velocity before the collision which is not quite equal to the velocity of M_B after the collision.[1] The difference between X_f^* and X_i depends upon this difference of the velocities of the two nuclei and, neglecting a correction of order m/M, is given by

$$X_i-X_f^*=-m\mathbf{V}(\theta)\cdot\mathbf{r}/\hbar\approx-(mv\theta/2\hbar)\hat{u}_\perp\cdot\mathbf{r}\,. \tag{3.6}$$

Failure to account for this velocity-dependent phase difference has, in the past, led to some incorrect statements about the velocity dependence of the quantum-mechanical knock-on capture cross section. In writing down Eq. (3.5) we have assumed that the transition takes place when the separation between the nuclei M_A and M_B is zero. This is not quite correct; classically there is a distance of closest approach which, however small, is finite; quantum-mechanically, we expect from the uncertainty principle that M_A and M_B must approach one another to within a distance of order $\hbar/Mv$—they may have to come much closer—to be able to exchange momentum of the order $M\mathbf{v}$ and therefore to backscatter at this distance. However, since v is large, the correction due to the finite separation of the nuclei during the transition is, in general, negligible. An exception occurs when $\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$ are orthogonal and $\theta=0$, for then $P(0)=0$ according to Eqs. (3.5) and (3.6) and the correction due to the finite separation of the nuclei becomes important, though it is not necessarily the leading correction. However, we need not consider this correction in evaluating the *total* cross section since for $\theta=\theta_{max}$ we have $X_i-X_f^*=(mv_{m>}/\hbar)\hat{u}_\perp\cdot\mathbf{r}$, which is of order unity for the maximum value of r that is relevant, and so $P(\theta_{max})$ need not be small even when ψ_i and ψ_f are orthogonal.

The differential *k*nock-*o*n cross section, $d\sigma_{ko}$, for m to be captured, with M_B backscattered through an angle $\pi-\theta$ into the differential solid angle $d\Omega$, is therefore

$$d\sigma_{ko}=P(\theta)d\sigma_{bs}=(\pi^2M^2/\hbar)\,|\tilde{W}_{AB}(-M\mathbf{v})|^2P(\theta)\theta\,d\theta\,, \tag{3.7}$$

where we have replaced $\mathbf{q}(\theta)$ by $-M\mathbf{v}$ and $d\Omega$ by $2\pi\theta\,d\theta$. The total cross section σ_{ko} for capture in the backward direction is obtained by integrating over the angular range $0\leq\theta\leq\theta_{max}$. If we change the variable of integration from θ to $s=mv\theta/2\hbar$, we obtain

$$\sigma_{ko}=\left(\frac{\pi^2M^2}{\hbar}\right)|\tilde{W}_{AB}(-M\mathbf{v})|^2\int_0^{\theta_{max}}P(\theta)\theta\,d\theta$$
$$=\hbar\left(\frac{2\pi M}{mv}\right)^2|\tilde{W}_{AB}(-M\mathbf{v})|^2\int_0^{s_{max}}s\,ds\,|f(s)|^2\,, \tag{3.8}$$

where

$$f(s)=\int d^3r e^{-is\hat{u}_\perp\cdot\mathbf{r}}\psi_f^*(\mathbf{r})\psi_i(\mathbf{r})\,. \tag{3.9}$$

The integral over s of Eq. (3.8) is independent of v and

[1]See Bates and McCarroll (1958) for a discussion of translational phase factors.

has the dimension of $(1/\text{length})^2$. In this integral we can replace the upper limit of integration $s_{max} = mv_{m>}/\hbar$ by ∞. The justification for this is as follows. Since $1/s_{max}$ is of the order of the dimension of the smaller of the "atoms" described by ψ_i and ψ_f, the main contribution to the integral of Eq. (3.9) comes from the region $r \leq 1/s_{max}$. (As r increases beyond $1/s_{max}$ the integrand decays exponentially.) It follows that $f(s)$ decreases rapidly for $s > s_{max}$ because of the presence of the oscillatory exponential function in the integrand of Eq. (3.9). Therefore the region $s > s_{max}$ does not contribute appreciably to the integral of Eq. (3.8), and, with little error, s_{max} can be replaced by ∞. If this is done the asymptotic form for the knock-on capture cross section given by Eq. (3.8) is (to leading order in m/M) identical to that obtained by Dettmann and Leibfried (1969) using the first Born approximation.

Note that if $\tilde{W}_{AB}(-M\mathbf{v})$ decreases more rapidly than $1/Mv$ with increasing v, the expression on the right-hand side of Eq. (3.8) contains M in the denominator and is therefore small. If the two nuclei interact via a pure Coulomb potential, we have, using Eq. (2.2),

$$\sigma_{ko} = 8\pi\left(\frac{Z_A Z_B e^2 \hbar}{mMv^3}\right)^2 \int_0^\infty s\, ds\, |f(s)|^2. \tag{3.10}$$

The cross section is small, and for capture into an s state the knock-on process is always dominated by the radiative capture process when the interactions are pure Coulombic.

Explicit values of $\sigma_{ko}(1s \to n'l')$ for $n'l' = 1s$ and $2p$ are given in Sec. VI. A. In Sec. VII we consider $\sigma_{ko}(nl \to n'l')$ for $n \gg 1$ and l rather larger than 1. The results in that domain can be given a classical interpretation and give some new insights into the results obtained above. Thus the relative speed of m and M_B after the collision is $(\frac{1}{2}v)\theta$, and θ_{max} can be interpreted as the angle beyond which $(\frac{1}{2}v)\theta$ exceeds the escape velocity.

•[2]In discussing the knock-on process we treated the nuclei as distinguishable particles. We now consider *identical* nuclei. Roughly speaking, each nucleus can be described by a wave packet whose linear dimensions (in coordinate space) are of order $\hbar/Mv$; each nucleus cannot be localized to a volume whose linear dimensions are smaller than $\hbar/Mv$ if the quantum-mechanical uncertainty in the relative speed of the nuclei is to be small compared to v. Provided that the two nuclei do not approach one another to within a distance of order $\hbar/Mv$, the wave packets of the nuclei will not overlap appreciably, and the nuclei can be distinguished even when they are identical. However, in the knock-on process the two nuclei must approach one another to within this distance in order to exchange momentum $M\mathbf{v}$, and therefore in this process identical nuclei cannot be treated as distinguishable; for identical nuclei, not spin polarized, the knock-on process cannot be distinguished from the direct process in which the incident nucleus passes by the target nucleus with an impact parameter of order $\hbar/Mv$ or less without picking up the light particle. Of course, when the nuclei are identical the knock-on process contributes to the total elastic scattering cross section, but its contribution is small in proton–hydrogen atom scattering, for example. The knock-on process can be clearly distinguished from the direct process when the nuclei are not identical as, for example, in the case of a ^{3}He nucleus incident upon the atom $(e + {}^3\text{H})$, or a ^{14}C nucleus incident upon an ion consisting of a single electron bound to an ^{14}N nucleus. However, it should be noted that in these two examples the knock-on process cannot be distinguished from the process in which there is forward scattering, with the target nucleus and the projectile changing their identities by single pion exchange. In fact, the single pion exchange cross section becomes much larger than the Rutherford backscattering cross section as the relative velocity increases.

The nuclear force plays no role in the radiative and double-scattering processes since, as will be seen in the following sections, the range of impact parameters that contributes to these processes is much larger than the range of the nuclear force.

Equation (3.10) may be readily generalized to target atoms having more than one electron. If the target nucleus is knocked forward with a high speed in the lab frame, the target electrons will remain behind and some may be captured while others will be set free. The form of Eq. (3.10) (and, in particular, the v dependence) remains valid, but in the function $f(s)$ of Eq. (3.9) the single particle wave functions must be replaced by their multiparticle counterparts. For capture of a specified number of electrons ψ_f would be a wave function for that number of electrons bound with the remaining electrons being in the continuum. $\mathbf{r}$ in the exponent would be replaced by the sum over all (free and continuum) electron coordinates.

IV. RADIATIVE CAPTURE

A. Derivation of the cross section

In radiative capture at high impact velocities, the target[3] nucleus M_A plays essentially no role and the total radiative capture cross section at asymptotically high energies can be determined by assuming that the light particle m is free initially, the initial binding ultimately becoming negligible.[4] Radiative capture is then simply the inverse photoelectric effect—"the subsystem" $(m + M_B)$ spontaneously emits a photon and becomes bound. Invoking detailed balance with the appropriate density of states the asymptotic form of the total *r*adiative *c*apture cross section, σ_{rc}, can therefore be ob-

[2]This symbol (•) indicates a paragraph which may be skipped without breaking continuity in reading. It generally indicates somewhat more specialized material.

[3]By the *target* nucleus we mean the nucleus to which m is bound intially.

[4]This point has often been insufficiently stressed in the literature. For example, Oppenheimer (1928) discusses both nonradiative charge transfer and the radiative recombination of electrons and protons, but he never notes that the result derived for radiative recombination is relevant to charge transfer. That it is was stressed by Raisbeck and Yiou (1971), who extended the result to radiative charge transfer at relativistic energies. Note that the target nucleus plays a significant role in radiationless capture.

tained from the well-known formulae for the photoelectric effect (Bethe and Salpeter, 1957). However, as it is not difficult, and since it is more instructive, we shall obtain σ_{rc} directly.

Ignoring M_A altogether, treating M_B as infinitely massive, and proceeding nonrelativistically, we work in the projectile frame F in which M_B is at rest. In this frame, m initially moves with a velocity roughly equal to $-\mathbf{v}$ and is *approximately* (see below) described by a plane wave $(1/V)^{1/2}\exp(-im\mathbf{v}\cdot\mathbf{r}/\hbar)$ which is normalized to unity in a volume V, and generates a flux v/V. If m spontaneously "decays" into the final bound state f represented by $\psi_f(\mathbf{r})$, the rate at which photons of polarization $\hat{\lambda}$ are emitted into the solid angle $d\Omega$ is, treating the electromagnetic field as a small perturbation and using first-order perturbation theory (Dirac, 1958),

$$d\Gamma=\left(\frac{\hbar\omega e^2}{2V\pi m^2c^3}\right)\left|\int d^3r\psi_f^*(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\lambda}\cdot\vec{\nabla}e^{-im\mathbf{v}\cdot\mathbf{r}/\hbar}\right|^2 d\Omega$$

$$=\left(\frac{4\omega\pi^2e^2\hbar^2}{Vc^3}\right)(\hat{\lambda}\cdot\mathbf{v})^2|\tilde{\psi}_f(-m\mathbf{v}-\hbar\mathbf{k})|^2d\Omega. \qquad (4.1)$$

Here ω is the angular frequency of an emitted photon and $\hbar\mathbf{k}=\hbar\hat{k}\omega/c$ is its momentum. The value of ω follows from energy conservation; since the final (as well as the initial) binding energy is assumed to be very much less than the initial kinetic energy of m in the frame F, we have $\hbar\omega=mv^2/2$. Since the flux is v/V the differential cross section for radiation of polarization $\hat{\lambda}$ to be emitted when m is captured into the state f is

$$\frac{d\sigma_{rc}}{d\Omega}=\frac{V}{v}\frac{d\Gamma}{d\Omega}$$

$$=\left(\frac{2\pi^2mve^2\hbar}{c^3}\right)(\hat{\lambda}\cdot\mathbf{v})^2\left|\tilde{\psi}_f\left(-m\mathbf{v}-\frac{mv^2\hat{k}}{2c}\right)\right|^2. \qquad (4.2)$$

Note that due to the factor $(\hat{\lambda}\cdot\mathbf{v})^2$ in Eq. (4.2), the emitted light is preferentially polarized along the beam axis. Note also that, although we treat m nonrelativistically, the momentum $(mv^2/2c)\hat{k}$ of the photon need not be neglected in the argument of $\tilde{\psi}_f$ in Eq. (4.2) since its relative contribution to the differential cross section is of order v/c, whereas a relativistic treatment of m would give corrections of order $(v/c)^2$. However, the relative contribution of the photon momentum to the integrated cross section σ_{rc} should be dropped since it is of order $(v/c)^2$. This can be seen by expanding $|\tilde{\psi}_f(\mathbf{p})|^2$ as a Taylor series about the value $|\tilde{\psi}_f(-m\mathbf{v})|^2$, with $\mathbf{p}=-m\mathbf{v}-mv^2\hat{k}/2c$; the expansion is a power series in v/c and the second term is odd under the reflection $\hat{k}\to-\hat{k}$ so that, since $(\hat{\lambda}\cdot\mathbf{v})^2$ is even under $\hat{k}\to-\hat{k}$, it vanishes when the integration over $\hat{k}$ is performed. Summing over all polarizations of the emitted radiation, integrating over $\hat{k}$ (neglecting the photon momentum), and using

$$\sum_{\hat{\lambda}}\int d\hat{k}(\hat{\lambda}\cdot\mathbf{v})^2=v^2\int d\hat{k}\sin^2\theta=\frac{8\pi v^2}{3},$$

we obtain the total cross section for radiative capture to the state f,

$$\sigma_{rc}=(2^4\pi^3m\hbar e^2v^3/3c^3)|\tilde{\psi}_f(-m\mathbf{v})|^2. \qquad (4.3)$$

Note that the factor $|\tilde{\psi}_f(-m\mathbf{v})|^2$ is consistent with the fact that the photon carries away only a negligible amount of momentum; m must be captured into a high-momentum component of the final bound state. High-momentum components are generated by the coordinate wave function $\psi_f(\mathbf{r})$ only for r very small, and the higher the angular momentum of m in the state f, the less likely it is that we shall find m near M_B. For ψ_f a Coulomb wave function, $|\tilde{\psi}_f(-m\mathbf{v})|^2$ behaves as $v^{-8-2l'}$. Note also that $\tilde{\psi}_i$ and $\tilde{\psi}_f$ do not enter into the expression for the cross section symmetrically—in fact, $\tilde{\psi}_i$ does not enter at all. This does not violate time-reversal invariance since the time-reversed process involves the absorption of a photon, and therefore radiative capture from state f to state i, which necessarily involves the emission of a photon, is not related by time reversal to radiative capture from state i to state f.

Equation (4.3) is effectively identical to the result obtained in a three-body approach by Briggs and Dettmann (1974) and Kleber and Jakubassa (1975) in the same high-energy limit. (The Compton profile factor, the only difference, is of no significance in this limit.)

Unfortunately Eq. (4.3) is not quite correct in the asymptotic limit when $l'\geq 1$ unless $W_B(r)$ is less singular than the Coulomb potential at $r=0$. The treatment of (three-body) radiative capture as (two-body) radiative recombination introduces no error in the asymptotic limit, but the subsequent neglect of the effect of $W_B(r)$ on the initial state, that is, the replacement of the initial state of m by a plane wave state, is inadequate when $l'\geq 1$. The reason is the following. Rather than being captured into a high momentum component of the final state, m can scatter from M_B, lose most of its large momentum $-m\mathbf{v}$ *before* being captured, and be captured into a low momentum component of the final state. Such scattering corresponds to a considerable distortion of the plane wave and can occur only if m gets close to M_B in the initial state. It will be sufficient to consider the dipole approximation, for which only the $l=l'\pm 1$ components of the initial continuum wave function of m contribute to radiative recombination. For $l'=0$, only the $l=1$ component contributes, and the correction to Eq. (4.3) is negligible, but for $l'\geq 1$ one can have $l=l'-1$; the centrifugal barrier is then lower in the initial than in the final state. Thus, for $l'\geq 1$, m can more easily get close to M_B in the initial state than in the final state. It is not difficult to show that the reduced barrier compensates for the additional scattering if $l'\geq 1$ [and $W_B(r)$ has a Coulomb singularity at $r=0$], that is, that it is roughly as "efficient" for m to scatter from M_B and lose most of its momentum before being captured as it is for m to be captured directly into a high momentum component of the final state. When this additional possibility is taken into account, the over-all numerical coefficient in Eq. (4.3) is altered if $l'\geq 1$, but the v dependence is unaffected. We shall not generally incorporate this modification since it is rather complicated to do so and since the problem has been carefully analyzed (Bethe and Salpeter, 1957, Sec. IVb). Further, Eq. (4.3) not only gives the correct v dependence but, at least for the Coulomb case, can give the correct dependence upon n' and Z_B for l' fixed and a sum over μ'; on the other hand, Eq. (4.3) tends to give incorrect angular distributions. We note that σ_{rc} ($1s\to$bound) for $v\sim\infty$ will be given correctly by Eq. (4.3) since the dominant contributions, $\sigma_{rc}(1s \to ns)$, are given correctly by Eq. (4.3). We also note that a number of recent papers obtained $\sigma_{rc}(1s \to n', l' \geq 1)$ incorrectly for they ignored the possibility of the preliminary scattering of m. Further, we remark that, as for double versus single scattering in radiationless forward capture, it follows from the above discussion that for radiative capture into a state with $l' \geq 1$ via a singular interaction, a higher term in the Born expansion does not become negligible as the incident energy goes to infinity.

If, to be concrete, we consider a bare nucleus incident on H, we might ask if we can indeed neglect the effect of the target proton on m. Two separate questions arise. (i) The correct asymptotic form of the wave function is a product of a hydrogenic function and of a plane wave describing the relative motion. The relative motion is *not* asymptotically Coulombic, and one might question whether the preliminary Coulomb scattering of the electron by the nuclear projectile, discussed in the previous paragraph, is the correct description. To see that it is, we note first that the electron and the projectile have a large relative momentum and that the wave function of relative motion therefore has many wavelengths within the shielding, (a_0/Z_A), and, second, that the significant aspect of the Coulomb interaction is here not its long range character but rather its singularity at the origin. (ii) In its initial state, m has high momentum components, and one might ask if these components could (as for the high momentum components generated in a preliminary scattering of m by M_B) make it easier for m to be captured into a high momentum component. The answer is no, and is related to the difficulty of then conserving both energy and momentum. The replacement of the three-body radiative capture problem by the two-body radiative recombination problem makes it possible to extend the analysis in a number of directions. For example, one can directly take over everything known about the photoelectric effect; thus, one can almost immediately obtain the relativistic version of $d\sigma_{rc}/d\Omega$ (Raisbeck and Yiou, 1971). As a second example consider the radiative capture of an electron initially bound in a hydrogen atom by an ion with one or more electrons, He^+ for instance. The process $He^+ + H \to He + p + \gamma$ would then be equivalent to $He^+ + e \to He + \gamma$; one could approach this much simpler problem theoretically, or use data for the inverse (photoelectric) process. For this second example, where M_B is not a bare nucleus, still another process could conceivably dominate in some energy range. One might imagine—this is a point we have not checked—that at high v, though not in the asymptotically high v limit, the dominant capture process for sufficiently large Z might be through dielectronic recombination. In the frame F the incident electron would excite an inner electron, the two electrons then each being in excited Rydberg bound states while the system as a whole would be in a bound state embedded in the continuum, a bound state which could either auto-ionize *or* decay by the emission of a photon to a true bound state. As a final example, consider the case in which there are two or more electrons bound to M_A. To be concrete, compare the capture of an electron from a helium atom by a proton with the capture of an electron from a hydrogen atom by a proton. One would expect σ_{rc} for $p + He \to H + He^+$ to be twice σ_{rc} for $p + H \to H + p$ since details of the binding play no role, either of the two electrons can be captured from He, and there should be no interference between the amplitude for the capture of one electron and the amplitude for the capture of the other electron since the spin projection of the electron which is captured (or the electron which is not) could in principle be measured.

B. The impact-parameter dependence

Though it is not necessary to do so since we already know σ_{rc}, it will provide some further physical insight if we obtain the impact-parameter dependence of the radiative capture cross section. We first note that the collision between m and M_B must be almost head-on since the effective collision time is short and a large impulse is needed to cause m to emit a photon of energy $mv^2/2$. Therefore m must initially be on the path of M_B. In other words, if M_B is incident with an impact parameter between b and $b+db$ relative to the target nucleus M_A, the component of the vector joining m and M_A in the direction perpendicular to the beam axis must initially be between b and $b+db$. The normalized probability $dP(b)$ that this condition is satisfied is determined by the initial bound-state wave function. If we introduce cylindrical coordinates ρ, ϕ, z, with the z axis chosen as in Fig. 1, and if we write $|\psi_i(\rho, z)|^2$ in place of $|\psi_i(\mathbf{r})|^2$, assuming, as is generally the case, that $|\psi_i(\mathbf{r})|^2$ is independent of the azimuthal angle we have

$$dP(b) = 2\pi b\,db \int_{-\infty}^{\infty} dz\,|\psi_i(b,z)|^2. \tag{4.4}$$

[Note that $\int_0^\infty dP(b)$ is unity since $\psi_i(\mathbf{r})$ is normalized to unity.] Given that radiative capture takes place, $dP(b)$ is the probability that it takes place for an impact parameter between b and $b+db$. Therefore, with respect to impact parameter, the differential cross section is

$$\frac{d\sigma_{rc}}{db} = \sigma_{rc}\frac{dP(b)}{db} = \left(\frac{2^5\pi^4 m b \hbar e^2 v^3}{3c^3}\right) |\tilde{\psi}_f(-m\mathbf{v})|^2 \int_{-\infty}^{\infty} dz\,|\psi_i(b,z)|^2. \tag{4.5}$$

With some manipulation this result also follows from Eq. (9) of Briggs and Dettmann (1974), as sketched in Appendix A of this article. It is apparent from the integral of Eq. (4.5) that the significant values of b with regard to radiative capture range from zero to the order of the average radius of the initial orbit of m, and this range, of course, is independent of the speed v. Thus the radiative process explores all but the outer regions of the target atom $(m + M_A)$. Note that the target nucleus M_A does play a role in the determination of the impact-parameter dependence of the cross section.

C. Linewidth

The emphasis in this paper is on the development of simple interpretations of and insights into the mechanisms for charge transfer, with a total of three particles involved, at asymptotically high velocities. In this subsection, however, we digress and discuss matters of more direct concern to experimentalists. We use the dipole approximation throughout this section.

Analysis of radiative capture rather than of radiative recombination is an excellent approximation for the determination of σ_{rc} at asymptotically high velocities. The photon emitted, for a monochromatic incident beam, will then also be monochromatic, with an energy $\hbar\omega = mv^2/2$, neglecting the binding energy of m in the final state. In reality, the photons will of course have a spread in energy. To determine the width of the spread, it will be necessary to take into account the momentum distribution of m in its initial state. (Here again the target nucleus M_A plays a role—it generates the initial momentum distribution.) To be concrete, we assume that a nucleus of charge $Z_B|e|$ is incident with velocity $\mathbf{v}$ on a nucleus of charge $Z_A|e|$ which binds one electron. (The result will be derived in a form approximately applicable to many-electron atoms.)

The problem can be attacked at a number of levels. In the crudest approximation the momentum $\mathbf{p}_m$ of the electron, with respect to the target nucleus which binds it, has a spherically symmetric angular distribution and is of fixed magnitude p_m. The range of the kinetic energy T of the electron with respect to the incident nucleus is then given by

$$(p+p_m)^2/(2m) \leq T \leq (p-p_m)^2/(2m)\,, \tag{4.6}$$

where $p \equiv mv$. The energy spread of T, a measure of the width of the line, is then $2pp_m/m$, which we can rewrite as $4\{T_m(p^2/2m)\}^{1/2}$; $T_m \equiv p_m^2/(2m)$ will be of the order of the ionization energy of the electron and the target nucleus.

An analysis along the above lines was given by Sohval (1975) and by Sohval *et al.* (1976). They also went further by considering more realistic momentum distributions, $\tilde{\phi}^2(p_m)$, where $\int \tilde{\phi}^2(p_m)d^3p_m = 1$. [If $\tilde{\phi}^2(\mathbf{p}_m)$ is not spherically symmetric, it can be replaced by the spherically symmetric function obtained by averaging over angles, for the target atoms are randomly oriented.] If $n(T)dT$ represents the normalized distribution of energies of the electron with respect to the incident nucleus, we then have

$$n(T) = \int 2\pi p_m^2\, dp_m d\mu \tilde{\phi}^2(p_m)\delta\{T - T(p_m,\mu)\}\,, \tag{4.7}$$

where $\mu \equiv \hat{p}\cdot\hat{p}_m$ and

$$T(p_m,\mu) \equiv \frac{(\mathbf{p}-\mathbf{p}_m)^2}{2m} = \left(\frac{pp_m}{m}\right)\left[\left(\frac{p}{2p_m}\right)+\left(\frac{p_m}{2p}\right)-\mu\right].$$

There will be a value of μ between -1 and $+1$ for which $T - T(p_m,\mu) = 0$ if and only if p_m lies in the range defined by Eq. (4.6), namely, if and only if

$$|(2mT)^{1/2} - p| \leq p_m \leq (2mT)^{1/2} + p\,. \tag{4.8}$$

We thereby arrive at

$$n(T) = \left(\frac{2\pi m}{p}\right)\int p_m \tilde{\phi}^2(p_m)dp_m\,,$$

with the range of integration of p_m given by Eq. (4.8).

Sohval *et al.* (1976) used a Fock momentum distribution, appropriate to a hydrogenlike state of principle quantum number n and of average kinetic energy T_n. The number T_n was taken to be an open parameter, to be determined experimentally. (This is equivalent to using an effective charge in the approximation in which the electrons of a many-electron atom are considered to be independent.) They measured the linewidth for stripped and partially stripped oxygen nuclei incident with energies 30 to 65 MeV on targets ranging from the H_2 molecule to the O_2 molecule. In their analysis, they used for σ_{rc} Eq. (4.3) generalized to include the effect on the incident wave function of the Coulomb interaction between the incident charged nucleus and the electron to be captured. Furthermore, they corrected for instrumental broadening, for Doppler broadening, for the energy dependence of σ_{rc}, and for the distribution of charged states of the ^{16}O beam within the gas target cell. The T_n thereby deduced experimentally were in good agreement with theoretical estimates. [Incidentally, the line is of course centered not about $\frac{1}{2}mv^2$ but about $\frac{1}{2}mv^2 + E_B$, where E_B is the difference between the binding energies of the final and initial states.]

More recently Spindler *et al.* (1977) measured the radiative capture linewidth for partially stripped copper ions incident on carbon and aluminum foils with an energy up to 450 MeV. The observed linewidth was well accounted for by using highly accurate momentum distributions for the target electrons.

The above analysis is sufficient for present purposes, but we note that within the context of the Born approximation, a rigorous treatment of the three-body problem was given by Briggs and Dettmann (1974).

It should be clear that folding in the momentum distribution of the electron not only provides an estimate of the linewidth for a monochromatic incident beam, but also provides an estimate of $d\sigma_{rc}/d\omega$, the differential cross section for radiative capture with the emission of a photon with frequency between ω and $\omega + d\omega$. Since $T = \hbar\omega - mv^2/2$, so that $dT = \hbar d\omega$, we have, ignoring as above the slight dependence of σ_{rc} on the initial velocity distribution of the electron, $d\sigma_{rc}/d\omega = \hbar d\sigma_{rc}/dT = \hbar n(T)\sigma_{rc}$.

D. Galilean invariance for processes involving photons

In their evaluation of the radiative capture cross section σ_{rc} for $p + \mathrm{H} \to \mathrm{H} + p + \gamma$, with the particles treated nonrelativistically, Briggs and Dettmann (1974) found that σ_{rc} depended upon the frame of reference used for their calculation if the relative motion were described by the Born approximation. This may not seem surprising, since we are concerned with the emission of a photon, and electromagnetic theory is Lorentz invariant rather than Galilean invariant[5]; therefore we might not expect σ_{rc} to be Galilean invariant. (σ_{rc} would, of course, be Lorentz invariant if the particles were treated relativistically.) Despite the presence of the photon, it was found that σ_{rc} was Galilean invariant if the relative motion of p and H were described more accurately. That σ_{rc} and, more generally, the cross sec-

[5]A very enlightening discussion of the nonrelativistic limit of electromagnetic theory has been given by Le Bellac and Levy-LeBlond (1973).

tions for a number of other radiative processes are Galilean invariant under specified circumstances was recently pointed out by the present authors, and we shall touch briefly on this subject.

We begin by remarking that the particle-electromagnetic interaction is proportional to $\omega^{-1/2}$, to the polarization vector $\hat{\lambda}$, and to $\exp(\pm i\mathbf{k}\cdot\mathbf{r})$. But the Doppler shift of ω and the aberration of $\hat{\lambda}$ as seen by observers with relative velocity $\mathbf{u}$ will be or order u/c and can be neglected; further, in the dipole approximation we replace the exponential by unity. There is little left therefore of the structure of the photon, and in the above approximation we have what might be called a nonrelativistic quantum theory of photons.[5] (One can also surely find conditions under which *classical* radiative processes have Galilean invariant cross sections. Further, since the gravitational field has spin two, as opposed to the spin one of the electromagnetic field, we should expect to obtain a nonrelativistic theory of gravitational radiation on using the quadrupole approximation.) It turns out that σ_{rc} is indeed Galilean invariant in this nonrelativistic limit *if* the initial and final wave functions describing the motion of the particles are orthogonal. If the initial and final wave functions are not orthogonal, Galilean invariance does not, in general, follow. This can be understood as follows.

It is well known that a free particle cannot radiate. The mathematical proof of this result is that the quantum-mechanical matrix element for the radiation by a free particle contains, as a factor, the product of an energy-conserving delta function and a momentum-conserving delta function; the arguments of both delta functions cannot vanish simultaneously and so the matrix element must vanish. A free particle that has internal degrees of freedom, to be referred to as a free system, such as a He^+ ion, can of course radiate if the free system is in an internal state of excitation. However, one should not expect the c.m. of the free He^+ ion to be able to radiate, at least if, as we assume, the photon momentum can be neglected. (If the photon momentum is not neglected, the c.m. of the ion will recoil, and therefore radiate, if the ion undergoes an internal radiative transition.) The proof that the c.m. of a free system cannot radiate does not follow from the impossibility of the arguments of the energy- and momentum-conserving delta functions vanishing simultaneously. In fact, of course, both arguments *can* vanish simultaneously if the free system is initially in an excited internal state (which includes continuum states), since energy conservation can be satisfied merely by allowing the free system to undergo an internal transition. It is the orthogonality of the wave functions describing the internal state of the system before and after the transition which precludes radiation from the c.m. If this orthogonality is not preserved when approximate wave functions are used to describe the internal state of a system, the c.m. of the system will, in general, seem to radiate. As one might expect, the matrix element for spurious c.m. radiation is proportional to the current generated by the c.m.; the constant of proportionality is zero only if the initial and final internal wave functions are orthogonal. Since the current generated by the c.m. of a system depends on the frame of reference being used (unless the system is electrically neutral, in which case the current is zero in all frames), it follows that if the initial and final internal wave functions of the system are not orthogonal, the cross section for the system to undergo any radiative transition will not be Galilean invariant in the natural nonrelativistic limit.

This point has been discussed in detail by the present authors elsewhere (Shakeshaft and Spruch, 1977) and so we shall not enter into further details here; however, we should remark that had we performed the calculation of Sec. IV.A in any frame other than the frame F, we would have obtained an erroneous result. The reason, of course, is that the wave functions which we used to describe the initial and final internal states of $(m+M_B)$ are not orthogonal. (The final state was described exactly, but the initial continuum state was described by a plane wave rather than by a Coulomb wave function.) We obtained the correct result only because in the frame F the c.m. of $(m+M_B)$ is at rest and therefore generates no current, so that the possibility of spurious radiation does not arise. The correct result can be obtained in a frame other than F, but one must use a better approximation ψ_{it} to the initial continuum wave function ψ_i than a plane wave; we need not have $(\psi_{it},\psi_f)=0$, but (ψ_{it},ψ_f) must vanish "sufficiently rapidly" as v increases for the error introduced by the lack of orthogonality to be irrelevant.

V. DOUBLE SCATTERING

In this section we discuss the double scattering mechanism, so called because m is captured after undergoing two binary collisions. It should be noted that the knock-on process and the double scattering process are two very different mechanisms for radiationless capture. In fact, the knock-on process is really not of great interest since it is never observed in customary "electron" capture experiments, where, in the lab frame, only those "atoms" moving with high velocity in the forward direction are detected. (Recall that in the knock-on process the incident nucleus comes to rest in the lab frame.) In the double scattering mechanism the incident nucleus is only barely deflected owing to the extremely small ratios m/M_A and m/M_B; in other words, the incident nucleus is scattered into the *forward* direction through a very narrow range of angles with little change in speed.

As in the preceding two sections the emphasis in this section is on the "physical" interpretation. Indeed it is even more to the point for the present mechanism than for the previous two to develop further insights since the present mechanism is a much more complicated one and one can perform the full quantum-mechanical three-body calculation of the forward capture cross section without gaining much feeling as to what "happened." Our viewpoint in this section is the following. In the days of the old quantum mechanics, and even in the early days of modern quantum mechanics when the theory was not yet properly understood, one was often guided by concepts such as the correspondence principle; such concepts enabled one to utilize one's knowledge of classical mechanics. We should like not to reverse but to update the procedure. Guided by our classical *and* quantum-mechanical knowledge, we should like to develop a simple but accurate picture for the complicated double scattering process. To develop such a picture we shall decompose the process into elements and we shall use classical concepts to evaluate the elements where possible, that is, where there is no violation of the (higher) laws of quantum mechanics; the uncertainty principle, in particular, will ever be in our minds. Apart from satisfying an inner need, the above approach will enable us, using considerable hindsight, to rederive the asymptotic form of the forward capture cross section in a fashion very much simpler than that of treating the problem as a full quantum-mechanical three-body problem; it is not merely that the analysis and integrations are simpler, but that there are no integrations of any kind to be performed! [In the full quantum-mechanical treatment, the matrix element at one stage is a 24-dimensional integral. See Eq. (8.4.5) of McDowell and Coleman (1970). This book, incidentally, contains an excellent discussion of the single scattering and double scattering processes. Furthermore, as is to be expected from its title, the book *Theory of Charge Exchange* (Mapleton, 1972) contains a wealth of information on charge transfer processes.] However, our approach is not quite rigorous. It should be possible to make it rigorous, but at present its full justification must rely upon agreement with earlier and more rigorous calculations; more significantly, it might be difficult to obtain the exact numerical coefficient with the present approach. On the other hand, the present viewpoint should clarify the limits of validity of existing calculations, and should suggest whether possible extensions—to target atoms or ions with more than one electron, to incident nuclei that are not bare, or to the relativistic domain, for example—could be validly treated with merely minor modifications or whether these extensions would require a far more elaborate calculational procedure. (With regard to relativistic corrections, note that the light particle m never achieves a speed much exceeding that of the incident heavy nucleus M_B so that m can be treated nonrelativistically if M_B can.)

A. Some historical remarks

The double scattering process was suggested by Thomas (1927) as the mechanism for forward capture at high impact velocities. Thomas performed the first calculation of the forward capture cross section; it was a *tour de force* based on a classical treatment of double scattering. We shall describe Thomas's calculation in some detail in Sec. V.C. For the present we briefly note that Thomas supposed that for capture to take place m must acquire a velocity very close to the velocity $\mathbf{v}$ of the incident nucleus M_B; the latter moves with essentially constant velocity. This requires (from conservation of energy and momentum, as explained below) that, in the lab frame, m first be knocked by M_B towards the target nucleus M_A with a speed very close to v and in a direction making an angle α_1 of just about 60° with the direction of motion of M_B, as shown in Fig. 3; m then scatters from M_A through an angle α_2 of just about 60°, without change of speed, and emerges with a velocity very close to $\mathbf{v}$. The mutual attraction between m and M_B then serves to bind them. Using classical mechanics, Thomas predicted that the cross section for forward capture by protons from hydrogen atoms should behave as $1/v^{11}$ for asymptotically high v.

The first quantum-mechanical calculation of forward capture was performed by Brinkman and Kramers (1930). Their calculation differed from the first Born approximation only in that the internuclear potential was omitted. The justification for neglecting the internuclear potential is as follows: To order m/M_A the internuclear coordinate is the same as the coordinate connecting M_B to the c.m. of $(m+M_A)$; but an interaction between two systems which depends only on the coordinate connecting the centers of mass of the two systems cannot directly affect the internal state of either system—in particular, it cannot directly induce charge transfer. For further discussion of this point see Dettmann (1971). The internuclear potential is, of course, essential to knock-on capture; it is for this reason that the velocity-independent coefficient is so much smaller for σ_{ko} than for σ_{ds}. Within this approximation, Brinkman and Kramers predicted that the cross section for forward capture by protons from hydrogen atoms should behave as $1/v^{12}$ for asymptotically high v, in clear disagreement with the Thomas result. The Brinkman-Kramers result was naturally favored, since quantum mechanics, though still a new theory then, had already been enormously successful in explaining phenomena that classical mechanics could not. Nevertheless, despite the overwhelming predilection for quantum mechanics, the disagreement between the Thomas and Brinkman–Kramers results was not viewed without consternation by Bohr and others; it was difficult to understand why the conditions for the validity of the classical treatment were not satisfied since, in the Thomas picture, m is scattered through *large angles* with *high speed*, and since the classical Rutherford cross section happens to be correct. (The extent to which the double scattering process *can* be treated classically is discussed in Secs. V.B. 2 and VII. A.) For many years it was incorrectly thought that the classical treatment failed to yield the Brinkman–Kramers result because it neglected subtle interference effects. Even as late as 1948 Bohr (1948), in commenting on the supposed inadequacy of the classical treatment, wrote: "It must be realized, however, that in the capture phenomena we have not simply to do with two separate collisions, the individual effects of which .... are defined by the wave functions at large distances from the scattering centre. On the contrary, electron capture presents us with an intricate collision process for the result of which the interference of the scattered wavelets during the overlapping of the atomic fields may be decisive." A correct understanding of the discrepancy between the classical and quantum-mechanical results was not achieved until 1955 when Drisko (1955) reasoned that classical double scattering is a two-step process which should therefore correspond to a *second* Born term in a quantum-mechanical treatment; the first Born term corresponds to single scattering. Drisko calculated the contribution from the second Born term—the Born again term, Prof. Paul Berman has called it—to the forward capture cross section and indeed found

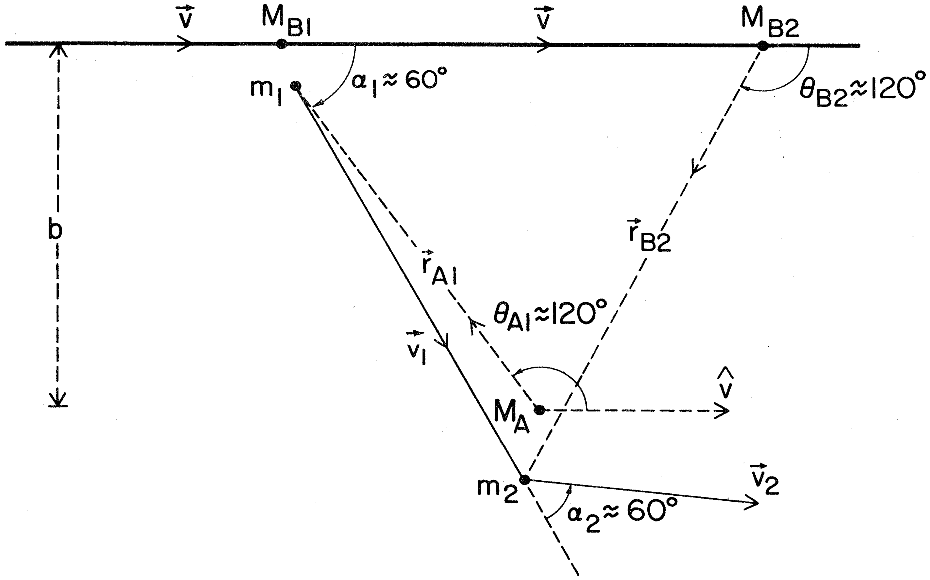

FIG. 3. Schematic diagram depicting the motion of m and M_B in the lab frame for the double scattering process. The paths of m and M_B are indicated by thin and thick lines, respectively. The initial speed of m is very much less than v and will be neglected. M_A remains effectively at rest, and M_B moves with effectively constant velocity $\mathbf{v}$ at an impact parameter of about b relative to M_A. The dots labeled m_1 and M_{B1} and the dots labeled m_2 and M_{B2} represent the positions of m and M_B at the times of the first and second collisions, respectively. Note that m_1, m_2, and M_{B2} form an approximately equilateral triangle with sides of length $2b/\sqrt{3}$. The position vector of m with respect to M_A, indicated by a dashed line, is $\mathbf{r}_A \equiv (r_A, \theta_A, \phi_A)$ with the polar axis parallel to $\mathbf{v}$. The value of $\mathbf{r}_A$ for the initial collision is roughly $\mathbf{r}_{A1} = (2b/\sqrt{3},\ 2\pi/3,\ \phi_A)$. The position vector of m with respect to M_B, also indicated by a dashed line, is $\mathbf{r}_B \equiv (r_B, \theta_B \phi_B)$ with the polar axis again parallel to $\mathbf{v}$. At the time of the second collision m is very close to M_A—roughly at the break in the thin line—and $\mathbf{r}_B \approx \mathbf{r}_{B2} = (2b/\sqrt{3},\ 2\pi/3,\ \phi_A)$, setting $\phi_B = \phi_A$. The velocities of m after the first and second collisions are $\mathbf{v}_1$ and $\mathbf{v}_2$, respectively. Note that, as opposed to the classical case, the uncertainty principle prevents us from knowing whether the trajectory of m passes above or below M_A.

that for p–H atom scattering it behaves as $1/v^{11}$ for asymptotically high v. Quantum and classical mechanics were thereby largely reconciled. However, the classical numerical coefficient is incorrect by an order of magnitude; this point is discussed in Sec. VII B.)

More recently, Dettmann and Leibfried (1969) and Dettmann (1971) showed that for a system of three particles interacting via a wide range of potentials the contribution from the second Born term to the forward capture cross section dominates over the contribution from any other Born term at asymptotically high velocities. However, we should stress that in the absence of a proof that the Born series is at least an asymptotic series, it does not immediately follow that the asymptotic velocity dependence of the forward capture cross section is truly determined by the second Born term. Unfortunately, almost nothing is known about the convergence properties of the Born series for three-body scattering. It is known (Aaron *et al.*, 1961; Rosenberg, 1963) that the Born expansion of the full three-body Green's function $G(E)$ in terms of the free three-body Green's function $G_0(E)$ diverges in some region of momentum space no matter how large E is. However, it does not follow from this that the Born series for the scattering amplitude diverges, since in the expression for the amplitude $G(E)$ appears inside a weighted integral over momentum space. Indeed, if the interactions are sufficiently short-ranged, $G(E)$ appears between *square-integrable* functions. This point has been emphasized by Dettmann and Leibfried (1966) and by Corbett (1968), who investigated a one-dimensional three-body problem involving delta-function potentials and showed that for this case the Born series for the amplitude *does* converge for sufficiently high E. The present authors attempted to avoid convergence questions by expanding the scattering amplitude in a Born series only up to a certain term and then bounding the remainder. So far it has proved to be possible to do this only within the impact parameter approximation where the nuclei are treated as infinitely massive, and then only for certain potentials. Within this approximation it was shown (Shakeshaft and Spruch, 1973), using variational bounds on transition amplitudes developed earlier by Spruch (1969),[6] that for a certain class of potentials the

[6]In this reference bounds and variational bounds were derived on the transition amplitudes for any system governed by a time-dependent Hamiltonian. (Note that in the impact-parameter approximation the nuclei become moving centers of force which subject the light particle to a time-dependent perturbation.) The only unknown in the exact expression for an amplitude is the time-translation operator U. This operator was eliminated by using the Schwarz inequality and the isometric property $U^\dagger U = 1$. Contrast the boundedness of the (unknown) operator U that characterizes transition processes with the singular nature of the (unknown) Green's function G that characterizes time-independent cross sections; the non-normalizable plane wave describing the relative motion of the nuclei does not appear in the impact-parameter approximation.

remainder, written as one (explicit) term rather than as an infinite series, decreases more rapidly with increasing velocity than the second Born term. Combined with the work of Dettmann and Leibfried this then proves that, at least within the impact parameter approximation, the second Born term truly does determine the asymptotic form of the forward capture cross section for the class of potentials considered.[7]

Before proceeding further, we should like to make it perfectly clear that the treatment of the double scattering process that follows is not classical; rather, we isolate certain factors which can be treated classically. Indeed, it is not possible to treat scattering by a target atom in a $1s$ state classically, and various attempts to do so lack justification. Double scattering capture from an atom initially in a *high* Rydberg state *can* be treated classically; this is done in Sec. VII. We note that the expression to be derived below, Eq. (5.12), has been derived within the quantum-mechanical second Born approximation. The derivation below has, we believe, heuristic value, but while the mathematics involved is at an extremely low level, there are many small details associated with the many uses of the uncertainty principle. Any reader who is satisfied with the mathematical derivations in the literature can simply accept Eq. (5.12) and start reading again at that point, though the reader might read subsections V.B. 1 and V.B. 2 and skim V.B.3 through V.B.6.

B. "Physical" derivation of the cross section

1. Classical aspects of the problem

We let M_B be incident with a velocity $\mathbf{v}$ and impact parameter between b and $b+db$ relative to M_A. With little loss in applicability, we assume azimuthal symmetry so that the cross section is independent of the azimuthal angle, with $\hat{v}$ defining the polar axis. If it is to be possible to treat M_B classically as well as quantum mechanically, db must be large compared to $\hbar/M_B v$; since v is to be arbitrarily large, this in no way prevents us from imposing the further condition that $db \ll b$ for all relevant b and $db \ll$ the linear dimensions of the "atoms" $(m+M_A)$ and $(m+M_B)$. Furthermore, it is *a priori* reasonable, and will be made quite clear shortly, that the change in momentum of M_B due to its collision with m will be of order mv, which is negligible compared with $M_B v$. The change in momentum of M_B due to its interaction with M_A is, for all $b \gg \hbar/M_B v$, also negligible in comparison with $M_B v$. For present purposes we can therefore take M_B to move with constant velocity $\mathbf{v}$ within the thin cylindrical shell defined by b and $b+db$.

We assume that M_A is initially localized to within a region of linear dimensions large compared to $\hbar/M_A v$, but very small compared to b and to the linear dimensions of the "atoms"; then in the lab frame the initial speed of M_A can, and will, be assumed to be negligible compared to v. Since, further, for all $b \gg \hbar/M_A v$, M_A will absorb momentum which too is only of order mv, we are free to think of M_A as remaining effectively stationary in the lab frame throughout the double scattering process.

Now there is clearly an enormous advantage to treating the nuclei as classical particles, for then the full quantum problem reduces to a one-body problem. There is, however, a disadvantage, and that is that the nuclei, when treated classically, must be treated as external sources which follow classical trajectories and subject m to a potential which is time dependent. Fortunately, in the present analysis, it is possible to extract the advantage without introducing the disadvantage. Speaking very loosely, we note that the nuclei can be treated classically *or* quantum-mechanically and we shall talk about "when" the nuclei are at such and such a position.

Even in the study of the light particle m, much of the description can be classical. Each collision will involve a momentum transfer to m of order mv—which is large for a particle of mass m—so that each collision will be a close one. Since, in addition, the wavelength of m between the two collisions will be of order $\hbar/mv$, which is very much smaller than the separation of the nuclei for almost all relevant values of b, the motion of m between collisions is essentially classical. Thus each collision is truly a binary one; interference effects between the two collisions are negligible, and we can work with probabilities rather than amplitudes.

We defer the discussion of the explicitly quantum-mechanical aspects of the motion of m until after a discussion of the kinematics of the problem. The kinematics are of course the same classically and quantum-mechanically.

2. Kinematics

Let $\mathbf{v}_1$ and $\mathbf{v}_2$, respectively, denote the velocities of m in the *lab* frame after the first and second collisions. (Throughout, the subscripts 1 and 2 denote quantities which are related to conditions immediately after the first and second collisions, respectively.) Let α_1 and α_2 denote the acute angles between $\mathbf{v}_1$ and $\mathbf{v}$ and between $\mathbf{v}_2$ and $\mathbf{v}$, respectively. We neglect the initial energy and momentum of m. It is precisely because we can here neglect the high-velocity components of m in its initial state—and also in its final state, as discussed below—that double scattering can dominate over single scattering. If we also neglect corrections of order m/M_B, it follows immediately from energy and momentum conservation that

$$v_1 = 2v\cos\alpha_1 . \tag{5.1}$$

Since $m/M_A \ll 1$, the energy transferred to m during the second collision is negligible in the lab frame. Therefore, in the lab frame, m scatters from M_A without change of speed so that $v_2 = v_1$. Combined with Eq. (5.1) and the requirement $\mathbf{v}_2 \approx \mathbf{v}$, this leads to $v_1 \approx v$ and $\alpha_1 \approx \alpha_2 \approx \pi/3$, as indicated in Fig. 3.

We must of course allow a small spread, of absolute magnitude $d\alpha_1$, in the "scattering" angle α_1. (We refer to α_1 as the "scattering" angle, although in the lab

[7]The class of potentials is as follows: $W_A(r)$ and $W_B(r)$ are local, spherically symmetric, decrease faster than $1/r^{18}$ as $r\to\infty$, are bounded for all r, and have Fourier transforms which for large k have an asymptotic expansion in $1/k$. (Unfortunately Coulomb potentials are not included.)

frame m is not scattered through any well-defined angle since it is at rest initially.) This spread gives rise to a spread, of absolute magnitude dv_1, in the speed v_1; from Eq. (5.1) we have

$$dv_1 = 2v\sin\alpha_1 d\alpha_1 . \tag{5.2}$$

It will turn out that, apart from requiring $v \gg dv_1 \gg$ the orbital speed of m about either nucleus, we shall not need to specify dv_1. Let $\mathbf{r}_A = (r_A, \theta_A, \phi_A)$ denote the coordinates of m with respect to M_A, with the polar axis defined by $\hat{v}$. Since m must undergo a very large momentum transfer in each collision, each collision will be almost head-on, and we therefore find that at the time of the first collision r_A and θ_A must have the values $r_{A1} \approx b/\sin\alpha_1 \approx 2b/\sqrt{3}$ and $\theta_{A1} \approx \pi - \alpha_1 \approx 2\pi/3$, respectively.

3. Quantum-mechanical considerations and formulation of the problem

Quantum-mechanically we know the region from which m is scattered in the first collision only to within the accuracy permitted by the uncertainty principle. This region, to be denoted by $d\tau_1$, is centered about the point specified by $\mathbf{r}_{A1} \equiv (2b/\sqrt{3}, 2\pi/3, \phi_A)$. The actual size of $d\tau_1$ is related to the quantum-mechanical uncertainty in the velocity $\mathbf{v}_1$ of m after the first collision. The uncertainty in this velocity, in any direction, can be assumed to be small compared to v but large compared to the orbital speed of m before the collision. Thus $d\tau_1$ can be assumed to be small compared to the size of the "atom" $(m+M_A)$, and the initial bound-state wave function of m will be roughly constant over the region $d\tau_1$.

In the second collision m strikes M_A and emerges into a small solid angle with a velocity $\mathbf{v}_2$ close to $\mathbf{v}$. Let $d\sigma_2$ denote the cross section for this second scattering. The target M_A *effectively* presents an area $d\sigma_2$ upon which m must impinge. Classically, one knows precisely where this area must be located. Quantum-mechanically, however, one knows the position of the area only insofar as m is localized during the collision; roughly speaking, the area $d\sigma_2$ can be anywhere on a disc whose plane is perpendicular to $\mathbf{v}_1$, whose center is at M_A, and whose radius is, for sufficiently high v, very small compared to b and to the linear dimensions of the "atoms" $(m+M_A)$ and $(m+M_B)$, but somewhat larger than $\hbar/mv$ and very much larger than the linear dimensions of $d\sigma_2$. Note that, for Rutherford scattering, the differential cross section decreases as $1/v^4$ with increasing v, and for interactions less singular than Coulomb it decreases even faster; therefore the linear dimensions of $d\sigma_2$ will be extremely small for high v. Now if we treat the motion of m as classical between collisions, m can impinge upon the area $d\sigma_2$, for a given

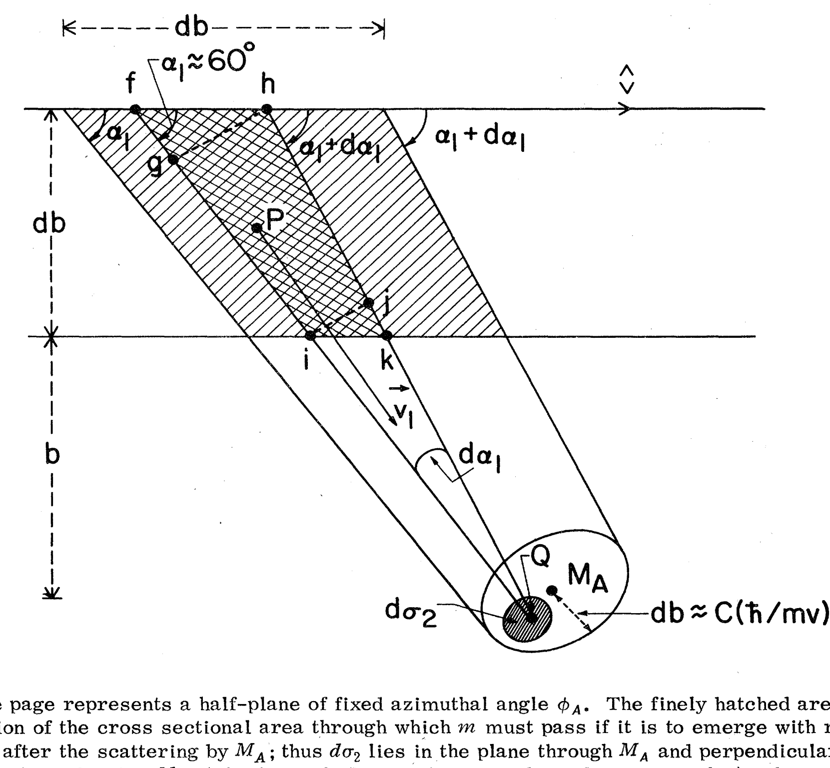

FIG. 4. The plane of the page represents a half-plane of fixed azimuthal angle ϕ_A. The finely hatched area denoted by $d\sigma_2$ represents one possible location of the cross sectional area through which m must pass if it is to emerge with reasonable probability of being captured by M_B after the scattering by M_A; thus $d\sigma_2$ lies in the plane through M_A and perpendicular to $\mathbf{v}_1$ in a circle centered on M_A and with a radius of order db. (The figure has not, of course, been drawn to scale.) The point Q is an arbitrary point on $d\sigma_2$. The hatched and crosshatched regions at the top of the figure are, respectively, the projections of $d\tau_1$ and $d\tau_1'$ onto the plane of the page. The point P within the crosshatched region is a possible initial location of m if m is to be scattered by M_B to the point Q so as finally to emerge with a velocity close to $\mathbf{v}$; m must be scattered through an angle between $\alpha_1 \approx 60°$ and $\alpha_1 + d\alpha_1$ and pass through the particular area $d\sigma_2$ under consideration. For m to pass through *any* $d\sigma_2$ which leads to a reasonable probability of capture—which is all that we can ever be sure happened if m is captured—m can initially be in the much larger volume $d\tau_1$. The dimension db is somewhat larger than $\hbar/mv$, by a velocity-independent factor C. (C might be of the order of 100, say.)

position of this area, only if m is scattered in the first collision from a certain subregion $d\tau_1'$ of the volume $d\tau_1$. This is indicated in Fig. 4 and will be discussed further in Sec. V.B. 5. Therefore the cross section for m to finally emerge after the second collision with a velocity close to $\mathbf{v}$ is $P_{1oc}d\sigma_1$ where $d\sigma_1$ is the cross section for the first scattering and where P_{1oc} is the probability that m is scattered from the "appropriate" *loc*ation in the first collision.

Even if m finally emerges with a velocity close to $\mathbf{v}$ it will be *cap*tured into a particular final state by M_B only with a certain conditional probability, to be denoted by P_{cap}. The actual *d*ouble *s*cattering cross section for m to be captured when M_B is incident with an impact parameter between b and $b+db$ is therefore

$$d\sigma_{ds} = P_{1oc}\, d\sigma_1 P_{cap}\,. \tag{5.3}$$

We now study the quantities P_{1oc}, $d\sigma_1$ and P_{cap}.

4. Analysis of $d\sigma_1$ and $d\sigma_2$, the binary differential cross sections

Let $d\Omega_1$ denote, in the c.m. frame of m and M_B (which is not the lab frame), the solid angle into which m is knocked in the first collision; let $d\Omega_2$ denote, in the c.m. frame of m and M_A (which *is*, essentially, the lab frame), the solid angle into which m is knocked in the second collision. With $W_A(r)$ and $W_B(r)$ denoting the interactions between m and M_A and between m and M_B, respectively, let $\tilde{W}_A(p)$ and $\tilde{W}_B(p)$ be the associated Fourier transforms, defined by Eq. (2.1). The momenta transferred to m during the first and second collisions are $m\mathbf{v}_1$ and $m(\mathbf{v}_2-\mathbf{v}_1)$, respectively. We note that $|m\mathbf{v}_1| \approx mv$ and $|m(\mathbf{v}_2-\mathbf{v}_1)| \approx mv$, and that the cross sections $d\sigma_1$ and $d\sigma_2$ are adequately described by the first Born approximation (since for *potential* scattering the first Born approximation becomes increasingly accurate as the energy increases for the class of potentials we allow.) We can now write

$$d\sigma_1 = (2m^2\pi/\hbar)\,|\tilde{W}_B(mv)|^2 d\Omega_1\,, \tag{5.4}$$

and

$$d\sigma_2 = (2m^2\pi/\hbar)\,|\tilde{W}_A(mv)|^2 d\Omega_2\,. \tag{5.5}$$

Let $d\Omega_1(\text{lab})$ denote the solid angle corresponding to $d\Omega_1$ in the lab frame, that is, in the frame in which M_A is at rest. It is not difficult to see that $d\Omega_1 \approx 4\cos\alpha_1 d\Omega_1(\text{lab}) \approx 2d\Omega_1(\text{lab})$. Now, in order for m to scatter into $d\Omega_2$ in the second collision, m must impinge upon the area $d\sigma_2$. Since the linear dimensions of the area $d\sigma_2$ are much smaller than the distance r_{A1} of m from M_A at the time of the first collision, we see from Fig. 5 that $d\Omega_1(\text{lab}) \approx d\sigma_2/r_{A1}^2$. From $r_{A1}^2 \approx 4b^2/3$ and $d\Omega_1 \approx 2d\Omega_1(\text{lab})$ we obtain

$$d\Omega_1 \approx (3/2b^2)d\sigma_2\,. \tag{5.6}$$

The only unknown in $d\sigma_1$ is therefore the solid angle $d\Omega_2$. We need never determine $d\Omega_2$; it will be eliminated below by using the uncertainty principle.

5. Analysis of P_{loc}, the appropriate location probability

The "scattering" angle of the first collision lies between $\alpha_1 \approx \pi/3$ and $\alpha_1 + d\alpha_1$. Referring to Fig. 4, the first scattering must, in the half-plane defined by any fixed azimuthal angle ϕ_A, take place somewhere within the intersection of the pair of lines diverging from any point Q on $d\sigma_2$, at angles α_1 and $\alpha_1 + d\alpha_1$, and the pair of lines defined by b and $b+db$. Since the distance of the point Q from M_A is very much less than b, the area of intersection (that is, the area of the crosshatched region *ifhk* in Fig. 4) will be roughly the same for all of the allowed points Q, and in estimating the area of intersection we can, with negligible error, take the point Q to coincide with M_A. Furthermore, neglecting only corrections of order $1/v$, we can approximate the area of the region *ifhk* by the area of the region *ighj*. We conclude that the area of intersection is approxi-

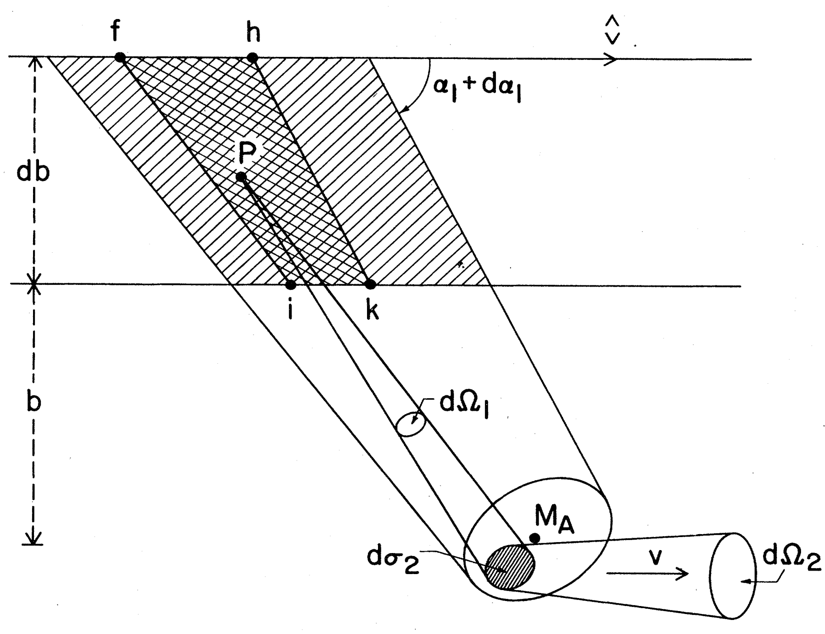

FIG. 5. m is initially at the point P within the crosshatched region defined by *ifhk*. It is scattered by M_B, with a cross section $d\sigma_1$, into the solid angle $d\Omega_1$, centered about a "scattering angle" of $\frac{1}{3}\pi$. m is then scattered by M_A, with a cross section $d\sigma_2$, into the solid angle $d\Omega_2$ centered about an axis which is parallel to $\mathbf{v}$ and which passes very close to M_A.

mately

$$\left(\frac{b}{\sin\alpha_1}\right)d\alpha_1 \times \left(\frac{db}{\sin\alpha_1}\right) \approx \frac{4bdbdv_1}{(3\sqrt{3}v)},$$

where in the right-hand side of this equation we have set $\alpha_1 \approx \pi/3$ and used Eq. (5.2) to replace $d\alpha_1$ by $dv_1/\sqrt{3}v$. It follows that, for a fixed position of $d\sigma_2$, m must be scattered in the first collision from within a volume

$$d\tau_1' \approx bd\phi_A \times 4bdbdv_1/(3\sqrt{3}v). \tag{5.7}$$

The probability that m is initially within the volume $d\tau_1$ defined earlier is $|\psi_i(\mathbf{r}_{A1})|^2 d\tau_1$, where as noted above, $\mathbf{r}_{A1} = (2b/\sqrt{3}, 2\pi/3, \phi_A)$, where ψ_i is the initial wave function of m, and where we have used the fact that ψ_i is roughly constant over the region $d\tau_1$. The probability that if m is within the region $d\tau_1$ it is actually within the subregion $d\tau_1'$ is $d\tau_1'/d\tau_1$. Therefore, if M_B is incident with an impact parameter between b and $b+db$, the probability that m is initially in the appropriate location to be scattered in the first collision in such a fashion as to emerge from the second collision with a velocity close to $\mathbf{v}$ is

$$P_{1oc} = |\psi_i(\mathbf{r}_{A1})|^2 d\tau_1 \left(\frac{d\tau_1'}{d\tau_1}\right) = |\psi_i(\mathbf{r}_{A1})|^2 \frac{8\pi b^2 dbdv_1}{3\sqrt{3}v}, \tag{5.8}$$

where we have used Eq. (5.7) and we have integrated over all azimuthal angles assuming that m has a well-defined component of angular momentum along $\hat{v}$ in the initial state i so that $|\psi_i(\mathbf{r}_A)|^2$ is independent of ϕ_A.

Our use of two different volumes, $d\tau_1$ and $d\tau_1'$, to describe the initial location of m is essential for a quantum-theoretical justification of the calculation, and we shall comment further on these two volumes in Appendix B.

6. Analysis of P_{cap}, the conditional probability of capture

Let $\mathbf{r}_B = (r_B, \theta_B, \phi_B)$ be the spherical coordinates of m with respect to M_B, with the polar axis defined by $\hat{v}$, and let $\Psi_2(\mathbf{r}_B)$ be the (normalized) wave function that describes m immediately after the second collision. (The reduction in the intensity of the twice-scattered beam with respect to the incident beam is accounted for by other factors, including $d\sigma_1$ and $d\Omega_2$.) The probability that m will be captured into the final state f, characterized by the normalized wave function $\psi_f(\mathbf{r}_B)$, from the state characterized by the wave function $\Psi_2(\mathbf{r}_B)$, is defined as P_{cap}. We have

$$P_{cap} = \left| \int \psi_f^*(\mathbf{r}_B)\Psi_2(\mathbf{r}_B)d^3r_B \right|^2. \tag{5.9}$$

Since m and M_B travel at roughly the same speed v, and therefore cover roughly the same distance during the interval between the first and second collisions, and since $\alpha_1 \approx \pi/3$, the significant values of the coordinates r_B and θ_B at the time of the second collision are, respectively, $r_{B2} \equiv 2b/\sqrt{3}$ and $\theta_{B2} \equiv 2\pi/3$. Denoting the region in which $\Psi_2(\mathbf{r}_B)$ is non-negligible by $d\tau_2$, we therefore have

$$P_{cap} \approx |\psi_f(\mathbf{r}_{B2})|^2 \left| \int \Psi_2(\mathbf{r}_B)d^3r_B \right|^2, \qquad \le |\psi_f(\mathbf{r}_{B2})|^2 d\tau_2, \tag{5.10}$$

where $\mathbf{r}_{B2} \equiv (r_{B2}, \theta_{B2}, \phi_B)$. In the first step we recognized that the linear dimensions of the volume $d\tau_2$ of the wave packet that emerges after the second collision are sufficiently small compared to the linear dimensions of the "atom" $(m + M_B)$ that ψ_f can be treated as a constant over the volume $d\tau_2$ and can therefore be taken outside the integral; we also assumed that in the final state m has a well-defined component of angular momentum along $\hat{v}$ so that $|\psi_f|^2$ is independent of the azimuthal angle ϕ_B. The second step follows from the Schwarz inequality. This inequality will be a rough equality if Ψ_2 is nodeless, a property Ψ_2 will possess if, as we assume, Ψ_2 represents a nearly *minimum* wave packet.[8]

7. The final result

Combining Eqs. (5.3)–(5.6), (5.8), and (5.10), we obtain

$$d\sigma_{ds}/db \approx (16\pi^3 m^4/\sqrt{3}v\hbar^2) \times |\tilde{W}_A(mv)\tilde{W}_B(mv)\psi_i(\mathbf{r}_{A1})\psi_f(\mathbf{r}_{B2})|^2 \times dv_1 d\Omega_2 d\tau_2. \tag{5.11}$$

We now evaluate the factor $dv_1 d\Omega_2 d\tau_2$. We can assume that the uncertainty in the speed of m after the first collision is essentially dv_1. Since m scatters without change of speed from M_A, the uncertainty dv_2 in the speed of m after the second collision must be equal to dv_1. Noting that $v_2 \approx v$ we therefore have $dv_1\, d\Omega_2 = dv_2\, d\Omega_2 \approx d^3v_2/v^2$. Now from the uncertainty principle we know that $d^3v_2\, d\tau_2 \approx (h/m)^3$; we shall comment in a moment on the use of $h(=2\pi\hbar)$ rather than $\hbar$, and on the replacement of an inequality by an equality. It follows that $dv_1\, d\Omega_2\, d\tau_2 \approx h^3/m^3v^2$. Using this result in Eq. (5.11) we obtain the essential result

$$d\sigma_{ds}/db \sim (2^7\pi^6 m\hbar/\sqrt{3}v^3) \times |\tilde{W}_A(mv)\tilde{W}_B(mv)\psi_i(\mathbf{r}^*)\,\psi_f(\mathbf{r}^*)|^2 \tag{5.12}$$

where

$$\mathbf{r}^* = (2b/\sqrt{3}, 2\pi/3, \phi).$$

It follows that

$$\sigma_{ds} \sim (2^6\pi^6 m\hbar/v^3)\,|\tilde{W}_A(mv)\,\tilde{W}_B(mv)|^2 \times \int_0^\infty dr\,|\psi_i(r, 2\pi/3, \phi)\psi_f(r, 2\pi/3, \phi)|^2. \tag{5.13}$$

For the atomic case we have, using Eq. (2.2),

[8]A minimum (Gaussian) wave packet has the property that the product of the uncertainty in position and uncertainty in momentum is a minimum. If the description of m presented here is to be at all meaningful, we must assume that after the first collision m is described by an almost minimum wave packet. Therefore $\Psi_2(\mathbf{r}_B)$ is assumed to be a product of exp $[im(\mathbf{v}_2 - \mathbf{v})\cdot\mathbf{r}_B/\hbar]$ and three Gaussian or Gaussian-like functions. The wavelength of oscillation of the exponential function is roughly equal to the width of the Gaussian functions, and therefore the presence of the exponential function does not invalidate the argument. If one were able to determine exactly the leading term in powers of $1/v$ of $\int \Psi_2(\mathbf{r}_B)d^3r_B$, the final result, Eq. (5.12), would contain all of the relevant "physics" *and* the numerical coefficient would be precisely determined.

$$\sigma_{ds}(nl\mu \to n'l'\mu') \sim (2^8\pi^4 Z_A^2 Z_B^2 \hbar^3 e^8/m^7 v^{11}) \times |Y_{l\mu}(2\pi/3,\phi)Y_{l'\mu'}(2\pi/3,\phi)|^2 \times \int_0^\infty dr R_{nl}^2(r) R_{n'l'}^2(r) . \quad (5.14)$$

Averages over μ and/or sums over μ' follow immediately. For example, we have, averaging over μ and summing over μ'

$$\sigma_{ds}(nl \to n'l') \sim (2^4\pi^2 Z_A^2 Z_B^2 \hbar^3 e^8/m^7 v^{11}) \times (2l'+1) \int_0^\infty dr R_{nl}^2(r) R_{n'l'}^2(r) . \quad (5.15)$$

Note that apart from the requirement $m/M_A \ll 1$ and $m/M_B \ll 1$, these results are independent of the masses M_A and M_B. Note also that the entire range of impact parameters, from zero to the order of the smaller of the characteristic radii of the two "atoms" $(m+M_A)$ and $(m+M_B)$, contributes to the cross section.

It might be noted that once one has deduced the absolute-magnitude factor in Eq. (5.11), and recognized that the coefficient of this term can be a function of m, h, and v only, it is no longer necessary to use the uncertainty principle to obtain the form of the coefficient and thereby of $d\sigma_{ds}/db$; it follows from dimensional analysis. This is not to the point, however, for the deduction of the absolute-magnitude factor requires the uncertainty principle for its proper justification.

C. Discussion

The result (5.12) is identical to the asymptotic form of the differential cross section with respect to impact parameter obtained in the impact-parameter representation of the quantum-mechanical second Born approximation (Shakeshaft, 1974a; see also Appendix C). We expected, of course, that the foregoing analysis would yield the correct dependence of the asymptotic form of $d\sigma_{ds}/db$ on its various parameters, but we should not have expected to obtain the correct numerical coefficient. That we did was due to our "foresightedness" in arbitrarily setting $d^3v_2 d\tau_2$ equal to $(h/m)^3$. The uncertainty principle tells us only that $d^3v_2 d\tau_2 \geq (\hbar/2m)^3$ and we might, for example, have set $d^3v_2 d\tau_2$ equal to $(\hbar/m)^3$. It is satisfying that we obtained the correct numerical coefficient using a value of $d^3v_2 d\tau_2$ above the minimum value, but it scarcely proves anything, especially since we used an *upper* limit in arriving at Eq. (5.10).

In the foregoing analysis we borrowed the basic picture from the ingenious analysis of Thomas (1927). Our analysis differs from that of Thomas in that an attempt has been made to build in all of the essential elements of a proper quantum-mechanical calculation. In addition to any conceptual insights gained by the present derivation, our results are an improvement over those of Thomas in the following three computational respects: (i) Thomas assumed that m can initially be found only on the surface of a sphere whose radius is equal to the characteristic radius a, say, of $(m+M_A)$; his only use of quantum theory was in the input value of a. (This point, which has been the source of some confusion in the literature, will be elaborated on in Sec. VII.B.) We assume that m can initially be found in any region of space with a probability determined by the initial wave function ψ_i of $(m+M_A)$. (ii) Thomas calculated the differential cross sections for the first and second scatterings from classical mechanics, whereas we use quantum mechanics. His analysis is thereby limited to the case of Rutherford scattering, for which the classical cross section is correct. (iii) Thomas did not account for any quantum-mechanical uncertainty in the speed of m. In his analysis the spread dv_1 in the speed v_1 after the first collision was set equal to the spread dv_2 in the speed v_2 after the second collision, and the factor $dv_1 d\Omega_2$ was eliminated by supposing that the vector $\mathbf{v}_2$ should lie within a sphere of radius u (centered at $\mathbf{v}$, in velocity space), where u is the escape velocity of m in the field of M_B. Thus Thomas supposed that $d^3v_2 \approx (4\pi/3)u^3$, with u determined from the equation

$$\tfrac{1}{2}mu^2 + W_B(a) = 0 .$$

Therefore Thomas could determine only the sum of cross sections for capture into individual states; we determine the cross section for capture into any particular final state f characterized by ψ_f, and we eliminate the factor $dv_1 d\Omega_2$ by using the uncertainty principle. (However, $\sigma_{ds}(1s \to n')$ can be calculated for a particular n' along the lines of Thomas' original approach. See Sec. VII.B, where it is done for capture via double scattering from a high Rydberg state in a way which could be applied, though again not quite legitimately for an initial state a $1s$ state, to capture via double scattering from the $1s$ state.)

• In discussing the quantum-mechanical aspects of the problem, in Sec. V.B.3, we did not consider the effect that the principle of indistinguishability might have in the case that the nuclei are identical. We now pause to consider this point. We assume that the nuclei are identical and examine whether forward capture can be distinguished from direct scattering where capture does not occur, but where M_B gives up most of its kinetic energy in the lab frame to $(m+M_A)$, knocking this "atom" forward with a velocity roughly equal to $\mathbf{v}$, and exciting it to the final state of interest; this direct process differs from the knock-on process discussed above in that m is not captured by M_B but remains attached to M_A. Note first that since the nuclei are highly localized their wave packets will not overlap appreciably, and they are effectively distinguishable, for all impact parameters $b \gg \hbar/Mv$, where $M \equiv M_A = M_B$. Now the range of impact parameters $b \lesssim \hbar/Mv$ contributes negligibly to the double scattering cross section, as can be seen from Eq. (5.12); on the other hand, it is this range of impact parameters which provides the major contribution to the direct scattering cross section, since in the direct process under consideration the two nuclei must collide almost head-on to exchange momentum of order $M\mathbf{v}$. Therefore capture via double scattering can, for practical purposes, be distinguished from direct scattering. Forward capture via single scattering (described by the Brinkman–Kramers approximation) can for practical purposes also be distinguished from direct scattering, but only because of the small ratio m/M since, as discussed in Appendix D, forward capture via single scattering occurs for impact parameters $b \lesssim \hbar/mv$. [To estimate the cross section for the indistinguishable direct scattering process, note that the characteristic exchange of momentum in forward capture, whether it is via single or double scattering, is of order of magnitude mv. Therefore in forward capture the stripped nucleus M_A should not have a final momentum greatly exceeding mv in the lab frame. This means that direct scattering will be indistinguishable from forward capture only if, in direct scattering, the incident nucleus M_B has a final momentum of order mv in the lab frame, in which case $(m+M_A)$ must be knocked into a solid angle of order $(m/M)^2$ with a velocity roughly equal to v. The cross section for this latter event can be calculated in a fashion very similar to that used to derive the knock-on capture cross section in Sec. III. For pure Coulomb interactions the cross section for indistinguishable direct scattering behaves with increasing v as $1/v^{12+2l'}$, the coefficient being proportional to $(m/M)^4$; here l' is the orbital angular momentum quantum number of the final state—we assume that the initial state is the ground state. This cross section is negligible.]

It is interesting to note that although the discussions of P_{loc} and P_{cap} proceeded along quite different lines, the explicit form of the final expression for $d\sigma_{\text{ds}}/db$, given by Eq. (5.12), is symmetric in the sense that it is invariant under the interchange of the subscripts i and f. This symmetry has its origins in the kinematics rather than in the dynamics, and it does not represent detailed balance; indeed detailed balance follows merely from the requirement that the interactions be invariant under time reversal. The symmetry of the kinematics is perhaps most evident in the frame in which the heavy nuclei have equal and opposite velocities. In this frame M_B is incident with a velocity $\mathbf{v}/2$ and, as drawn in the figures, impact parameter b "above" M_A; m is initially above M_A by a distance b, and ahead of M_A by a distance $b/\sqrt{3}$ and m and M_A are initially traveling with a velocity $-\frac{1}{2}\mathbf{v}$. After the first collision m travels *straight down* (its velocity is perpendicular to v) with a speed $(\sqrt{3}/2)v$, while M_A continues to move with a velocity $-\mathbf{v}/2$. Then m strikes M_A and is captured by M_B at a distance b below M_B and behind M_B by a distance $b/3$. We should like to thank Professors U. Fano and B. Lippmann for a useful remark on symmetry.

The present analysis of the double scattering mechanism can be extended in a number of directions. We briefly mention two. The first extension is to arbitrary masses. [The classical analysis of Thomas was extended to arbitrary masses by Bates *et al.* (1964)]. One can consider, for example, electron capture from hydrogen atoms by positrons. For this example, energy and momentum conservation, and the condition that the electron and positron finally have the same velocity, require that the positron be deflected in the first collision through an angle of 45° in the lab frame; the electron is knocked towards the target proton in a direction making an angle of 45° relative to the incident direction $\hat{v}$, and it then scatters from the target proton through an angle of 90°. One could also consider the capture of an atom from a diatomic molecule. The second extension is to ions or atoms with more than one electron. When the target "atom" has more than one electron there is the possibility that the electron to be captured scatters in the second collision from a second target electron rather than from the target nucleus; the second electron is then ejected. This case does not seem to have been analyzed. One can also consider molecular targets. Forward capture from the hydrogen molecule has been studied within the first Born approximation (Tuan and Gerjuoy, 1960) but not within the second Born approximation, nor at asymptotically high velocities.

The double scattering mechanism seems to be the dominant mechanism (within the nonrelativistic framework) for radiationless capture into the forward direction. It is therefore highly plausible that the second Born term gives the correct nonrelativistic asymptotic form for the radiationless forward capture cross section, whether or not the Born series converges. However, a variety of other asymptotic forms for the forward capture cross section have been suggested; some of these are presented and briefly discussed in Appendix D. We conclude this section with two remarks. First, although it should be possible to detect double scattering experimentally, as discussed in Secs. VI.C and VII.B, the significance of the double scattering mechanism perhaps lies more in what it teaches us about the high-energy behavior of nonrelativistic many-body Green's functions and scattering amplitudes—for example, the fact that the second Born term can dominate over the first Born term[9]—

[9]This is not the only example in which the second Born term can dominate over the first Born term. Another example is the *excitation* of an "atom" (m_1+m_2) with m_1 *infinitely massive*, by a fast-moving particle m_3 in the limit of high-momentum transfer to m_3. This can be understood as follows. Since m_1 is infinitely massive it does not recoil, and since m_2 must remain bound to m_1 the momentum transferred to or from m_2 must be relatively small. Therefore the large momentum transferred to m_3 must come from the scattering of m_3 from m_1. But the interaction between m_3 and m_1 does not contribute to the excitation cross section in the first Born approximation owing to the orthogonality of the initial and final wave functions; as a consequence the second Born term dominates. This result was first discussed in detail by Potapov (1972) and has been extended to the case where all three masses are arbitrary by Shakeshaft (1977). Note that the total excitation cross section, integrated over all values of the momentum transfer, is given correctly by the first Born approximation in the limit of high impact velocity. (If the other conditions are retained, the present example can be extended to include ionization or breakup, provided the momentum with which m_2 emerges is small.) Another example of a case in which the second Born term dominates over the first, under certain circumstances, is the high-velocity limit of the exchange process $m_3+(m_1+m_2) \to m_2+(m_1+m_3)$, where m_2 and m_3 are identical, and m_1 is infinitely massive (e.g., Potapov, 1972; Bonham, 1972; Joachain, 1977; Shakeshaft, 1978a). Again, the total cross section, obtained by integrating over all values of the momentum transfer, is given correctly by the first Born approximation at high impact velocities. In contrast, in the capture problem it is not only the differential cross section that is governed by the second Born term, at certain values of the scattering angle (or, equivalently, momentum transfer), but also the *total* cross section (disregarding kock-on, which only occurs when $M_A=M_B$).

than in the particular application. Second, it is conceivable that in some circumstances double scattering becomes the dominant radiationless mechanism for forward capture only at relativistic velocities; if that is the case, our nonrelativistic description of double scattering can be characterized, to quote Georges Temmer on hearing our description, as "anschaulich but nonphysical."

VI. RELATIVE IMPORTANCE OF THE DIFFERENT MECHANISMS FOR CAPTURE FROM THE GROUND STATE

In this section we examine the relative importance of the different capture mechanisms discussed in the previous sections. We consider only the case when m is an electron whose interactions with the nuclei are pure Coulombic, this case being of great interest in atomic physics. We restrict the initial state to be the 1s (ground) state, but the final state can be the 1s or 2p (or, for σ_{BK} or σ_{ds}, the n', $l'=n'-1$) state; for the particular case $Z_A=2Z_B=1$ we also give the sum over *all* final bound states. In addition, we discuss "capture to the continuum." We begin by giving the asymptotic form of the cross section for each mechanism. In Eqs. (6.1)–(6.4) below, the cross section for capture to the 2p state is summed over all magnetic substates, but in Eqs. (6.5)–(6.7) we give the contributions from the individual magnetic substates. In this section m is the electron mass and $a_0=\hbar^2/me^2$ denotes the Bohr radius of the hydrogen atom.

A. Asymptotic forms of the cross section

1. Knock-on capture

For this mechanism we assume that $M\equiv M_A=M_B$. It follows from Eq. (3.10) that the total cross section for knock-on capture into the particular states under consideration is given by

$$\frac{\sigma_{ko}(1s\to 1s)}{\pi a_0^2}\sim\frac{2^8Z_A^5Z_B^5}{3(Z_A+Z_B)^4}\left(\frac{m}{M}\right)^2\left(\frac{e^2}{\hbar v}\right)^6, \tag{6.1a}$$

$$\frac{\sigma_{ko}(1s\to 2p)}{\pi a_0^2}\sim\frac{2^{11}Z_A^5Z_B^7}{5(2Z_A+Z_B)^6}\left(\frac{m}{M}\right)^2\left(\frac{e^2}{\hbar v}\right)^6. \tag{6.1b}$$

The results of Eq. (6.1) were obtained by integrating over all scattering angles in the c.m. frame, but only c.m. angles between π and $\pi-\theta_{max}$ are significant, where $\theta_{max}=2Z_{max}(e^2/\hbar v)$ and where Z_{max} is the larger of Z_A and Z_B. For $Z_A=Z_B=1$ the cross section summed over all final bound states is

$$\frac{\sigma_{ko}(1s\to bd)}{\pi a_0^2}\sim 6.86\left(\frac{m}{M}\right)^2\left(\frac{e^2}{\hbar v}\right)^6; \tag{6.1c}$$

capture to the 1s state represents about 78% of this cross section.

2. Radiative capture

From Eq. (4.3) we have, for the total cross section for radiative capture into the states under consideration,

$$\frac{\sigma_{rc}(1s\to 1s)}{\pi a_0^2}\sim\frac{2^7}{3}Z_B^5\left(\frac{e^2}{\hbar c}\right)^3\left(\frac{e^2}{\hbar v}\right)^5, \tag{6.2a}$$

$$\frac{\sigma_{rc}(1s\to 2p)}{\pi a_0^2}\sim\left[\frac{3}{4}\right]\frac{2^4}{3}Z_B^7\left(\frac{e^2}{\hbar c}\right)^3\left(\frac{e^2}{\hbar v}\right)^7. \tag{6.2b}$$

Note that the 1$s\to$1s and 1$s\to$2p cross sections have different velocity dependences. They are also independent of Z_A, which is consistent with the assumption that the target nucleus plays no role. Equation (4.3) would give Eq. (6.2b) without the factor of 3/4, which has been placed in square brackets. Equation (6.2b) is correct as it stands, with the factor 3/4, which accounts for the contribution which arises from the scattering of the incident electron by the projectile before capture of the electrom by the projectile. The results of Eq. (6.2) were obtained by summing over all polarizations and integrating over all directions of emission of the photon; it is unnecessary to explicitly integrate over the scattering angle of M_B. Note that the emission of photons is not sharply peaked in any direction; in fact, in the dipole approximation the photons have a $\sin^2\gamma$ distribution, where γ is the angle of emission of the photon relative to $\hat{v}$. On the other hand, the scattering of M_B is very sharply peaked in the forward direction; indeed, the scattering angle is zero if the photon momentum is neglected and if m is treated as initially free and at rest in the lab frame. To obtain a nonzero scattering angle we must take into account the momentum of the photon and/or the initial momentum distribution of m. Neglecting the Doppler shift, the momentum of the photon in the lab frame is of magnitude $\hbar\omega/c\approx mv^2/2c$. The magnitude of the average initial momentum of m is $mZ_Ae^2/\hbar$. Therefore the maximum momentum which can be imparted to M_B is roughly of magnitude $mv^2/2c+mZ_Ae^2/\hbar$. The scattering of M_B will be greatest when this momentum is imparted in the direction transverse to $\hat{v}$, in which case the scattering angle is roughly $(m/M_B)[(v/2c)+(Z_Ae^2/\hbar v)]$, which is a very small angle.

For radiative capture the cross section can be summed over all final bound states in closed form, using a sum rule derived by May (1964). We obtain

$$\sigma_{rc}(1s\to bd)\sim 1.202\sigma_{rc}(1s\to 1s), \tag{6.2c}$$

with Z_A and Z_B arbitrary; therefore capture to the 1s state represents about 83% of the cross section for radiative capture to all bound states for the large velocities under consideration.

3. Double scattering

In this mechanism M_B is again essentially undeflected and only small scattering angles—of order m/M_B—are important. The differential cross section actually peaks at a nonzero, albeit small, scattering angle. This angle, known as the critical angle (Dettmann and Leibfried, 1969), is the angle through which the incident nucleus must scatter in the first collision in order to knock m towards the target nucleus with speed v in a direction making an angle of $\pi/3$ radians with $\hat{v}$. Since the transverse momentum imparted to M_B is about $mv\sin(\pi/3)$, the critical angle is about $(m/M_B)\sin(\pi/3)$, which for electron capture by protons is about 1.6′. For all inelastic processes the differential cross section integrated over angle is the same, to order m/M_A or m/M_B, as the differential cross section integrated over impact parameter (Wilets and Wallace, 1968). Performing the integration of Eq. (5.15) we have, for the total cross section for double scattering,

$$\frac{\sigma_{ds}(1s \to 1s)}{\pi a_0^2} \sim 2^7 \pi \frac{Z_A^5 Z_B^5}{(Z_A + Z_B)} \left(\frac{e^2}{\hbar v}\right)^{11}, \tag{6.3a}$$

$$\frac{\sigma_{ds}(1s \to 2p)}{\pi a_0^2} \sim 2^4 \pi \frac{Z_A^5 Z_B^7}{(2Z_A + Z_B)^3} \left(\frac{e^2}{\hbar v}\right)^{11}. \tag{6.3b}$$

For large n' and for $Z_A = Z_B = 1$, Shakeshaft (1974b) showed that $\sigma_{ds}(1s \to n') \sim (210/n'^3)(e^2/\hbar v)^{11} \pi a_0^2$. Thus to evaluate the cross section summed over all bound states, $\sigma_{ds}(1s \to bd)$, we use Eq. (5.15) for small n' and we use the preceding result for large n'. We obtain, for $Z_A = Z_B = 1$,

$$\sigma_{ds}(1s \to bd)/\pi a_0^2 \sim 243(e^2/\hbar v)^{11}; \tag{6.3c}$$

capture to the 1s state represents about 83% of this cross section.

A result (Shakeshaft and Spruch, 1978b) which includes Eqs. (6.3a) and (6.3b) is

$$\frac{\sigma_{ds}(1s \to n',\ l' = n' - 1)}{\pi a_0^2} \sim \frac{2^7 \pi Z_A^5 Z_B^{2n'+3}}{n'^3 (n' Z_A + Z_B)^{2n'-1}} \left(\frac{e^2}{\hbar v}\right)^{11}.$$

4. Brinkman-Kramers approximation

For the purpose of comparison we give the asymptotic form of the total cross section obtained in the Brinkman–Kramers approximation. Again only small scattering angles, of the order of m/M_B, are important. [For example, for $1s \to 1s$ capture half of the contribution to the total cross section comes from scattering angles less than 0.074 (m/M_B) radians in the lab frame.] We have, to order m/M_A and m/M_B,

$$\frac{\sigma_{BK}(1s \to 1s)}{\pi a_0^2} \sim \left(\frac{2^{18}}{5}\right) Z_A^5 Z_B^5 \left(\frac{e^2}{\hbar v}\right)^{12}, \tag{6.4a}$$

$$\frac{\sigma_{BK}(1s \to 2p)}{\pi a_0^2} \sim \left(\frac{2^{16}}{3}\right) Z_A^5 Z_B^7 \left(\frac{e^2}{\hbar v}\right)^{14}. \tag{6.4b}$$

Equations (6.4a) and (6.4b) are encompassed in the more general result

$$\frac{\sigma_{BK}(1s \to n',\ l' = n' - 1)}{\pi a_0^2} \sim \frac{2^{6n'+13} (n'!)^2 Z_A^5}{n'(2n'+8)(2n'-2)!} \times \left(\frac{Z_B}{n'}\right)^{2n'+3} \left(\frac{e^2}{\hbar v}\right)^{2n'+10}.$$

The Brinkman–Kramers approximation does not give the correct coefficient of either the $1/v^{12}$ term (for $1s \to 1s$ capture) or the $1/v^{14}$ term (for $1s \to 2p$ capture) in the asymptotic expansion of the forward capture cross section developed from the Born series; contributions from the second- and third-order Born amplitudes significantly modify these coefficients. For example, in the case of $1s \to 1s$ capture the contribution from the first three Born terms is, through order $(e^2/\hbar v)^{12}$ and neglecting corrections of order m/M_A and m/M_B (Shakeshaft, 1978b),

$$\sigma \sim [0.319 + 5\pi 2^{-11} \hbar v/(Z_A + Z_B) e^2] \sigma_{BK}.$$

This formula, and the asymptotic formulae given in Eqs. (6.1)–(6.4) above are valid only when v is much greater than the initial and final orbital velocities of the electron, and when $v^2/c^2 \ll 1$.

Recently Briggs and Dubé (1978) evaluated the asymptotic contribution of the sum of the first and second order Born amplitudes to the cross section for $1s \to n'l'\mu'$ capture with n', l', and μ' arbitrary. The leading term in the asymptotic expansion of the cross section is, of course, a $1/v^{11}$ term; the next term in the expansion behaves as $1/v^{12}$ if $l' = 0$ or $1/v^{13}$ if $l' > 0$, with third and higher order Born amplitudes neglected. (The $1/v^{13}$ contribution comes solely from the second Born term.) It can be shown that the interference of the second and third order Born amplitudes gives a $1/v^{12}$ contribution for all l', but the velocity independent coefficient is numerically very small.[10]

5. Capture into states of given orbital angular momentum projection

Each cross section given above for capture into the $2p$ state is a sum of contributions from states with projections of the angular momentum $\mu' = \pm 1$ and 0. It can be of interest to know the individual contributions; this will be the case if, for example, we wish to know the polarization(s) of the photon(s) that can be emitted after capture into an excited state. We shall now consider the individual contributions for each of the three mechanisms.

In the knock-on process, it follows directly from Eqs. (3.9) and (3.10), on expanding the exponential, that

$$\sigma_{ko}(1s \to n'l'\mu') \propto |Y_{l'\mu'}(\hat{u}_\perp)|^2 = |Y_{l'\mu'}(\tfrac{1}{2}\pi, \phi)|^2.$$

[Therefore $\sigma_{ko}(1s \to n'l'\mu')$ is zero if $l' - \mu'$ is odd.] This equation can be given a physical basis as follows. The linear momentum transferred to m in the knock-on process is $m\mathbf{V}(\theta)$, where $\mathbf{V}(\theta)$, defined by Eq. (3.4), is roughly $(v\theta/2)\hat{u}_\perp$. The angular momentum transferred to m therefore has zero projection in the direction of $\hat{u}_\perp$, and so, since the initial state is isotropic, the projection of the final angular momentum on an axis parallel to $\hat{u}_\perp$ is zero. Since the final state has angular momentum quantum numbers l' and o with respect to $\hat{u}_\perp$ as polar axis, the final bound-state wave function has an angular dependence which is proportional to $P_{l'}[\cos(\frac{1}{2}\pi - \theta)]$. Expanding this in terms of the $Y_{l'\mu'}(\theta, \phi)$ using the addition theorem,

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[10]The $1/v^{12}$ contribution from the interference of the second and third order Born amplitudes represents the second order Born correction to the cross section for one of the two two-body collisions in the double-scattering process. Each two-body collision may occur off the energy shell owing to the presence of the third particle, but corrections from far off the energy shell are insignificant. The entire range of impact parameters $b \lesssim a_0$ contributes. In contrast, the $1/v^{12}$ (or $1/v^{13}$) contribution from the square of the second order Born amplitude alone represents corrections from far off the energy shell. When each two-body collision occurs far off the energy shell, the momentum transfer to the electron is not restricted by the constraint of energy conservation. However, each two-body collision can occur far off the energy shell only if the third particle is very close by, which requires b to be very small; indeed, only the range $b \lesssim \hbar/mv$ contributes.

one finds that the coefficients in the expansion are proportional to $Y_{l'\mu'}(\frac{1}{2}\pi, \phi)$, in agreement with the above equation. For the $2p$ case of interest, and indeed for any p state, we have

$$\sigma_{ko}(1s \to n'po) = 0 , \tag{6.5}$$

and

$$\sigma_{ko}(1s \to n'p \pm 1) = \tfrac{1}{2}\sigma_{ko}(1s \to n'p) . \tag{6.6}$$

In the radiative capture process, it would follow from Eq. (4.3) that, for a fixed l',

$$\sigma_{rc}(1s \to n'l'\mu') \propto |Y_{l'\mu'}(0, \phi)|^2 \tag{6.6}$$

so that the entire contribution comes from the $\mu' = 0$ state. However, Eq. (4.3) and therefore the above equation are incorrect for $l' \geq 1$. When the correction to the incident plane wave of the electron is included, one finds, for example, that the entire contribution for $l' = 1$ comes from the $\mu' = 0$ state, *but* with $\hat{\lambda}$ rather than $\hat{v}$ chosen as the quantization axis (Bethe and Salpeter, 1957).

Turning now to the double scattering process, it follows directly from Eq. (5.14) that

$$\sigma_{ds}(1s \to n'l'\mu') \propto |Y_{l'\mu'}(2\pi/3, \phi)|^2 ;$$

we immediately obtain

$$\sigma_{ds}(1s \to n'p \pm 1) = (3/4)\sigma_{ds}(1s \to n'po) = (3/10)\sigma_{ds}(1s \to n'p) . \tag{6.7}$$

Note that for all three mechanisms the cross sections are independent of the sign of μ'. This can be understood by observing that, to the extent that the approximations used above are valid, the relative motion of the heavy nuclei takes place in a fixed plane; the Hamiltonian is invariant under a reflection in this plane, a reflection which changes the sign of μ'.

6. Charge transfer to the continuum; the cusp and its asymmetry

We have thus far restricted ourselves to true capture, in which the electron and projectile nucleus emerge bound to one another; we have ignored the ionization process. This process is, of course, very important, but it is not of such great interest in the context of the present paper since the total ionization cross section is determined, at asymptotically high velocities, by the first Born term, as is the differential ionization cross section for *most* velocities of the ejected electron. However, if the relative velocity of the emergent electron and the incident nucleus is sufficiently small—we will be more precise in the following paragraph—we expect by reason of continuity that ionization may, at asymptotically high projectile velocities, proceed via a mechanism analogous to the double scattering mechanism for true capture.

In line with standard usage we use the phrase "capture to the continuum" if the emergent electron is moving relative to the projectile nucleus with a (positive) energy that is small compared to the ionization energy of the electron–projectile subsystem. There has been considerable interest in charge transfer to the continuum since Salin (1969) and Macek (1970) demonstrated that this mechanism provides a qualitative explanation for the forward peak observed by Rudd *et al.* (1966) in the angular distribution of electrons ejected from helium atoms by 300 keV protons, at electron velocities comparable to the proton velocity. For references to more recent work see the paper by Vane *et al.* (1978).

The quantity of experimental interest is the differential cross section for the electron to emerge into a narrow forward cone of specified semiangle with a speed v_e close to v. Let $\mathbf{v}_e$ denote the velocity of the emergent electron in the lab frame, and define $\mathbf{k}$ by $\hbar\mathbf{k} \equiv m(\mathbf{v}_e - \mathbf{v})$. Let $\psi_{\mathbf{k}}(\mathbf{r})$ denote the continuum Coulomb wave function, that is,

$$\psi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-3/2} e^{\eta\pi/2}\Gamma(1 + i\eta)e^{i\mathbf{k}\cdot\mathbf{r}} \times {}_1F_1[-i\eta, 1, -i(kr + \mathbf{k}\cdot\mathbf{r})] , \tag{6.8}$$

where $k = |\mathbf{k}|$ and

$$\eta \equiv Z_B/(a_0 k) .$$

Let θ_e and ϕ_e denote the polar and azimuthal angles of $\mathbf{v}_e$, with $\mathbf{v}$ the polar axis. To obtain the double scattering differential cross section for the electron to emerge with a speed between v_e and $v_e + dv_e$ into a cone of specified semiangle θ_0, where $\theta_0 = K(e^2/\hbar v)$ with the constant $K \ll 1$ and independent of v, we simply replace $|\psi_f(\mathbf{r}^*)|^2$ in Eq. (5.12) by $|\psi_{\mathbf{k}}(\mathbf{r}^*)|^2 dN$, where $dN = (m/\hbar)^3 d^3v_e$, $d^3v_e = v_e^2 dv_e d\Omega_e$ and $d\Omega_e = \sin\theta_e \, d\theta_e \, d\phi_e$, and we integrate over θ_e and ϕ_e with $0 \leq \theta_e \leq \theta_0$ and $0 \leq \phi_e \leq 2\pi$; this range of integration will henceforth be understood. Note that since $\int |\psi_f(\mathbf{r})|^2 d^3r = 1$, we normalize $\psi_{\mathbf{k}}(\mathbf{r})$ so that $\int \psi_{\mathbf{k}}^*(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r}) d^3r = \delta(\mathbf{k} - \mathbf{k}')$. dN is the number of cells in phase space. [Note also that in arriving at Eq. (5.12) we integrated over the azimuthal angle of $\mathbf{b}$ assuming that $|\psi_i|^2$ and $|\psi_f|^2$ are independent of that angle; $|\psi_i|^2$ is of course here again independent of that angle, as is $\int |\psi_{\mathbf{k}}|^2 d\phi_e$.] Since we are interested in

$$\hbar^2 k^2/2m \ll (Z_B e)^2/2a_0 ,$$

or, equivalently, $\eta \gg 1$, we can write

$$e^{\eta\pi}|\Gamma(1 + i\eta)|^2 = 2\pi\eta/(1 - e^{-2\pi\eta}) \sim 2\pi\eta . \tag{6.9}$$

We can also replace v_e^2 in d^3v_e by v^2. Furthermore, since the initial state is a $1s$ state, $r^* \equiv |\mathbf{r}^*|$ is effectively restricted by the initial wave function to satisfy $r^* \lesssim a_0/Z_A$. Now if $\hbar^2k^2/2m \ll Z_B e^2/r^*$ for the significant range of r^*, that is, if $\eta^2 \gg Z_B/2Z_A$, the energy in the Schrödinger equation for $\psi_{\mathbf{k}}(\mathbf{r}^*)$ can be neglected, and $\psi_{\mathbf{k}}(\mathbf{r}^*)$ depends upon $\mathbf{k}$ only through the boundary conditions so that one expects the form of $\psi_{\mathbf{k}}(\mathbf{r}^*)$ to simplify. Indeed, with $\eta \gg (Z_B/2Z_A)^{1/2}$ we can use Eq. (13.3.2) of Abramowitz and Stegun (1970) to arrive at

$$|\psi_{\mathbf{k}}(\mathbf{r}^*)|^2 \sim (\eta/4\pi^2)\{J_0[2(Z_B\chi r^*/a_0)^{1/2}]\}^2 , \tag{6.10}$$

where

$$\chi = 1 + \hat{k}\cdot\hat{r}^* . \tag{6.11}$$

Equation (5.12) therefore becomes, using also Eq. (2.2),

$$\frac{d\sigma_{\rm ds}}{db\,dv_e}(1s\to{\rm cont})\sim\frac{2^7\pi Z_A^5 Z_B^3 a_0}{3^{1/2}}\left(\frac{e^2}{\hbar v}\right)^9 \times\int d\Omega_e\frac{1}{|\mathbf{v}_e-\mathbf{v}|}e^{-2Z_A r^*/a_0} \times\{J_0[2(Z_B\chi r^*/a_0)^{1/2}]\}^2. \qquad (6.12)$$

The kinematics are similar to those for double scattering capture, and so $r^*=b/\sin 60°$. Performing the integration over b using Eq. (6.615) of Gradshteyn and Ryzhik (1965), we obtain (Shakeshaft and Spruch, 1978a)

$$\frac{d\sigma_{\rm ds}}{dv_e}(1s\to{\rm cont})\sim 2^5 Z_A^4 Z_B^3\left(\frac{e^2}{\hbar v}\right)^9(\pi a_0^2)I(v_e), \qquad (6.13)$$

where

$$I(v_e)=\int d\Omega_e\frac{1}{|\mathbf{v}_e-\mathbf{v}|}J_0\left[i\left(\frac{Z_B}{Z_A}\right)\chi\right]\exp\left[-\left(\frac{Z_B}{Z_A}\right)\chi\right]. \qquad (6.14)$$

Note that this result differs from that obtained by Dettmann *et al.* (1974) for double scattering capture to the continuum; we believe that their result is incorrect, the error originating in Eq. (4.25) of their paper.

Although we cannot evaluate analytically the double integral $I(v_e)$, the following properties can be readily obtained:

(i) $I(v_e)$ behaves as v^{-2} with increasing v since the solid angle into which the electron emerges is roughly $\pi\theta_0^2=\pi K^2(e^2/\hbar v)^2$. [The denominator $|\mathbf{v}_e-\mathbf{v}|$ in the integrand of $I(\mathbf{v}_e)$ does not affect the v dependence since its range, $0\le|\mathbf{v}_e-\mathbf{v}|\le Z_B e^2/\hbar$, is independent of v.] Therefore the v dependence of the differential cross section is v^{-11}.

(ii) $I(v_e)$, and therefore the differential cross section, have a cusp at $v_e=v$.

(iii) $I(v)$ may be reduced to a one-dimensional integral.

(iv) If $\psi_{\mathbf{k}}(\mathbf{r})$ is approximated by its s-wave component, $I(v_e)$ can be reduced to a closed-form expression.

A cusp in the differential cross section for charge transfer to the continuum was predicted by Dettmann *et al.* (1974) using an approximation analogous to the Brinkman–Kramers approximation for true capture. They obtained the result

$$\frac{d\sigma_{\rm BK}}{dv_e}(1s\to{\rm cont})\sim\frac{2^{17}}{5}Z_A^5 Z_B^3\left(\frac{e^2}{\hbar v}\right)^{10}\left(\frac{1}{v^2}\right) \times\{[(v_e-v)^2+(v\theta_0)^2]^{1/2}-|v_e-v|\}(\pi a_0^2), \qquad (6.15)$$

and they verified the presence of the cusp by measuring the differential cross section for ionization of carbon and gold foils by fast light ions. Note that the v dependence of the cross section in Eq. (6.15) is v^{-12}, and therefore at sufficiently high velocities (extremely high, however) the double scattering mechanism for charge transfer to the continuum is important.

However, at very high velocities the dominant mechanism for charge transfer to the continuum is the one analogous to radiative capture to a bound state. To obtain the differential cross section for radiative capture to the continuum one simply replaces $|\tilde{\psi}_f(-m\mathbf{v})|^2$ in Eq. (4.3) by $|\tilde{\psi}_{\mathbf{k}}(-m\mathbf{v})|^2(m/\hbar)^3 d^3v_e$. The Fourier transform of the continuum Coulomb wave function $\psi_{\mathbf{k}}(\mathbf{r})$ is given by Eq. (9.12) of Bethe and Salpeter (1957); there is no difficulty in taking the limit implied in this equation since $mv>\hbar k$. We find that for electrons ejected into a cone of semiangle θ_0,

$$\frac{d\sigma_{\rm rc}}{dv_e}(nl\to{\rm cont})\sim\frac{2^6}{3}Z_B^3\left(\frac{e^2}{\hbar c}\right)^3\left(\frac{e^2}{\hbar v}\right)^3\left(\frac{1}{v^2}\right) \times\{[(v_e-v)^2+(v\theta_0)^2]^{1/2}-|v_e-v|\}(\pi a_0^2). \qquad (6.16)$$

Note that the v dependence of this differential cross section is v^{-5}. Comparing Eqs. (6.15) and (6.16) we find that for $Z_A=1$ the radiative mechanism begins to dominate over the Brinkman–Kramers mechanism when $(\hbar v/e^2)\approx 23$, that is, at proton energies of about 13 MeV.

The cusps noted above arise from the factor $2\pi\eta$ in the square of the Coulomb wave function. We see from Eq. (6.15) that the cusp in $d\sigma_{\rm BK}/dv_e$ is symmetric about $v_e=v$ (that is, invariant under a change of sign of v_e-v). This is because the probability for capture via the Brinkman–Kramers mechanism into a component of the continuum with $l'>0$ decreases relative to the probability for capture into the component with $l'=0$ as $1/v^{2l'}$; thus capture occurs predominantly to the s-wave component and, to leading order in $1/v$, the Brinkman–Kramers contribution is therefore isotropic in the vector $\mathbf{v}_e-\mathbf{v}$. In contrast, the relative probability for continuum capture via the double scattering mechanism into components of different l' is independent of v to leading order in $1/v$; many different angular momentum components of the continuum are important (and interfere with one another since the angular region for capture to the continuum is less than the full solid angle, and indeed is very small). Thus the double scattering contribution depends on both the magnitude *and* the direction of the vector $\mathbf{v}_e-\mathbf{v}$ and, as a consequence, the cusp in $d\sigma_{\rm ds}/dv_e$ is asymmetric about $v_e=v$. This is apparent from Eqs. (6.11), (6.13), and (6.14), where $d\sigma_{\rm ds}/dv_e$ is seen to depend upon the direction of $\mathbf{k}=m(\mathbf{v}_e-\mathbf{v})/\hbar$ through the "asymmetry source factor" χ. We note that since χ appears multiplied by Z_B in Eq. (6.14) the asymmetry of the cusp becomes more prominent as Z_B increases, at least for Z_B not too large.

The condition for the validity of the asymptotic formulae for bound-state-to-bound-state capture is that v be much greater than the initial and final orbital velocities. For capture to the continuum the final "orbital" velocity $\mathbf{v}_e-\mathbf{v}$ is negligible (for $\eta\gg 1$) and so we require, for the validity of Eqs. (6.13)–(6.16), that $v\gg Z_A e^2/\hbar$. Note that v is not restricted by the projectile charge $Z_B|e|$ through this condition, but for double scattering a further condition on v involving Z_B, must be imposed. In arriving at Eq. (5.10) for $P_{\rm cap}$ we assumed that the spatial width ($\sim\hbar/mv$) of the emergent wave packet is small compared to the characteristic radius of the atom $(m+M_B)$. For the final state a continuum state, the characteristic radius becomes the wavelength of oscillation of $\psi_k(\mathbf{r})$ which, from Eq. (6.10), is of order $a_0/(Z_A Z_B)^{1/2}$ for large Z_B/Z_A and for $r^* \approx a_0/Z_A$. We therefore require $\hbar/mv \ll a_0/(Z_A Z_B)^{1/2}$, that is, $v \gg (Z_A Z_B)^{1/2} e^2/\hbar$.

B. Discussion

In Figs. 6 and 7 we have plotted $(\xi\sigma/\pi a_0^2)$ versus both $(\hbar v/e^2)$ and the lab energy per nucleon in MeV; here σ is the asymptotic form of the cross section for the appropriate mechanism, and ξ is a scaling factor chosen so that $\xi\sigma$ is independent of the charges of the nuclei, with $\xi = 1$ for $Z_A = Z_B = 1$. Figure 6 pertains to $1s \to 1s$ electron capture, and we consider this transition first. Evidently radiative capture is the dominant mechanism at sufficiently high velocities; nonradiative capture is eventually dominated by the knock-on mechanism, but nonradiative capture into forward scattering angles can occur only by single or double scattering. For electron capture by protons from hydrogen atoms radiative capture dominates at a proton lab energy of about 6 MeV, corresponding to $(v/c)^2 \approx 0.01$, and knock-on capture becomes the dominant mechanism for nonradiative capture at about 44 MeV, corresponding to $(v/c)^2 \approx 0.1$. Evidently double scattering does not play a very significant role in $1s \to 1s$ capture for the energy considered;

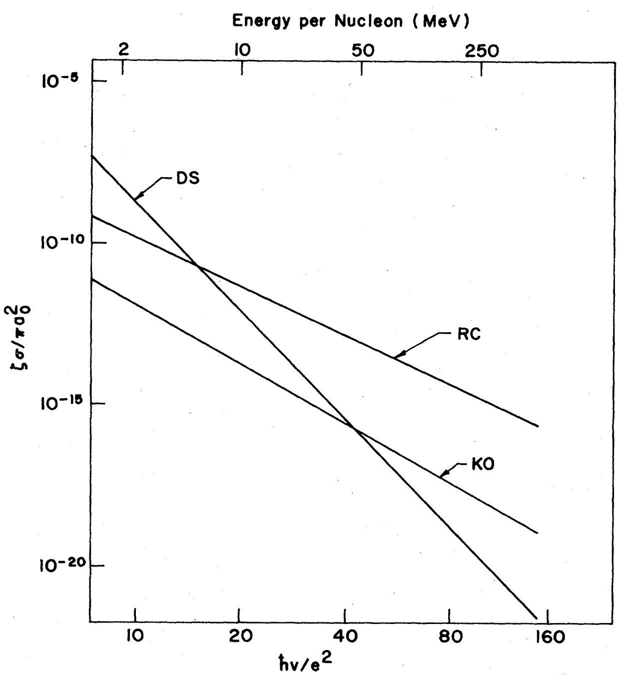

FIG. 6. This figure illustrates the relative importance of the three mechanisms for $1s \to 1s$ electron capture. We plot $(\xi\sigma/\pi a_0^2)$ versus both $(\hbar v/e^2)$ and the lab energy per nucleon in MeV; σ is the asymptotic form of the cross section for the appropriate mechanism and the ξ's are scaling factors chosen so that $\xi\sigma$ is independent of Z_A and Z_B and $\xi = 1$ for $A = Z_A = Z_B = 1$. Curve KO represents the knock-on mechanism, with $\xi = 2^{-4}(Z_A + Z_B)^4 (Z_A Z_B)^{-5} A^2$, where A is the nuclear mass number; curve RC represents radiative capture, with $\xi = Z_B^{-5}$; curve DS represents double scattering, with $\xi = 2^{-1}(Z_A + Z_B) \times (Z_A Z_B)^{-5}$.

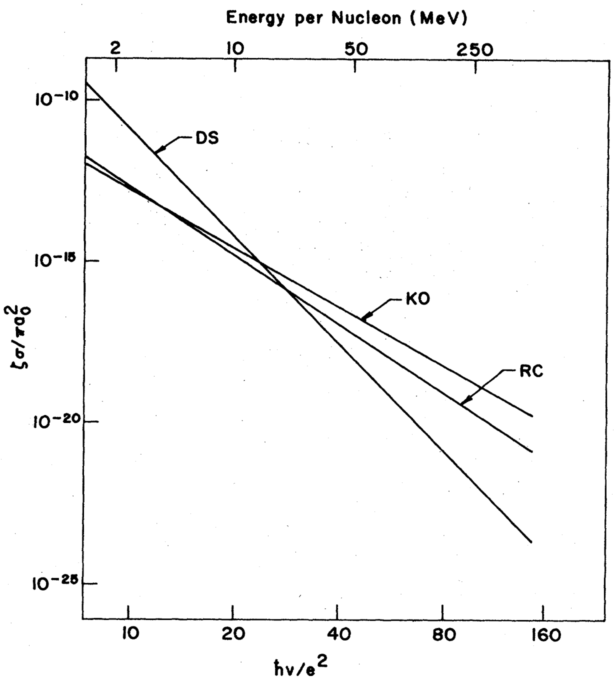

FIG. 7. This figure illustrates the relative importance of each mechanism for $1s \to 2p$ electron capture. The notation is the same as in Fig. 6. The scaling factors ξ are as follows: KO: $\xi = 3^{-6}(2Z_A + Z_B)^6 Z_A^{-5} Z_B^{-7} A^2$, where A is the nuclear mass number; RC: $\xi = Z_B^{-7}$; DS: $\xi = 3^{-3}(2Z_A + Z_B)^3 Z_A^{-5} Z_B^{-7}$.

it plays a more significant role in $1s \to 2p$ capture, as indicated in Fig. 7. For $1s \to 2p$ capture, the knock-on mechanism dominates at sufficiently high velocities; radiative capture still eventually dominates for forward scattering angles, but not until quite high velocities. Note that the cross section for radiative capture from the ground state decreases as $1/v^{5+2l'}$ with increasing v, where l' is the orbital angular momentum quantum number of the final state. Therefore for capture into states with $l' > 3$ radiative capture falls off faster than v^{-11} and will be dominated by double scattering at high velocities. For $1s \to 2p$ electron capture by protons from hydrogen atoms, knock-on capture becomes dominant at a proton energy of about 16 MeV, corresponding to $(v/c)^2 \approx 0.04$, and radiative capture becomes the dominant mechanism for scattering into forward angles at about 24 MeV, corresponding to $(v/c)^2 \approx 0.05$.

The Z_A dependences of the different mechanisms for the capture of an electron by a bare nucleus from an *outer* shell of a many-electron atom whose nucleus has charge $Z_A|e|$ warrants some comment. Apart from the applicability to a range of laboratory experiments, such capture cross sections are of astrophysical interest; for example, there is the possibility of detecting $K\alpha$ x-ray lines of Fe^{+25} emitted by astronomical sources; one way of populating the $2p$ state is by capture. Studies of the intensity and width of the line emitted for Fe ions passing through an ambient medium of stellar abundances, with energies in the range 1 to 300 MeV/amu, have been made recently by Bussard *et al.* (1977).

To obtain a crude estimate of the cross section for electron capture from the outer shell of an atom by a bare incident nucleus we can take as our initial electron wave function a Slater orbital (Slater, 1960). Thus if the outer electron is initially in a shell of principal quantum number n, we use the wave function $Nr^{n-1}\exp(-Z_A^* r/na_0)$, where N is a normalization factor and where $Z_A^*|e|$ is the effective charge that the electron sees, which is given by the Slater rules. To the extent that Z_A^* is independent of Z_A we can determine the Z_A dependences of the cross sections as follows. (The effective charge that an outer electron sees will vary with Z_A—it will oscillate—but it will not change dramatically. In contrast, the effective charge that a K shell electron sees increases monotonically with Z_A.) In the knock-on mechanism the capture cross section depends on Z_A only through the cross section for the backscattering of the nuclei. The Z_A dependence is therefore Z_A^2; the dependence on Z_A^* is through the wave functions. In the radiative mechanism there is no dependence on Z_A (nor on Z_A^*). In the double scattering mechanism the capture cross section depends on Z_A through the cross section for the electron to scatter from the target nucleus; the nucleus will be only barely screened during the collision and the Z_A dependence is therefore Z_A^2. In the Brinkman–Kramers approximation the cross section depends on Z_A through the square of the high-momentum component of the initial wave function. In this case the Z_A dependence is, for $l=0$, that of Z_A^2 multiplied by the probability density for the electron to be at the nucleus; the factor Z_A^2 originates in the cusp of the wave function (in coordinate space) when the electron is near the nucleus. Unfortunately we cannot use the Slater orbital to determine the probability density for the electron to be near the nucleus, since the Slater orbital is a very poor approximation in this region. To determine the electron density near the nucleus would require the use of far more elaborate wave functions than Slater orbitals. The density near the nucleus is expected to be very small because of the Pauli exclusion principle, thus enhancing the relative importance of double scattering versus Brinkman–Kramers. (For $l>0$ the density at the origin is zero and must be replaced by an expression involving derivatives of the coordinate wave function.)

C. Comparison of the second Born and Brinkman-Kramers cross sections

The Brinkman–Kramers cross section decreases as $1/v^{12+2l+2l'}$, where l and l' are the orbital angular momentum quantum numbers of the initial and final states, respectively. In contrast, the double scattering cross section decreases as $1/v^{11}$ for all l and l'. Therefore, for a fixed high velocity the Brinkman–Kramers cross section becomes increasingly inaccurate as l and l' increase; one must add the double scattering contribution. In Fig. 8 we compare σ_{ds} with σ_{BK} for electron capture from the ground state to the $1s$, $2p$, and $3d$ states. For $1s \to 1s$ capture σ_{ds} does not dominate over σ_{BK} until very high velocities, but this is not so

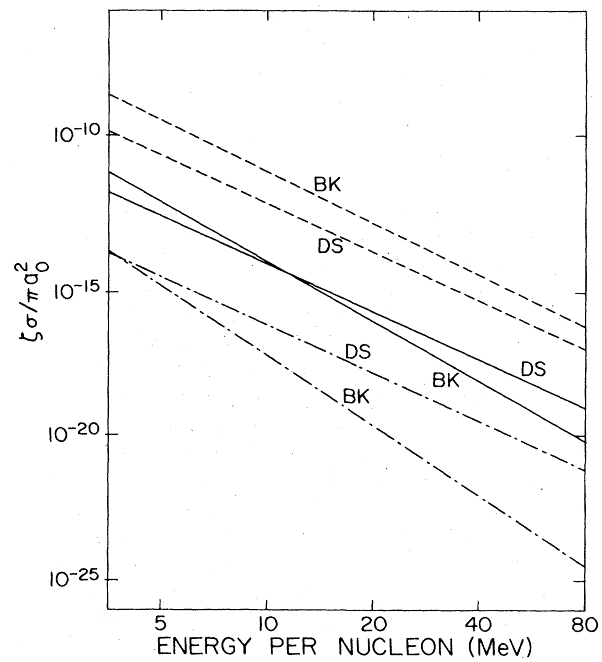

FIG. 8. The asymptotic forms of the double scattering cross section σ_{ds} and the Brinkman–Kramers cross section σ_{BK} for electron capture into various final states are plotted as functions of energy. The curves represent the following capture processes: $1s\to 1s$: — — — —; $1s \to 2p$: ————; $1s \to 3d$: —•—•—. All possible values of the final magnetic quantum number are summed over. The scaling factors ζ are as follows: $1s\to 1s$: $\zeta(\mathrm{DS})=2^{-1}(Z_A+Z_B)\,(Z_AZ_B)^{-5}$, $\zeta(\mathrm{BK})=(Z_AZ_B)^{-5}$; $1s\to 2p$: $\zeta(\mathrm{DS})=3^{-3}(2Z_A+Z_B)^3 Z_A^{-5}Z_B^{-7}$, $\zeta(\mathrm{BK})=Z_A^{-5}Z_B^{-7}$; $1s\to 3d$: $\zeta(\mathrm{DS})=2^{-10}(3Z_A+Z_B)^5 Z_A^{-5}Z_B^{-9}$, $\zeta(\mathrm{BK})=Z_A^{-5}Z_B^{-9}$. The cross sections for $1s\to 1s$ and $1s\to 2p$ capture are given in Eqs. (6.3) and (6.4) of the text. For $1s\to 3d$ capture we have $\sigma_{ds}/\pi a_0^2 \sim 2^7 3^{-3}\pi Z_A^5 Z_B^9 (3Z_A+Z_B)^{-5}(e^2/\hbar v)^{11}$ and $\sigma_{BK}/\pi a_0^2 \sim 2^{29}3^{-9}(1/7)Z_A^5Z_B^9(e^2/\hbar v)^{16}$.

for $1s \to 2p$ and $1s \to 3d$ capture. For example, for electron capture by protons from hydrogen atoms σ_{ds} dominates over σ_{BK} above a lab energy of about 13 MeV for $1s \to 2p$ capture and above 4 MeV for $1s \to 3d$ capture. (For a better theoretical estimate of the $1s \to n'l'$ capture cross sections one should, of course, evaluate the sum of the first two Born terms accurately. See Briggs and Dubé, 1978).

In Fig. 9 we have plotted the *differential* cross section as a function of laboratory scattering angle for $1s \to 1s$ electron capture by protons from hydrogen atoms. The impact velocity and energy in the lab frame are 40 a.u. and (very nearly) 40 MeV, respectively. The solid and dashed lines represent the differential cross section calculated from the sum of the first two Born terms and from the Brinkman–Kramers term, respectively. The second Born term was evaluated approximately using the high-velocity formula given by Eq. (52j) of Mapleton (1972). The contribution from the double scattering process is clearly evident as the second peak in the solid line; this peak becomes a delta function in the limit of infinite velocity. The peak maximizes at the critical angle (discussed in Sec. VI.A.3) of $(\sqrt{3}/2)(m/M_B)$ rad, i.e., 1.6′. It is

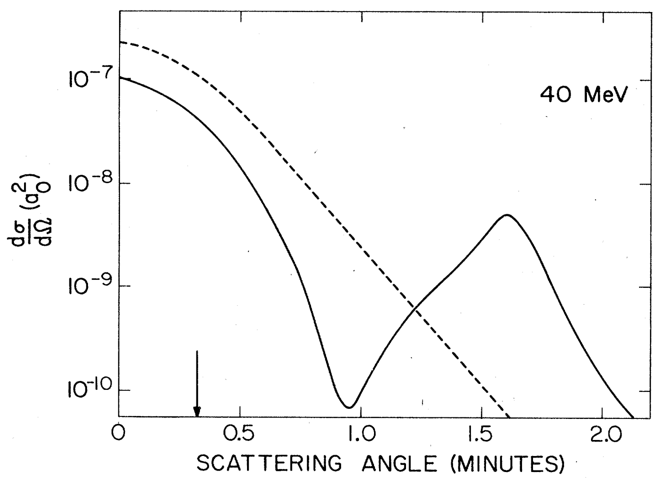

FIG. 9. The laboratory scattering differential cross section versus the angle in minutes is plotted for $p + H(1s) \to H(1s) + p$. The impact velocity in the lab frame is 40 a.u., that is, $40e^2/\hbar$, (corresponding to an impact energy of almost 40 MeV). The solid and dashed lines pertain to the differential cross section calculated from the sum of the first two Born terms and from the Brinkman–Kramers approximation, respectively. The second peak (in the solid line) at the critical angle of 1.6′ is due to the double scattering contribution. The differential cross section for radiative capture is very small for scattering angles beyond the vertical arrow marked on the horizontal axis. The knock-on process can be ignored.

conceivable that this peak could be seen even with the present limitations on the experimental angular resolution. Note that with the impact velocity fixed, the scattering angle scales as $1/M_B$ provided the scattering angle is small and $M_B \gg m$. It follows that if the projectile were a positive muon rather than a proton, the curves of Fig. 9 would be stretched along the abscissa by a factor of roughly 9, and the critical angle would be about 14.4′. The gain by a factor of 9 would not, however, compensate for the additional difficulties associated with using a muon rather than a proton beam. If it were possible, it would of course be even more advantageous, in this regard, to study the capture of electrons by fast positrons.

We have not plotted the differential cross section for radiative capture since this diminishes extremely rapidly with increasing angle—recall from Sec. VI.A.2 that the main contribution to the total radiative capture cross section comes from scattering angles less than of the order of $(m/M_B)[(v/2c)+(e^2/\hbar v)]$; this angle has been marked by a vertical arrow on the horizontal axis of Fig. 9. We have also not plotted the differential cross section for knock-on capture since the hydrogen atoms produced by knock-on capture are moving very slowly in the lab frame and will not be detected in a normal scattering experiment.

Charge transfer experiments with hydrogen atoms as targets can be plagued by the presence of contaminants with higher atomic number which have much larger charge transfer cross sections, as discussed in detail by Gardner (1978). Thus one might consider using targets other than hydrogen atoms. If the target atom has nuclear charge $Z_A|e|$, if we consider $1s \to 1s$ capture by an incident bare nucleus of charge $Z_B|e|$, and if we ignore the effect of outer electrons, the cross sections σ_{BK} and σ_{ds} for the capture of either of the two K-shell electrons increase relative to the corresponding cross sections for capture from a hydrogen atom target by factors of $2Z_A^5$ and $2Z_A^5(1+Z_B)/(Z_A+Z_B)$, respectively, assuming a fixed high velocity; the factor of 2 accounts for the two electrons in the K shell. However, the asymptotic forms of the cross sections do not become valid until $v \gg Z_A e^2/\hbar$, so that the lowest velocity at which they are valid increases linearly with Z_A; but increasing v by a factor of Z_A introduces factors of Z_A^{-12} and Z_A^{-11} into σ_{BK} and σ_{ds}, respectively, so that in fact the cross sections calculated at the lowest velocity at which the asymptotic forms are valid will decrease rapidly with increasing Z_A. One could use either helium atoms or hydrogen molecules as targets, though in the latter case it would be difficult to calculate σ_{BK} accurately. However, in either case the detection of a peak in the differential cross section at a nonzero scattering angle would indicate the presence of a double scattering contribution. There will, in fact, be two peaks. One peak will occur, in the lab frame, at $(\sqrt{3/2})(m/M_B)$ rad, and the other at m/M_B rad; this second peak arises from the possibility that the electron to be captured can, after being scattered by the incident ion, scatter from the other electron rather than from the helium target nucleus or from either target proton for the molecular hydrogen case. If the projectile is a proton the two peaks will occur, in the lab frame, at about 1.6′ and 1.9′, respectively. Note that if the second collision is between the two electrons, the electron that is not captured will be ejected from the target with a speed very nearly equal to v and in a direction that is almost perpendicular to the incident beam direction; these are simple consequences of the kinematics. Therefore if electrons ejected perpendicular to the beam direction were detected in coincidence with capture, there would be a peak in the energy spectrum of the electrons at roughly $\frac{1}{2}mv^2$; the width of the peak would be of order 1 a.u.

The possibilities just discussed of detecting the v^{-11} double scattering contribution to the cross section for electron capture at high impact velocities have been discussed in greater detail by Shakeshaft and Spruch (1978b). Perhaps the best possibility is to measure the cross section for capture from a high Rydberg state (Spruch, 1978); this is discussed briefly in Sec. VII. It is the qualitative, rather than the quantitative, changes introduced by the v^{-11} contribution that might be possible to detect. Except for very high v, the $1/v^{12}$ (or $1/v^{13}$) double scattering contribution is more significant quantitatively than the $1/v^{11}$ contribution, but the qualitative effects are less striking. However, Briggs and Dubé (1978) have suggested that it might be possible to detect the $1/v^{12}$ double scattering contribution by examining the polarization of the light emitted following $1s \to 2p$ capture. Another possibility is to examine the asymmetry in the cusp in the differential cross section for capture to the continuum (see Sec. VI.A.6); not only the v^{-11} but also the v^{-12} double scattering contribution is asymmetric. Indeed, the asymmetry in the cusp already observed for projectiles of high atomic number (Vane *et al.*, 1978; Suter *et al.*, 1978) may represent the first experimental confirmation of the importance of the double scattering contribution at high impact velocities. See Shakeshaft and Spruch (1978c) for further discussion of cusp asymmetries.

VII. CLASSICALLY DESCRIBABLE PROCESSES

A. General remarks

We have seen that the knock-on and double scattering capture mechanisms do not depend on the high-momentum components of the bound-state wave functions, whereas the radiative and Brinkman–Kramer mechanisms do. Now when the classical picture of an atom is valid, namely, when the atom is in a high Rydberg state, the (valence) electron moves in a fairly well-defined orbit and has a relatively narrow momentum distribution. It is reasonable to expect, therefore, that when the initial and final states are high Rydberg states, the knock-on and double scattering processes should be describable classically, and the cross sections for knock-on and double scattering capture should be very much larger than the cross sections for the nonclassical radiative and Brinkman–Kramers mechanisms. Furthermore, since the electron orbital velocity is small in the classical regime, we expect the asymptotic forms of the cross sections to be valid at much lower v than in the nonclassical regime.

In this section we turn our attention to high Rydberg states and assume, therefore, that $n \gg 1$. (Lasers have recently made these states accessible.) For later purposes it will be useful to record here a few of the properties of these states; at the same time we establish a notation. In the classical description of an electron bound to a nucleus of charge $Z|e|$, the electron orbit is characterized by semimajor and semiminor axes a and b, respectively; it will be convenient also to introduce $c \equiv (a^2 - b^2)^{1/2}$. There should be no confusion between the semiminor axis b and the impact parameter b, especially because most of those relations derived in this section that are used later are expressed in terms of a and c. We can express a and b in terms of the energy E and angular momentum L of the system and the constants Ze^2 and m, for we have

$$E = -\frac{Ze^2}{2a} \equiv -\frac{mv_0^2}{2}, \quad L = mv_0 b. \tag{7.1}$$

The distance r of the electron from the nucleus lies in the range

$$a - c \leq r \leq a + c. \tag{7.2}$$

The range of $v_m = |\mathbf{v}_m|$, where $\mathbf{v}_m$ is the electron orbital velocity, is given by

$$L/(a+c) \leq mv_m \leq L/(a-c), \tag{7.3}$$

or

$$v_{\min} \equiv v_0\{(a-c)/(a+c)\}^{1/2} \leq v_m \leq v_0\{(a+c)/(a-c)\}^{1/2} \equiv v_{\max}. \tag{7.4}$$

We can make the connection with the quantum results by setting

$$E = -Z^2e^2/(2n^2a_0), \tag{7.5}$$

and

$$L = (l + \tfrac{1}{2})\hbar. \tag{7.6}$$

[As is so commonly done in semiclassical studies, we use $(l+\frac{1}{2})^2$ rather than $l(l+1)$.] We then find

$$a = n^2a_0/Z, \quad b/a = (l+\tfrac{1}{2})/n, \quad v_0 = Ze^2/(n\hbar),$$
$$c/a = [1 - \{(l+\tfrac{1}{2})^2/n^2\}]^{1/2}. \tag{7.7}$$

We can now readily express the limits on r and v_m as functions of n and l.

• To obtain some idea of the values of the quantum numbers involved, at least for one particular case, we consider $c/a \ll 1$, for which the ellipse approximates a circle of radius a, and v_m is approximately constant, with the value L/ma. In quantum terms, $c/a \ll 1$ becomes $l \approx n \gg 1$. The distribution of v_m approaches a multiple of $\delta(v_m - \{Ze^2/n\hbar\})$, but only for very large values of l and n; even choosing $l = n-1$ requires n to be of the order of 15 to reduce the fractional spread in v_m, which is $2\,c/a$ for any value of c/a, to about 1 part in 2.

We now have the range of r (and of v_m) for a and c, or n and l, fixed. We will also need to know the range of values of a and c (and of n and l) for which the electron can be at a specified distance r. We have $0 \leq c \leq a$ and $a - c \leq r \leq a + c$. For fixed r, it follows that $r \leq a + c \leq 2a$, that is,

$$a \geq \tfrac{1}{2}r. \tag{7.8}$$

For fixed r and a, we start from $-c \leq r - a \leq c$; it follows that $c^2 \geq (a-r)^2$, or

$$(c/a)^2 \geq \{1 - (r/a)\}^2. \tag{7.9}$$

In terms of n and l, these two inequalities become

$$n^2 \geq (Zr/2a_0) \tag{7.10}$$

and

$$\frac{(l+\frac{1}{2})^2}{n^2} \leq \left(\frac{r}{a}\right)\left\{2 - \left(\frac{r}{a}\right)\right\}, \tag{7.11}$$

where $0 \leq r/a \leq 2$ and where, as above, $a = n^2a_0/Z$. The upper bound on $(l+\frac{1}{2})^2/n^2$ is unity, so that the requirement $l \leq n-1 (\approx n - \frac{1}{2})$ is effectively automatically satisfied.

We turn now to the normalized distributions in r and v_m, denoted by $f(r;a,c)$ and $g(v_m;a,c)$, for an orbit characterized by a and c. Letting dt represent the time the electron spends at a distance between r and $r+dr$, we have

$$f(r;a,c)dr = \frac{dt}{\frac{1}{2}\tau} = \frac{2}{\tau}\frac{dr}{dr/dt}, \tag{7.12}$$

where τ is the period and we divide by $\frac{1}{2}\tau$ rather than by τ since the range of the normalization integral,

$$\int_{a-c}^{a+c} f(r;a,c)dr = 1, \tag{7.13}$$

covers only half a period. The result for $f(r;a,c)$ can be obtained using only elementary mechanics; the derivation is not too tedious. One finds

$$f(r;a,c)dr=\frac{rdr}{\pi a[\{(a+c)-r\}\{r-(a-c)\}]^{1/2}}, \qquad (7.14)$$

where $a-c\leq r\leq a+c$ and $\mathbf{r}$ lies in the plane of the ellipse.

If we average over all orientations of the plane, the classical analog of averaging over the projection μ in quantum mechanics, we get a spherically symmetric probability density. It will be useful to have an average over all orientations and over the allowed range of c for r and a fixed, that is, $|r-a|\leq c\leq a$. To obtain this average we must use the appropriate weighting factor in c. This weighting factor can be obtained purely classically, but, especially for those whose training is primarily in quantum theory, it will be simpler to use quantum theory at an intermediate stage. Thus a and c are functions of n and l, and the average over orientations and c with r and a fixed is equivalent to an average over all μ and over all allowed l, for r and n fixed. We therefore have

$$f(r;a)dr=\sum_l (2l+1)f(r;a,c)dr/n^2$$

for the normalized probability of finding a particle moving in an ellipse of semimajor axis a with a weighted average over c at a distance r to $r+dr$; n^2 is the number of states for the given n. The sum is from $l=0$ to $l=n-1$, but the condition $a-c\leq r\leq a+c$ cuts down on the range of l that contributes; the upper limit on l is easily obtained, and follows from Eq. (7.11) above, but it need not here concern us since we shall convert from l to c and we already know the range of c. Thus we replace $\sum_l$ by $\int dl$, and then use Eq. (7.7) to obtain

$$2(l+\tfrac{1}{2})dl=-(n^2/a^2)2cdc\,.$$

We thereby arrive at

$$f(r;a)dr=-\left(\frac{2}{a^2}\right)dr\int_a^{|a-r|} f(r;a,c)cdc$$

$$=\left(\frac{2r}{\pi a^3}\right)(2ar-r^2)^{1/2}dr\,. \qquad (7.14)'$$

To obtain the normalized velocity distribution for a and c fixed, namely, $g(v_m;a,c)$, we note that

$$\int_{a-c}^{a+c} f(r;a,c)dr=\int_{v_{\min}}^{\max} g(v_m;a,c)dv_m\,, \qquad (7.15)$$

where $v_{\min}$ and $v_{\max}$ are defined by Eq. (7.4). Since $v_{\min}$ and $v_{\max}$ occur at $r=a+c$ and $r=a-c$, respectively, we have

$$g(v_m;a,c)dv_m=-f(r;a,c)dr\,. \qquad (7.16)$$

With some labor, we find, expressing r in terms of v_m,

$$g(v_m;a,c)dv_m$$

$$=\frac{8av_0^4v_mdv_m}{\pi(a^2-c^2)^{1/2}(v_m^2+v_0^2)^2\{(v_{\max}^2-v_m^2)(v_m^2-v_{\min}^2)\}^{1/2}} \qquad (7.17)$$

for $v_{\min}\leq v_m\leq v_{\max}$ and $\mathbf{v}_m$ in the plane of the ellipse.

If we average $g(v_m;a,c)dv_m$ over all orientations and over a weighted distribution in c, we obtain $g(v_m;a)dv_m$, the normalized probability of finding a particle in an ellipse of semimajor axis a and a distribution of values of c with a velocity (really a speed) between v_m and v_m+dv_m. It is simpler to obtain $g(v_m;a)$ by noting that

$$\int_0^\infty g(v_m;a)dv_m=\int_0^{2a} f(r;a)dr\,.$$

The limits on v_m are the smallest value of $v_{\min}$ and the largest value of $v_{\max}$, as a function of c for the allowed range of c; alternatively, we have $v_m=0$ at $r=2a$, and $v_m=\infty$ at $r=0$. We therefore have

$$g(v_m;a)dv_m=-f(r;a)dr\,,$$

and one then finds

$$g(v_m;a)dv_m=\frac{32v_0^5v_m^2dv_m}{\pi(v_m^2+v_0^2)^4}\,. \qquad (7.17)'$$

Some of the distributions obtained above have been derived (e.g., Mapleton, 1966 and 1972; Abrines and Percival, 1966—see also the review by Percival and Richards, 1975) using elegant but conceptually more difficult approaches; these same authors also derived distributions in the radial velocity and in the square of the orbital angular momentum.

The fact that the states with $l\approx n\gg 1$ are classically describable is well ingrained, but many of us may have forgotten its justification. We therefore record the properties that, apart from numerical coefficients of order unity, we have $\langle r\rangle\approx n^2a_0/Z$, $\Delta r\approx n^{3/2}a_0/Z$, $\langle p\rangle\approx(Z\hbar/na_0)$, and $\Delta p\approx(Z\hbar/n^{3/2}a_0)$, so that the ratios $\Delta r/\langle r\rangle\approx n^{-1/2}$ and $\Delta p/\langle p\rangle\approx n^{-1/2}$ vanish for $n\sim\infty$, while $\Delta r\Delta p\approx\hbar$. It follows that r and p can be rather accurately specified without violating the uncertainty principle. (The difference in form of the uncertainty principle for radial and Cartesian coordinates and momenta can here be ignored.)

Classical physics is obviously applicable to three astronomical objects interacting gravitationally. The relevant process will here be mass transfer rather than charge transfer—one member of a binary will be captured by an incident star—but the analysis will be almost identical. We shall comment briefly on this in subsection VII.D.

B. Double scattering capture from high Rydberg states

The result obtained by Thomas (1927) for double scattering capture of a bound electron that initially lies within a thin spherically symmetric shell of radius a is

$$\sigma_{\rm ds}(a\to{\rm bd})\sim\frac{2^{13/2}\pi Z_A^2Z_B^{7/2}}{3}\left(\frac{e^2}{mv^2}\right)^{11/2}\frac{1}{a^{7/2}}\,. \qquad (7.18)$$

The numerical value of the right-hand side of Eq. (7.18) is unfortunately very sensitive to the value of a. If, in the study of $\sigma_{\rm ds}$ for capture from the $1s$ state of H, $1/a^{7/2}$ is replaced by $1/a_0^{7/2}$, as was done by Thomas, the resulting estimate for $1s\to$ bd capture is about an order of magnitude smaller than the second Born result, while if $1/a^{7/2}$ is replaced by the expectation value, with respect to the ground state, of $1/r^{7/2}$ the resulting estimate is infinite. Furthermore, the v^{-11} dependence of the Thomas result is not completely justified. Bates and Mapleton (1966) showed that, in the course of his analysis, Thomas approximated the probability for capture by an expression which exceeds unity for small values of r; modifications which are reasonable, if arbitrary, lead to a v^{-9} or a v^{-7} dependence.

Of course, the question of the asymptotic v dependence of the classical double scattering cross section for capture to a bound state from the ground state may very well be an ill-posed question since the ground state is not completely describable classically. On the other hand, high Rydberg states are describable classically and it might be expected that the Thomas result gives a very good estimate for double scattering capture to a bound state from a high Rydberg state. (For this to be true it is of course necessary that capture to a bound state occurs predominantly *to* high Rydberg states; this will be shown to be the case.) Indeed, the classical estimate of the double scattering cross section for $nl\to$ bd capture becomes *exact,* that is, equivalent to the quantum-mechanical results.

In this section we briefly repeat the analysis of Spruch (1978) to derive an expression for $\sigma_{\rm ds}(nl\to{\rm bd})$ which becomes identical to the Thomas result, Eq. (7.18) above, as n, l, and v become infinite, if a is set equal to n^2a_0/Z_A. En route, we obtain simple expressions for $\sigma_{\rm ds}(nl\to n'l')$ and $\sigma_{\rm ds}(nl\to n')$ which become exact as n, l, n', l', and v become infinite.

We start from the quantum result given in Eq. (5.15), that

$$\sigma_{\rm ds}(nl\to n'l')\sim C\int dr R_{nl}^2(r,Z_A)\rho_{n'l'}(r,Z_B)\,, \qquad (7.19a)$$

where

$$C\equiv Z_A^2Z_B^2 2^4\pi^2(e^8\hbar^3/m^7v^{11})\,, \qquad (7.19b)$$

and where

$$\rho_{n'l'}(r,Z_B)\equiv(2l'+1)R_{n'l'}^2(r,Z_B) \qquad (7.19c)$$

represents the sum over μ' of the probability densities associated with the states $n'l'\mu'$. It will be convenient to define

$$\rho_{n'}(r,Z_B)\equiv\Sigma_{l'}\rho_{n'l'}(r,Z_B) \qquad (7.20)$$

and

$$\rho_{\rm bd}(r,Z_B)\equiv\Sigma_{n'}\rho_{n'}(r,Z_B)\,. \qquad (7.21)$$

We can then write

$$\sigma_{\rm ds}(nl\to X)\sim C\int dr R_{nl}^2(r,Z_A)\rho_X(r,Z_B)\,, \qquad (7.22)$$

where X represents $n'l'$, n', or bd.

Since we are interested in $n\gg1$, we can use the WKB approximation for R_{nl} (Bethe and Salpeter, 1957). We then have

$$R_{nl}^2(r,Z_A)\approx\frac{2Z_A^2}{\pi n^3a_0r^2}\left(\frac{2Z_Aa_0}{r}-\frac{Z_A^2}{n^2}-\frac{(l+\frac{1}{2})^2a_0^2}{r^2}\right)^{-1/2}\cos^2Q(r)\,. \qquad (7.23)$$

The precise form of $Q(r)$ need not concern us, other than to observe that, on integrating over the allowed range of r and/or summing over l, $\cos^2Q(r)$ will average to $\frac{1}{2}$. The allowed range of r, the classical region, is defined by the turning points, that is, by the zeroes of the quantity in parentheses in Eq. (7.23). As expected, the turning points are at $a\pm c$, and we can write

$$r^2R_{nl}^2(r,Z_A)\,dr=(r/\pi a)\{[(a+c)-r][r-(a-c)]\}^{-1/2}\times[2\cos^2Q(r)]\,dr\,. \qquad (7.24)$$

We turn now to the estimation of $\rho_X(r,Z_B)$. For $n'\gg1$, $R_{n'l'}^2(r,Z_B)$ is given by Eq. (7.23) with n, l, and Z_A replaced by n', l', and Z_B, respectively, and $\rho_{n'l'}(r,Z_B)$ follows immediately. The values of n' and l' for which the classical approximation to $R_{n'l'}^2(r,Z_B)$ does not vanish are given by equations analogous to (7.10) and (7.11), that is,

$$(Z_Br/2a_0)^{1/2}\le n'\le\infty \qquad (7.25)$$

and

$$0\le\frac{(l'+\frac{1}{2})}{n'}\le\left(\frac{r}{a'}\right)^{1/2}\left\{2-\left(\frac{r}{a'}\right)\right\}^{1/2}\equiv\varepsilon_0'\,, \qquad (7.26)$$

where

$$a'\equiv n'^2a_0/Z_B\,. \qquad (7.27)$$

The summation over l' required to determine $\rho_{n'}(r,Z_B)$ contains many slowly varying terms; it is therefore legitimate to approximate the sum over l' by an integral over l'. We then introduce a new variable of integration, $\varepsilon'\equiv(l'+\frac{1}{2})/n'$, where $0\le\varepsilon'\le\varepsilon_0'$, with ε_0' defined by Eq. (7.26). We find

$$\rho_{n'}(r,Z_B)=n'^2\frac{2^{3/2}}{\pi r^{1/2}(a')^{5/2}}\left(1-\frac{r}{2a'}\right)^{1/2}\,, \qquad (7.28)$$

for $r<2a'$, with the range of n' given by Eq. (7.25).

Similarly, in evaluating $\rho_{\rm bd}$, we approximate the sum over n' by an integral, with limits given by Eq. (7.25). [For small r, n' can be small, but we shall be using an approximation to $R_{n'l'}$ which is valid only for $n'>1$; in fact, however, the relevant regions of r will be large if n is large, and the dominant contributions to $\sigma_{\rm ds}(nl\to{\rm bd})$ will come from large n'—indeed, from $n'\approx n\gg1$ (and $l'\approx l$) if Z_A and Z_B do not differ greatly.] One easily finds

$$\rho_{\rm bd}(r,Z_B)=(2/3\pi)(2Z_B/ra_0)^{3/2}\,. \qquad (7.29)$$

Having obtained relatively simple expressions for R_{nl} and for the ρ_X, we are now in a position to estimate $\sigma_{\rm ds}(nl\to X)$ for $n\sim\infty$, $v\sim\infty$, and, when n' appears in X, for $n'\sim\infty$. For simplicity, however, we shall restrict ourselves to the case $l\approx n\gg1$. R_{nl} will then be sharply peaked about $r=a=n^2a_0/Z_A$, and we can approximate $\rho_X(r,Z_B)$ by $(r^2/a^2)\rho_X(a,Z_B)$. Using the normalization property of R_{nl}, we immediately obtain, from Eq. (7.22),

$$\sigma_{\rm ds}(nl\to X)\sim C\rho_X(a,Z_B)/a^2\,, \qquad (7.29')$$

where C and the ρ_X are given by Eqs. (7.19b), the analogs of (7.19c) and (7.23), (7.28), and (7.29).

In particular, we have, for $l\approx n\gg1$,

$$\frac{\sigma_{\rm ds}(nl\to{\rm bd})}{\pi a_0^2}\sim\frac{2^{13/2}Z_B^{7/2}}{3n^7}\left(\frac{Z_Ae^2/mv^2}{a_0}\right)^{11/2}. \qquad (7.30)$$

In arriving at this result, we have used $a=n^2a_0/Z_A$.

There is no ambiguity in the choice of a, since we started from a proper quantum-mechanical basis, and we are concerned with $l \approx n \gg 1$. If we replace n by $(Z_A a/a_0)^{1/2}$ in Eq. (7.30) we obtain the Thomas result, Eq. (7.18).

It is not only the final $\sigma_{\rm ds}(nl \to {\rm bd})$ which has a classical interpretation. On setting $2\cos^2 Q(r)$ equal to unity in Eq. (7.24), this equation, which represents the probability of finding m between r and $r+dr$, becomes exactly the classical probability, given by Eq. (7.14). Further, since there are n'^2 states with principle quantum number n', the coefficient of n'^2 in Eq. (7.28) represents the probability density averaged over l' and μ' of an electron in the n'th shell; the result is identical to the classical result quoted by Mapleton (1972, p. 159).

The results deduced above go beyond the results derived by Thomas in a direct classical approach; we obtained $\sigma_{\rm ds}(nl \to {\rm bd})$, $\sigma_{\rm ds}(nl \to n')$, and $\sigma_{\rm ds}(nl \to n'l')$ as the classical limits of quantum expressions, while Thomas derived only $\sigma_{\rm ds}(nl \to {\rm bd})$. However, one can easily adapt Thomas' approach to derive $\sigma_{\rm ds}(nl \to n')$ in a direct classical manner. Thus Thomas required the relative velocity $\mathbf{v}_2 - \mathbf{v}$ of the emergent electron with respect to the incident nucleus to be below the escape velocity,

$$\tfrac{1}{2}m(\mathbf{v}_2 - \mathbf{v})^2 \leq Z_B e^2/r\,, \tag{7.31}$$

and the probability of capture into a bound state, which we shall denote by $P_{\rm bd}$, was proportional to the allowable volume in velocity space, $V_{\rm bd}$. This gives

$$P_{\rm bd} \propto V_{\rm bd} = (4\pi/3)(2Z_B e^2/mr)^{3/2}\,.$$

The probability $P_{n'}$ of capture into the state n', for all l' and μ', is proportional to the volume $V_{n'}$ in velocity space, defined by

$$\begin{aligned}\frac{Z_B e^2}{r} - \frac{Z_B^2 e^2}{2a_0 n'^2} &\leq \frac{m}{2}(\mathbf{v}_2 - \mathbf{v})^2 \\ &\leq \frac{Z_B e^2}{r} - \frac{Z_B^2 e^2}{2a_0(n'+1)^2} \\ &\approx \frac{Z_B e^2}{r} - \frac{Z_B^2 e^2}{2a_0 n'^2} + \frac{Z_B^2 e^2}{a_0 n'^3}\,.\end{aligned} \tag{7.32}$$

One can readily show that $V_{n'}/V_{\rm bd} = \rho_{n'}/\rho_{\rm bd}$. Since the cross sections calculated in the direct classical approach are proportional to the volumes, while the cross sections calculated as the classical limits of the exact quantum expressions are proportional to the ρ's, it follows that our adaptation of the escape velocity condition gives the correct result for $\sigma_{\rm ds}(nl \to n')$. One can probably also get $\sigma_{\rm ds}(nl \to n'l')$ and $\sigma_{\rm ds}(nl \to n'l'\mu')$ in a direct classical approach by imposing the conditions that the magnitude of the angular momentum vector of the emergent electron with respect to the incident nucleus, $m\mathbf{r} \times \mathbf{v}_2$, lie between $l'\hbar$ and $(l'+1)\hbar$, and that its projection along $\hat{v}$ lie between $\mu'\hbar$ and $(\mu'+1)\hbar$.

At the end of the next subsection we compare the various mechanisms for capture from a high Rydberg state.

C. Knock-on capture from high Rydberg states

In Sec. III we showed that $\sigma_{\rm ko}$ could be written as

$$\sigma_{\rm ko} = \int d\Omega P(\theta)\frac{d\sigma_{\rm bs}(\pi-\theta)}{d\Omega}\,, \tag{7.33}$$

where $P(\theta)$ is the conditional probability for m to be captured by M_B, assuming M_A and M_B to have backscattered with differential cross section $d\sigma_{\rm bs}(\pi-\theta)/d\Omega$ into the solid angle $d\Omega$ centered about π-θ.

Starting from Eq. (7.33) we now derive classically the cross section for knock-on capture from a high Rydberg state, assuming that the masses M_A and M_B are equal. To simplify the analysis we average over the initial magnetic quantum number μ and we sum over all final bound states. We utilize the simple concept of escape velocity. As in Sec. III, the differential backscattering cross section $d\sigma_{\rm bs}(\pi-\theta)/d\Omega$ may be factored out of the integral of Eq. (7.33) since it is roughly constant over the region $\theta \approx 0$ where $P(\theta)$ is non-negligible. (This will be justified below.) We therefore have

$$\sigma_{\rm ko}(nl \to {\rm bd}) \sim \frac{d\sigma_{\rm bs}(\pi)}{d\Omega}P(nl \to {\rm bd})\,, \tag{7.34a}$$

where

$$P(nl \to {\rm bd}) = \int P(\theta)d\Omega\,. \tag{7.34b}$$

In Sec. III, $P(\theta)$ was evaluated using the quantum-mechanical sudden approximation. However, capture from a high Rydberg state will be primarily *to* high Rydberg states if, as is the case since $M_A = M_B$, Z_A and Z_B do not differ greatly. [The overlap integral of Eq. (3.5) will be very small unless n' and l' are comparable to n and l.] We therefore expect to be able to evaluate $P(\theta)$ classically.

As a preliminary orientation we take m to be initially at rest relative to M_A, that is, we ignore its initial velocity distribution. In the frame S, in which the c.m. of M_A and M_B is at rest, m retains its initial velocity of $-\mathbf{v}/2$ during the nuclear collision, but M_B emerges with a speed $v/2$ at an angle π-θ, while M_A emerges with with a speed $v/2$ at an angle θ. (See Fig. 2). Thus, immediately after the nuclear collision m and M_B have a relative velocity of only $(v\theta/2)\hat{u}_\perp$, where $\hat{u}_\perp$ is a unit vector in the plane perpendicular to $\mathbf{v}$, while M_A has a velocity close to $\mathbf{v}$ with respect to either m or M_B. Shortly thereafter M_A will be far removed from m and M_B and unable to affect their motions. Thus m will be captured by M_B if and only if the relative velocity of m and M_B does not exceed their escape velocity. For a given value of the separation r or m and M_B at the time of the nuclear collision—we shall later average the probability $P(\theta; r)$ over r—we have

$$\begin{aligned}&P(\theta;r) = 1\,, \quad 0 \leq \theta \leq \theta_{\max}^{\rm cl}(r)\,,\\ &P(\theta;r) = 0\,, \quad \theta > \theta_{\max}^{\rm cl}(r)\,,\end{aligned} \tag{7.35}$$

where, for the atomic case under consideration, $\theta_{\max}^{\rm cl}(r)$ is defined by the *cl*assical escape velocity condition

$$\left(\frac{m}{2}\right)\left(\frac{v\,\theta_{\max}^{\rm cl}(r)}{2}\right)^2 = \frac{Z_B e^2}{r}\,. \tag{7.36}$$

Before proceeding further we note that, for r a characteristic atomic dimension, the maximum allowed backscattering angle $\theta^{\rm cl}_{\rm max}(r)$ defined by Eq. (7.36) can readily be shown to be roughly the upper limit $\theta_{\rm max}$ that appeared in the quantum analysis of knock-on capture. We note further that $\theta^{\rm cl}_{\rm max}(r)$ is proportional to $1/v$; this justifies the neglect of the variation of the differential backscattering cross section with θ that was used in arriving at Eq. (7.34a).

Since the r in Eq. (7.35) is the separation of m and M_B at the time of the nuclear collision, it is also the separation of m and M_A at that time, for M_A and M_B are very close during the collision. We therefore replace Eq. (7.34b) by

$$P(nl\to{\rm bd})=\left\langle\int P(\theta;r)d\Omega\right\rangle=\int\int P(\theta;r)R^2_{nl}(r)r^2dr\,d\Omega\,, \tag{7.37}$$

where, as indicated by the presence of $R_{nl}(r)$, the brackets signify the weighted average with respect to the initial spatial distribution of m. Using Eqs. (7.35) and (7.36) we have

$$\begin{aligned}P(nl\to{\rm bd})&=\left\langle\int_0^{\theta^{\rm cl}_{\rm max}(r)}2\pi\sin\theta d\theta\right\rangle\\&\sim\langle\pi(\theta^{\rm cl}_{\rm max}(r))^2\rangle\\&=\{8\}(\pi Z_Be^2/mv^2)\langle 1/r\rangle\\&=\{8\}(\pi Z_AZ_B\,e^2/n^2mv^2a_0)\,.\end{aligned} \tag{7.38}$$

We put the coefficient 8 in curly brackets to indicate that it is not the correct numerical coefficient; the correct coefficient will be given shortly.

If capture is to occur the maximum allowable momentum difference between m and M_B, after the nuclear scattering process has occurred, is of the order of the initial characteristic orbital momentum of m. It follows that the neglect of the initial velocity distribution, while leading to a meaningful and even qualitatively correct estimate of $P(nl\to{\rm bd})$, is not fully justified. (Note that in the double scattering process the momentum transferred to m is much larger than either the initial or final characteristic orbital velocity of m, and so the velocity distribution can be ignored.) We therefore repeat the analysis, this time taking into account the initial velocity distribution of m. Equation (7.34a) remains valid, but Eq. (7.34b) must be replaced by

$$P(nl\to{\rm bd})=\int P(\theta;{\rm v}_m,r(v_m))G(v_m)d^3v_md\Omega\,, \tag{7.39}$$

where $G(v_m)=g(v_m)/(4\pi v_m^2)$, where $g(v_m)$ is defined by Eq. (7.17), and where Eq. (7.35) must be replaced by

$$\begin{aligned}&P(\theta;{\rm v}_m,r(v_m))=1\quad\text{if }\frac{m}{2}\left(\frac{v\theta}{2}\hat{u}_\perp-{\rm v}_m\right)^2\le\frac{Z_Be^2}{r}\\&P(\theta;{\rm v}_m,r(v_m))=0\text{ otherwise};\end{aligned} \tag{7.40a}$$

$r(v_m)$ denotes the value of r obtained from the equation

$$\tfrac{1}{2}mv_m^2-(Z_Ae^2/r)=-Z_A^2e^2/(2a_0n^2)\,. \tag{7.40b}$$

The integration of Eq. (7.39), subject to Eq. (7.40a), is not difficult to perform. The details are given in Spruch and Shakeshaft (1979). It turns out that it is unnecessary to know the form of $g(v_m)$. The result of performing the integration, assuming for simplicity that $Z_A=Z_B\equiv Z$, is

$$P(nl\to{\rm bd})\sim(20/3)(\pi Z^2e^2/n^2mv^2a_0)\,. \tag{7.41}$$

Thus the effect of introducing the initial velocity distribution is to reduce $P(nl\to{\rm bd})$ by the factor 5/6.

With $M_A=M_B\equiv M$ the Coulomb backscattering differential cross section is $(Z_AZ_Be^2/Mv^2)^2$. Inserting this in Eq. (7.34a), and using Eq. (7.41) for $P(nl\to{\rm bd})$, gives, for $Z_A=Z_B\equiv Z$ and $M_A=M_B\equiv M$,

$$\frac{\sigma_{\rm ko}(nl\to{\rm bd})}{\pi a_0^2}\sim\left(\frac{20}{3}\right)Z^6\left(\frac{m}{M}\right)^2\left(\frac{1}{n^2}\right)\left(\frac{e^2}{\hbar v}\right)^6. \tag{7.42}$$

Replacing n by $(Za/a_0)^{1/2}$, Eq. (7.42) becomes

$$\sigma_{\rm ko}(a\to{\rm bd})\sim(20\pi/3)(Z^5e^6)/(M^2mv^6a)\,. \tag{7.43}$$

The only property of the initial state that enters this last expression is $1/a$, and, in this form, the result is independent of $\hbar$.

The above analysis differs in some mathematical details from a classical derivation of $\sigma_{\rm ko}(1s\to{\rm bd})$ given previously in a brief but interesting paper by Bates and Mapleton (1965)—see also Mapleton (1972)—but the underlying physics is the same. There is an important difference, however; one does not know how accurate a classical analysis of capture from the ground state for asymptotically high velocities will be, for there is no true classical picture of the 1s state, while one has every reason to believe that a classical analysis of capture from a high Rydberg state becomes exact as n, l, and v become infinite. The agreement between the quantum and classical results, Eqs. (6.1c) and (7.42), for $\sigma_{\rm ko}(1s\to{\rm bd})$ is quite good—the numerical coefficients are 6.86 and $20/3\approx6.66$, respectively—but there are reasons to believe this agreement to be at least partially fortuitous. There is also the matter of the velocity distribution to be used for the electron in its initial state. The appropriate velocity distribution to be used in an analysis of $\sigma_{\rm ko}(nl\to{\rm bd})$ is given by $g(v_m;a,c)$ of Eq. (7.17), which depends on c or, equivalently, on l. Only if one is interested in the average over l for a given n, that is, $\sigma_{\rm ko}(n\to{\rm bd})$, can one use the "$n$-shell velocity distribution" $g(v_m;a)$ of Eq. (7.17)′. The latter distribution is, of course, appropriate for $\sigma_{\rm ko}(1s\to{\rm bd})$. As it happens, the results are independent of the velocity distribution. These and some other points are discussed in more detail in the article mentioned above (Spruch and Shakeshaft 1979).

We conclude this subsection by comparing $\sigma_j(nl\to{\rm bd})$ for $j=$ko, rc, ds, and BK, and for n and l both large. $\sigma_{\rm BK}$ depends upon the high-momentum components of the initial state and therefore decreases with increasing l—as v^{-12-2l}—and can be neglected for l sufficiently large. $\sigma_{\rm rc}$ is independent of the initial state and capture occurs predominantly to the 1s state so that $\sigma_{\rm rc}(nl\to{\rm bd})\approx\sigma_{\rm rc}(1s\to1s)$, given by Eq. (6.2a); this equation does not become applicable until $v=C(Ze^2/\hbar)$ where C is of order 20, and where for the purpose of the present discussion we set $Z_A=Z_B\equiv Z$. Since for the double scattering and knock-on mechanisms capture occurs predominantly to states with $n'\approx n$ and $l'\approx l$, the asymptotic formulae for $\sigma_{ds}(nl\to \text{bd})$ and $\sigma_{ko}(nl\to\text{bd})$, Eqs. (7.30) and (7.42), become applicable when $v=C(Ze^2/\hbar n)$, and for this value of v we have

$$\sigma_{ds}(nl\to\text{bd})\sim(2^{13/2}/3)Z^{-2}n^4C^{-11}(\pi a_0^2)$$
$$\approx 10Z^{-2}n^4C^{-11}(\pi a_0^2) \quad (7.43')$$

and, with A the nuclear mass number,

$$\sigma_{ko}(nl\to\text{bd})\sim(20/3)(m/M)^2n^4C^{-6}(\pi a_0^2)$$
$$\approx 10^{-6}A^{-2}n^4C^{-6}(\pi a_0^2)\,. \quad (7.43'')$$

Note the n^4 factor. σ_{ds} and σ_{ko} are proportional to the area $\pi(n^2a_0)^2$. To evaluate $\sigma_{rc}(1s\to 1s)$ for $v=C(Ze^2/\hbar n)$ we should use the exact Fourier transform in Eq. (4.3). We expect σ_{rc} to be negligible in comparison with σ_{ds} and σ_{ko} at this v.

D. Capture of a gravitationally bound astronomical object

It is simple to adapt the preceding classical formulae for knock-on and double scattering charge transfer to "mass transfer" between astronomical objects. Thus in this subsection we suppose that an object of mass M_B captures an object of mass m which had initially been gravitationally bound to an object of mass M_A. We need merely make the replacements

$$Z_AZ_Be^2\to -GM_AM_B\,,\quad -Z_Ae^2\to -GM_Am\,,\ -Z_Be^2\to -GM_Bm\,,$$

where G is the gravitational constant. For $m\ll M_A$ and $m\ll M_B$, requirements for the validity of Eqs. (7.18) and (7.43)—in the latter equation we recognize that Z^5e^6/M^2 arose from $(Z_AZ_Be^2)^2(Z_Be^2)/(M_AM_B)$—we immediately obtain

$$\sigma_{ko}(a\to\text{bd})\sim\frac{20\pi}{3}\frac{G^3M^3}{v^6a}\,, \quad (7.44)$$

$$\sigma_{ds}(a\to\text{bd})\sim\frac{2^{13/2}\pi}{3}\frac{G^{11/2}M_A^2M_B^{7/2}}{a^{7/2}v^{11}}\,; \quad (7.45)$$

a is the semimajor axis of the ellipse defining the original motion of m and M_A, and we have averaged over all possible orientations of the ellipse. Note that both σ_{ko} and σ_{ds} are independent of m. This is because in both processes the probability for capture requires the relative kinetic energy of m and M_B after the last collision to be less, in absolute magnitude, than their gravitational potential energy, GmM_B/a, a condition for which m drops out if $m\ll M_B$; in the formula for σ_{ds} there are also two Coulomb (or, rather, gravitational) cross sections, which are again independent of m, since $m\ll M_A, M_B$. The formulae (7.44) and (7.45) would be applicable to the capture of a planet of mass m bound initially to a star of mass M_A by a second star of mass M_B incident at velocities much greater than a characteristic initial relative velocity of m and M_A.

A more interesting possible application is to the question of how a neutron star, believed to be the result of a violent collapse, can be the component of a binary. Even if the star which collapsed to become a neutron star had been the component of a binary, one would expect the formation of the neutron star to be sufficiently violent to impart to the neutron star a kinetic energy sufficient to break the binary bond. Nevertheless, an appreciable fraction of the known neutron stars are binary components. One possible explanation (Hills, 1976, 1977) is that a neutron star, born as an isolated star, can become a binary component by capturing one of a binary pair of ordinary stars. All of the formulae we have written down assume that one of the three masses is very much smaller than the other two, which would not here be the case, but the adaptation to the case of comparable masses is relatively trivial, involving only kinematic details. It may be important to note that if the mass of the incident neutron star is rather close to the mass of one of the binary components, knock-on capture could play a far more significant role relative to double scattering capture than in atomic physics, where the factor $(m/M)^2$ that appears in σ_{ko} is less than 10^{-6}.

Another possible application is to the determination of the stability of large clusters of stars. It is known that in the course of time the binding energies of individual binaries increase, and that eventually the cluster breaks apart. Elaborate numerical codes have been written to study excitation, breakup, and capture processes involving binaries and isolated stars. For example, more than ten thousand calculations were performed by Hills (1975). The scattering of a massive object (more massive than a star) by a binary consisting of massive objects has also been studied as a "gravitational slingshot" in analyses of the structure of extragalactic radio sources (Saslaw *et al.*, 1974); ten thousand calculations were performed. Although capture processes at asymptotically high velocities play only a very minor role in these applications—in the cluster problem, the dispersion in velocity of the stars is small and one would not expect to find many stars incident on binaries at very high velocities—a knowledge of the asymptotic forms of the cross sections does provide a stringent test of the accuracy of the numerical codes.

Numerical calculations in classical domains of atomic physics—and in domains for which the classical calculations might at least be suggestive—have also been performed (e.g., Abrines and Percival, 1966). Some dialogue between atomic physicists and astrophysicists on these matters might be fruitful.

VIII. CONCLUSION

We have studied three different mechanisms for the capture of a light particle at asymptotically high velocities. We have derived, in a heuristic fashion, the asymptotic form of the cross section for each mechanism, and we have ascertained the relative importance of the different mechanisms for electron capture from hydrogenlike "atoms." We have not, however, precisely stated the range of validity of the asymptotic expressions presented here. To obtain a lower limit on v we should have to examine the proper asymptotic expansion of the cross section, if indeed there is one. This would, of course, be a formidable task; it is difficult to obtain even an asymptotic expansion of an individual Born term, other than the first Born term. However, it is reasonable to expect that the asymptotic forms will become valid when v is between one and two orders of magnitude greater than the initial and final orbital ve-

TABLE I. An outline of some results on charge transfer. *Row* (1): the prototype reactions; the photon γ is, of course, emitted only in the radiative process. *Row* (2): the cross sections, integrated over all angles—though only certain regions are significant—for $1s \to 1s$ capture. See the equations referred to for the numerical coefficients, and for the Z_A and Z_B dependences in the extension to nuclei other than protons. Note that the coefficient of the double scattering $(e^2/\hbar v)^{11}$ term is less than 10^{-2} times the coefficient of the Brinkman–Kramers $(e^2/\hbar v)^{12}$ term, and that the coefficients of the v^{-6} term in the knock-on mechanism and of the v^{-5} term in the radiative mechanism contain $(m/M)^2$ and $(e^2/\hbar c)^3$, respectively, each of these factors being of order 10^{-6}. Section VI.A contains results for $1s \to n'$, $l' = n'-1$, and $1s \to$ bd capture. *Row* (3): the velocity dependences of the integrated cross sections for arbitrary initial and final states. *Row* (4): the exponent of v depends upon $l(l')$ if and only if the reaction requires high-momentum components of the initial (final) state. *Row* (5): the integrated cross sections for capture from a high Rydberg state, summed over all final bound states. Here $a = n^2 a_0$ is the semimajor axis of the elliptic orbit that the electron describes in the classical approximation. Note that, in the double scattering and knock-on mechanisms, capture from a high Rydberg state occurs predominantly *to* high Rydberg states. *Row* (6): the analog of row (5) for the transfer of a light astronomical object between two massive astronomical objects. *Row* (7): the location of the maximum in the angular distribution of the outgoing atom. *Row* (8): the *rough* widths of the peak in the angular distribution of the outgoing atom. See the text for the extension to nuclei other than protons.

Row	Item	Mechanisms: Knock-on ($M_A = M_B \equiv M$)	Double scattering (second Born)	Brinkman–Kramers ("first Born")	Radiative capture
1	Prototype reactions	$p + \mathrm{H}(nl) \to \mathrm{H}(n'l') + p + \{\gamma\}$ $p + \mathrm{H}(nl) \to \mathrm{H}(\mathrm{bd}) + p + \{\gamma\}$			
2	$\frac{\sigma(1s \to 1s)}{\pi a_0^2}$	$\left(\frac{m}{M}\right)^2 \left(\frac{e^2}{\hbar v}\right)^6$ See Eq. (6.1a)	$\left(\frac{e^2}{\hbar v}\right)^{11}$ See Eq. (6.3a)	$\left(\frac{e^2}{\hbar v}\right)^{12}$ See Eq. (6.4a)	$\left(\frac{e^2}{\hbar c}\right)^3 \left(\frac{e^2}{\hbar v}\right)^5$ See Eq. (6.2a)
3	v dependence for arbitrary n, l, n', l'	v^{-6}	v^{-11}	$v^{-(12+2l+2l')}$	$v^{-5-2l'}$
4	High-momentum components needed	None	None	In both initial and final states	In final state only
5	$\sigma(nl \to \mathrm{bd})$ for $n, l \gg 1$ (High Rydberg states)	$\frac{20\pi}{3} \frac{e^6}{M^2 m v^6 a}$	$\frac{2^{13/2}\pi}{3} \left(\frac{e^2}{mv^2}\right)^{11/2} \frac{1}{a^{7/2}}$	No reaction in classical limit. See l-dependence above.	Independent of n and l, and dominated by capture to $1s$ state; thus $\sigma_{\mathrm{rc}}(nl \to \mathrm{bd}) \approx \sigma_{\mathrm{rc}}(1s \to 1s)$
6	Analog of row (5) for gravitational astrophysical phenomena (for $m \ll M_A, M_B$)	$\frac{20\pi}{3} \frac{G^3 M^3}{v^6 a}$	$\frac{2^{13/2}\pi}{3} \frac{G^{11/2} M_A^2 M_B^{7/2}}{v^{11} a^{7/2}}$	No reaction	Gravitational radiation normally negligible
7	Location of maximum of $d\sigma/d\Omega$	π rad. (in c.m. frame)	$\left(\frac{m}{M_B}\right) \sin\left(\frac{\pi}{3}\right)$ rad. (in lab frame)	0°	0°
8	Width of peak of $d\sigma/d\Omega$	$\frac{e^2}{\hbar v}$	$\left(\frac{m}{M_B}\right) \left(\frac{e^2}{\hbar v}\right)$	$\frac{m}{M_B}$	$\left(\frac{m}{M_B}\right) \left[\left(\frac{v}{2c}\right) + \left(\frac{e^2}{\hbar v}\right)\right]$

locities of m. This expectation is partly substantiated by the fact that one can evaluate the Brinkman–Kramers cross section exactly and show that, for example, for ground-state to ground-state electron capture by protons from hydrogen atoms the asymptotic expression given in Eq. (6.4a) is accurate to within 5% when v is twenty times greater than the Bohr velocity. Further evidence is provided in the case of radiationless forward capture by a comparison of the $1/v^{11}$ term with the $1/v^{12}$ term obtained from the first three Born terms, again for the reaction $\mathrm{H}^+ + \mathrm{H}(1s) \to \mathrm{H}(1s) + \mathrm{H}^+$; the $1/v^{11}$ term dominates over the $1/v^{12}$ term when v is about eighty-three times greater than the Bohr velocity. To obtain an upper limit on v we should have to examine relativistic and particle production effects. This again is a formidable task. Mittleman (1964) has generalized the Brinkman–Kramers approximation for $\mathrm{H}^+ + \mathrm{H}(1s) \to \mathrm{H}(1s) + \mathrm{H}^+$ to the relativistic domain and finds that relativistic corrections are about 3% at 10 MeV (at which energy v is about 20 times the Bohr velocity.) Raisbeck and Yiou (1971), using the known cross section for the relativistic photoelectric effect, have generalized the cross section for the radiative ground-state recombination of electrons and protons to the relativistic domain; using their expression, after correcting some obvious misprints,[11] we find that relativistic corrections are less

[11]The correct expression is simply a factor of $k^2/[(k+\mu)^2 - \mu^2]$ times the cross section for the relativistic photoelectric effect, where this cross section, and k and μ, are given by Eq. (17), Sec. 21, of Heitler (1954).

than 3% at 10 MeV.

In Table I we summarize some of the salient features of the various mechanisms for electron capture from a hydrogenlike atom by a bare ion. It is worth recalling here the origin of the dependences upon the velocity v shown in row (3) of the table. σ_{ko} factors into the Coulomb differential cross section $d\sigma_{bs}(\pi)/d\Omega$ for the nuclei to backscatter, which is proportional to $1/v^4$, and a conditional probability of capture, which is proportional to the solid angle $2\pi(\theta_{max}^2/2)$ of a cone with semiangle θ_{max}; the angle of scattering in the c.m. frame is $\pi-\theta$. θ_{max} is defined by the requirement that the maximum relative velocity of m and M_B after the nuclear scattering process, $v\theta_{max}/2$, be less than the escape velocity, which is v independent, and it follows that θ_{max} behaves as $1/v$ and therefore that the solid angle behaves as $1/v^2$. σ_{ds} contains as factors the product of two Rutherford 60° scattering differential cross sections, each proportional to $1/v^4$, and also contains a conditional probability of capture that is proportional both to the solid angle $d\Omega$ into which the electron must emerge after its second scattering if it is to be captured and to the volume element within which the electron must initially lie; the volume element is proportional to $1/v$ [see Eq. (5.7)] while the solid angle, as for knock-on, is proportional to $1/v^2$. Treating radiative capture as radiative recombination, σ_{rc} is the product of $1/F \propto 1/v$, where F is the incident electron flux, and the rate Γ for recombination. Γ is proportional to the density of final states, to $1/\omega$, and to the square of the matrix element of the current and therefore velocity operator. The density of final states is proportional to ω^2, and therefore to v^4 since ω is proportional to v^2, and the matrix element of the velocity operator is proportional to v multiplied by $\tilde{\psi}_f(m\mathbf{v}/\hbar)$, the latter behaving as $1/v^{4+l'}$. See the discussion of Appendix D for the origin of the v dependence of σ_{BK}. In that mechanism there is a single three-body collision, and the physical interpretations require rather more care.

It is also worth recalling the roles of the high-internal-(or orbital-) momentum components of the initial and final states. They play no role for either double scattering or knock-on. In the Brinkman–Kramers mechanism the high-momentum components of both the initial and final states are crucial but in radiative capture only the high-momentum components of the final state are crucial—the initial state, and therefore its high-momentum components, plays no role in the determination of σ_{rc}.

In the knock-on and double scattering mechanisms the matrix element for capture involves a product of the initial and final coordinate space wave functions, so that n' and l' must be roughly equal to n and l, respectively, if the matrix element is to be significant. That $\sigma_{ko}(nl\to bd)$ and $\sigma_{ds}(nl\to \text{bd})$ have classical limits for n and $l\sim\infty$ (with the main contribution coming from n' and $l'\sim\infty$) is a reflection of the fact that these reactions proceed without the requirement of high-momentum components, components not possessed by classically describable states of high quantum numbers. The situation is different for the Brinkman–Kramers and radiative mechanisms. For these mechanisms capture occurs predominantly to the 1s state, regardless of the initial quantum numbers n and l. This is because capture occurs to the high-momentum components of the final state, and for the electron to finally have a high momentum it must be close to the projectile nucleus, which is most likely if the final state is a 1s state. Note that for large l' the electron spends little time near the projectile nucleus. In the Brinkman–Kramers mechanism the electron must also have high momentum initially, and $\sigma_{BK}(nl\to \text{bd})$ decreases with increasing v as $1/v^{12+2l}$ and vanishes in the classical limit n, $l\to\infty$.

Accurate measurements of the cross section for electron capture from hydrogenlike "atoms" by bare ions are difficult to perform at high impact velocities. However, as discussed above, it might be feasible to measure cross sections for electron capture from helium atoms or hydrogen molecules. Such experiments might shed more light on the asymptotic form of the cross section, and lead to a better understanding of capture processes.

Notes added in proof:

(1) More and more people are using a notation with the subscripts P and T denoting projectile and target, respectively. We apologize for not having used this more descriptive notation.

(2) The two-step dielectronic recombination process mentioned in Sec. IV *is* important—see Y. Hahn, 1978, Phys. Lett. **67A**, 345.

(3) Bates *et al.* (1964) extended the Thomas double-scattering model and predicted, in particular, that H_2^+ ions would emerge from the reaction $H^+ + CH_4 \to H_2^+ + CH_3$ at an angle of about 45° relative to the beam direction for a beam energy above about 75 eV. This was strikingly verified in an experiment by C. J. Cook, N. R. A. Smyth, and O. Heinz, 1975, J. Chem. Phys. **63**, 1218. Note that the "orbital" (actually vibrational) velocity of the active H atom is small in both the initial and final states, and consequently the beam velocity need not be high for the picture to be valid. The classical estimate of the integrated cross section is about a factor of 10 larger than the experimental result; we stress again that a purely classical analysis of double scattering need not be valid unless the initial and final states are classically describable.

(4) In Sec. VI.C we suggested a coincidence experiment to look for a peak in the angle and energy of electrons ejected from He targets. This experiment was independently suggested, and is now being performed, by E. Horsdal Pederson at Aarhus. A quantum-mechanical calculation of the process was recently completed by J. S. Briggs and K. Taulbjerg (J. Phys. B, 1979, in press).

(5) Recent reviews include "Electron capture in high-energy ion-atom collisions," by Dz Belkić, R. Gayet, and A. Salin, scheduled to appear in Physics Reports, July, 1979; "Electron capture processes in ion-atom collisions," by D. Basu, S. C. Mukherjee, and E. P. Sural, 1978, Physics Reports **42C**, 147, and B. H. Bransden, Physicalia, to be published.

IX. ACKNOWLEDGMENTS

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APPENDIX A: IMPACT-PARAMETER DEPENDENCE OF RADIATIVE CAPTURE

We here briefly sketch a proof which shows that Eq. (4.5) of the present paper can also be derived (though very much less directly) starting with Eq. (9) of Briggs and Dettmann (1974). Let A be the amplitude for the capture of an electron, initially attached to M_A in state i, into state f attached to M_B, with the concomitant emission of a photon of polarization $\hat{\lambda}$ and propagation $\mathbf{k}$; M_B is incident with an impact parameter $\mathbf{b}$. In the dipole approximation, and neglecting the difference between the initial and final binding energies, Eq. (9) of Briggs and Dettmann (1974) is, in our notation,

$$A = e(\hbar\omega)^{-1/2}(\hat{\lambda}\cdot\mathbf{v})\tilde{\psi}_f(-m\mathbf{v}) \times \int d^3p\; \delta\left(\omega - \frac{\frac{1}{2}mv^2}{\hbar} + \frac{\mathbf{p}\cdot\mathbf{v}}{\hbar}\right) e^{i\mathbf{p}\cdot\mathbf{b}/\hbar}\tilde{\psi}_i(\mathbf{p})\,. \tag{A1}$$

We use Eq. (2.1) and the representation

$$\delta(vg) = \left(\frac{1}{v}\right)\delta(g) = \left(\frac{1}{2\pi v}\right)\int_{-\infty}^{\infty} dz' e^{igz'}$$

with

$$g = \frac{(\omega - \frac{1}{2}mv^2/\hbar + \mathbf{p}\cdot\mathbf{v}/\hbar)}{v}$$

to perform the integration over $\mathbf{p}$ in Eq. (A1) and obtain, after integrating over $\mathbf{r}$ and replacing z' by z,

$$A = \left(\frac{2\pi}{\omega}\right)^{1/2}\left(\frac{e\hbar}{v}\right)(\hat{\lambda}\cdot\mathbf{v})\tilde{\psi}_f(-m\mathbf{v})\int_{-\infty}^{\infty} dz\, e^{i(\omega/v - mv/2\hbar)z}\psi_i(b, z)\,. \tag{A2}$$

For radiative capture, the differential cross section with respect to impact parameter is given by

$$\frac{d\sigma_{\rm rc}}{db} = 2\pi b\int d^3k \sum_{\hat{\lambda}} |A|^2\,. \tag{A3}$$

Using

$$\int d^3k \sum_{\hat{\lambda}} (\hat{\lambda}\cdot\mathbf{v})^2 \ldots = \left(\frac{8\pi v^2}{3c^3}\right)\int_0^{\infty} \omega^2 d\omega \ldots$$

and using Eq. (A1) for A and the complex conjugate of Eq. (A2) for A^*, Eq. (4.5) follows from Eq. (A3) on integrating first over ω and then over $\mathbf{p}$. [In the last integration over $\mathbf{p}$ we neglect $\mathbf{p}\cdot\mathbf{v}$ in comparison with $\frac{1}{2}mv^2$ since $\tilde{\psi}_i(\mathbf{p})$ restricts the range of $\mathbf{p}$ and since $\mathbf{v}$ is large compared to the characteristic initial internal velocity.]

The impact-parameter dependence of the radiative capture cross section was also derived in a recent paper by Briggs and Dettmann (1977).

APPENDIX B: FURTHER REMARKS ON THE JUSTIFICATION OF THE DOUBLE SCATTERING ANALYSIS

We here remark further on the use of two volumes, $d\tau_1$ and $d\tau_1'$, to describe the initial location of m in the double scattering process. As indicated in Fig. 4, two of the linear dimensions of $d\tau_1$, in the half-plane defined by a fixed value of ϕ_A, are of order db. [We need not have chosen the dimension parallel to $\mathbf{v}$ to be equal to db. If we call this dimension db', we want db' large compared to $\hbar/M_Bv$ and small compared to b and to the dimensions of the "atoms" $(m+M_A)$ and $(m+M_B)$. Subject to these restrictions, restrictions which we can assume to be satisfied by db, the final answer will be independent of our choice of db'.] Now $d\phi_A$ is the spread in the azimuthal angle ϕ_A that helps define $d\tau_1$. The dimension of $d\tau_1$ in the direction perpendicular to the half-plane is therefore $bd\phi_A$; choosing $d\phi_A = db/b$, this dimension will also be of order db. (Once again, our choice is a matter of convenience. There is some latitude in the choice of $d\phi_A$, a latitude which in no way will affect the final answer.) The wave packet describing m immediately after the first collision will therefore have a spread db in each dimension. Because of the restrictions imposed upon db, a spread db leads to a spread in the velocity $\mathbf{v}_1$ of magnitude small compared to v, so that there is no violation whatever of the uncertainty principle in stating that m travels in a rather well-defined path between collisions. We turn now to the much smaller volume $d\tau_1'$. Two of its dimensions are of order db, but its third dimension (see Fig. 4) is of order $bd\alpha_1$, that is, of order bdv_1/v. If m is to reach some given point Q on $d\sigma_2$, for a given location of $d\sigma_2$, then m must originate at some point P in $d\tau_1'$. If we really knew that m originated in $d\tau_1'$ there would be an inconsistency, for then the component of the quantum-mechanical uncertainty in $\mathbf{v}_1$ in the direction perpendicular to $\hat{v}_1$ could not be much less than v. But we do not know exactly where $d\sigma_2$ is; the center of $d\sigma_2$ can be anywhere on a circle centered on M_A and with a radius of order $C\hbar/mv$, where C is rather large compared to 1. Thus, although in calculating the probability of m passing through the point Q we can assume the point P to be in $d\tau_1'$ and write $P_{\rm loc} = |\psi_i|^2 d\tau_1'$, the volume $d\tau_1'$ can be anywhere within $d\tau_1$ and all we actually know about the location of P is that it lies within $d\tau_1$. The whole scheme is made consistent by choosing db to be $db = C(\hbar/mv)$, where C, the constant defined just above, is independent of v, and large compared to 1. The exact value chosen for C plays no role, but to be concrete let us consider $C = 100$. We then have $d\tau_1 = 100 d\tau_1'$. More significantly, each dimension of $d\tau_1$ is of order db

$=100(\hbar/mv)$, so that the uncertainty in any component of the velocity of the wave packet emerging after the first collision is $\hbar/mdb=v/100$, which, as required, is rather small compared to v.

One further remark about the two volumes is essential. Since each linear dimension of the wave packet that emerges from the first collision is of order db, each linear dimension of the wave packet that emerges from the second collision will also be of order db. This latter wave packet therefore has linear dimensions small compared to b and to the linear dimensions of the "atom" $(m+M_B)$ but large enough for the magnitude of the spread in the velocity $\mathbf{v}_2$ to be small compared to v. These last two facts allow $P_{\rm cap}$ to be evaluated in the manner of Sec. V.B.6.

APPENDIX C: MATHEMATICAL DERIVATION OF $d\sigma_{\rm ds}/db$

We sketch, very briefly, a mathematical derivation of Eq. (5.12), the asymptotic expression for $d\sigma_{\rm ds}/db$.

Let $\hbar\mathbf{K}$ be the difference between the final momentum of the system M_B+m multiplied by $M_B/(m+M_B)$ and the initial momentum of the projectile (that is, the "average" final momentum less the initial momentum of the projectile). With $K=|\mathbf{K}|$, let $A_{\rm ds}(K)$ denote the full quantum-mechanical second-order Born amplitude for capture from a bound state i to a bound state f. The asymptotic form of $A_{\rm ds}(K)$ for $H^+ + H(1s) \rightarrow H(1s) + H^+$ was first derived by Drisko (1955). Drisko's result was generalized by Dettmann and Liebfried (1969) and Dettmann (1971) to cover a large class of interactions, but with the initial and final states isotropic. An expression which is valid for arbitrary initial and final states was given by Shakeshaft (1978b); we start with this expression here, but with many notational changes.[12] We have

$$\sigma_{\rm ds}=(2\pi\hbar^2v^2)^{-1}\int_{q/2}^{\infty}|A_{\rm ds}(K)|^2K\,dK\,,$$

where

$$A_{\rm ds}(K)\sim -i(2\pi)^3\hbar m\tilde{W}_A(\hbar K)\tilde{W}_B(\hbar K)\times\int_0^{\infty}ds\,e^{i/2\,Ds}\psi_f^*(-s\mathbf{T})\psi_i(s\mathbf{K})\,, \qquad \text{(C1)}$$

where we have neglected corrections of the order of m/M_A and m/M_B, and where

$$\mathbf{T}\equiv\mathbf{q}+\mathbf{K}\,,\quad \mathbf{q}\equiv m\mathbf{v}/\hbar\,,\quad D\equiv q^2-K^2\,, \qquad \text{(C2)}$$

with $q=|\mathbf{q}|$. The second-order Born amplitude, $A_{\rm ds}(b)$, in the impact-parameter representation (see, for example, Wilets and Wallace, 1968) is

$$A_{\rm ds}(b)\sim i^{\nu}\frac{1}{2\pi\hbar v}\int_0^{\infty}K_\perp dK_\perp J_\nu(bK_\perp)A_{\rm ds}(K)\,, \qquad \text{(C3)}$$

where $\nu=\mu-\mu'$ is the difference between the final and initial magnetic quantum numbers, and where $K_\perp=\hat{u}_\perp\cdot\mathbf{K}$, the projection of $\mathbf{K}$ on a unit vector $\hat{u}_\perp$ perpendicular to $\hat{v}$. It follows from energy and momentum conservation that $\hat{v}\cdot\mathbf{K}=-\frac{1}{2}q$ (plus a term of order $e^2/\hbar v$, which we neglect) and therefore $\hat{v}\cdot\mathbf{T}=\frac{1}{2}q$, $K=(K_\perp^2+q^2/4)^{1/2}$, and $D=(3/4)q^2-K_\perp^2$. Now for "most" values of $K_\perp$, D is proportional to v^2 and so the integrand of Eq. (C1) is highly oscillatory. Therefore $A_{\rm ds}(K)$ is largest when $D=0$, that is, when $K_\perp=K_{\perp C}\equiv(3^{1/2}/2)q$ $(=q\sin\frac{1}{3}\pi$, the value of $K_\perp$ corresponding to the critical angle). Hence the main contribution to the integral over $K_\perp$ in Eq. (C3) comes from the region near $K_\perp=K_{\perp C}$, and, since most of the contribution to $\sigma_{\rm ds}$ comes from $b\gg\hbar/mv$, we have $bK_\perp\gg1$. We can therefore replace the Bessel function by its asymptotic form and we obtain, combining Eqs. (C1) and (C3),

$$A_{\rm ds}(b)\sim -2i^{\nu+1}(2\pi)^{3/2}\left(\frac{m}{vb^{1/2}}\right)\int_0^{\infty}dK_\perp\int_0^{\infty}ds\,K_\perp^{1/2}\times\tilde{W}_A(\hbar K)\tilde{W}_B(\hbar K)\psi_f^*(-s\mathbf{T})\psi_i(s\mathbf{K})\exp(\tfrac{1}{2}iDs)\times\cos(bK_\perp-\tfrac{1}{2}\nu\pi-\tfrac{1}{4}\pi)\,, \qquad \text{(C4)}$$

where $\mathbf{K}=-\frac{1}{2}\mathbf{q}+K_\perp\hat{u}_\perp$. Interchanging the order of integration and performing the integration over $K_\perp$ using the method of stationary phase (the point of stationary phase is $K_\perp=b/s$) we obtain[13]

$$A_{\rm ds}(b)\sim-(2\pi)^2\frac{m}{v}\int_0^{\infty}ds\left(\frac{1}{s}\right)\tilde{W}_A(\hbar K)\tilde{W}_B(\hbar K)\times\psi_f^*(-s\mathbf{T})\psi_i(s\mathbf{K})\exp\left[i\left(\frac{3}{8}\right)q^2s+i\left(\frac{b^2}{2s}\right)\right]\,, \qquad \text{(C5)}$$

where now $\mathbf{K}=-\frac{1}{2}\mathbf{q}+(b/s)\hat{u}_\perp$. The method of stationary phase may again be used to evaluate this last integral over s. The point of stationary phase is $s=b/K_{\perp C}$ and therefore $K_\perp=K_{\perp C}$, $\hbar K=mv$, and $\hbar|\mathbf{T}|=mv$. It follows that

$$\mathbf{K}=-\tfrac{1}{2}q\hat{u}_z+K_{\perp C}\hat{u}_\perp\,,$$

and hence that $s\mathbf{K}=(b/K_{\perp C})\mathbf{K}=\mathbf{r}_{A1}$. Similarly, at the point of stationary phase, $-s\mathbf{T}=\mathbf{r}_{B2}$. Integrating over s and using $d\sigma_{\rm ds}/db=2\pi b|A_{\rm ds}(b)|^2$ we obtain Eq. (5.12).

APPENDIX D: SOME DIFFERENT ASYMPTOTIC FORMS FOR THE RADIATIONLESS FORWARD CAPTURE CROSS SECTION

Radiationless forward capture at high impact velocities has been treated in a variety of approximations, each leading to a different asymptotic form for the cross section. In this appendix we present, along with a few brief remarks, five different estimates of the asymptotic form of the cross section for ground-state to ground-state radiationless forward electron capture by protons from hydrogen atoms. We use atomic units. The modified Bessel function $K_n(x)$ is defined as $(\frac{1}{2}\pi i)\exp(\frac{1}{2}in\pi)H_n^{(1)}(x)$, where $H_n^{(1)}(z)$ is the Hankel function of the first kind.

Brinkman–Kramers approximation (Brinkman and Kramers, 1930; see McDowell and Coleman, 1970)

[12]Note the misprint in Eq. (3.8e) of Shakeshaft (1978b); the 2 should be deleted in the term $\hbar^2\beta\mathbf{K}_f/2\nu_A$.

[13]The integral of Eq. (C5) may diverge at its lower limit. This can be avoided by replacing the lower limit on s in Eq. (C4) by a small positive quantity.

$$d\sigma/db \sim 2^7\pi b^5 v^{-6}[K_2(bv/2)]^2\,, \tag{D1a}$$

$$\sigma \sim (2^{18}\pi/5)v^{-12}\,. \tag{D1b}$$

First Born approximation (Jackson and Schiff, 1953)

$$d\sigma/db \sim 2^7\pi b v^{-10}[(bv)^2K_2(\tfrac{1}{2}bv) - 4K_0(\tfrac{1}{2}bv)]^2\,, \tag{D2a}$$

$$\sigma \sim (127/192)(2^{18}\pi/5)v^{-12}\,. \tag{D2b}$$

As opposed to the Brinkman–Kramers approximation, the first Born approximation includes the proton–proton interaction.

Second Born approximation (Drisko, 1955)

$$d\sigma/db \sim (2^9\pi^2/\sqrt{3})v^{-11}\exp(-8b/\sqrt{3})\,, \tag{D3a}$$

$$\sigma \sim 2^6\pi^2 v^{-11}\,. \tag{D3b}$$

Continuum distorted-wave approximation (Cheshire, 1964)

$$\frac{d\sigma}{db} \sim \left(\frac{2^9\pi^2}{\sqrt{3}}\right)v^{-11}\left(1-\frac{2b}{\sqrt{3}}\right)^2\exp\left(\frac{-4b}{\sqrt{3}}\right)\,, \tag{D4a}$$

$$\sigma \sim 2^6\pi^2 v^{-11}\,. \tag{D4b}$$

Variational continuum distorted-wave approximation (Shakeshaft, 1974c)

$$\frac{d\sigma}{db} \sim \left(\frac{2^9\pi^2}{\sqrt{3}}\right)v^{-11}\left(1+\frac{2b}{\sqrt{3}}\right)^{-2}\exp\left(\frac{-4b}{\sqrt{3}}\right)\,, \tag{D5a}$$

$$\sigma \sim 2^6\pi^2\Gamma v^{-11}\,. \tag{D5b}$$

where $\Gamma = 4\exp(2.0)E_2(2.0) = 1.109$, and where $E_2(x)$ is the exponential integral.

Note that the differential cross sections in Eqs. (D3a)–(D5a) are the same through terms of order b. Note also that the total cross sections in Eqs. (D3b) and (D4b) are identical; however, this is fortuitous, and the continuum distorted-wave approximation would seem to be inadequate even at very high velocities. (See also the recent discussion of Belkić, 1977).

The modified Bessel functions $K_0(x)$ and $K_2(x)$ decrease exponentially as x increases. Therefore only the narrow range of impact parameters $b \lesssim 1/v$ contributes significantly to the total cross section in the Brinkman–Kramers and first Born approximations. This can be understood as follows. Consider the "prior" form of the Brinkman–Kramers approximation in which the perturbation is the interaction of the electron with the incident nucleus. Momentum is transferred only between m and M_B, and for capture to occur momentum and energy conservation require that the initial velocity of m relative to the target nucleus M_A be roughly $\frac{1}{2}\mathbf{v}$. Therefore there can be a significant probability of capture only if m happens to be within a distance of order $\hbar/mv$ from M_A. (We use arbitrary units now.) For capture to occur m must receive an impulse of order $\frac{1}{2}m\mathbf{v}$ from M_B, and this requires almost a direct collision between m and M_B; more precisely, M_B must pass within a distance of order $\hbar/mv$ from m, and hence from M_A. Therefore only the range of impact parameters $b \lesssim \hbar/mv$ is significant. Similar arguments can be given for the "post" form of the Brinkman–Kramers approximation and both the "post" and "prior" forms of the first Born approximation.

Although only a single collision is involved in the Brinkman–Kramers approximation, this collision is not a binary one since the effect of the third particle cannot be ignored. (The collision takes place far off the energy shell.) Without going into details, the v dependence of σ_{BK} can be understood as follows: The probability for m to have an initial velocity of roughly $\frac{1}{2}\mathbf{v}$ relative to M_A is proportional to $|\tilde{\psi}_i(m\mathbf{v}/2)|^2$, which, for pure Coulomb interactions, behaves as $1/v^{8+2l}$; the Coulomb differential cross section for m to receive an impulse of roughly $\frac{1}{2}m\mathbf{v}$ behaves as $1/v^4$; the probability for m to be finally at a distance of roughly $\hbar/mv$ from M_B is proportional to $|\psi_f(\hbar\hat{r}/mv)|^2$, which, for pure Coulomb and other interactions, behaves as $1/v^{2l'}$. Multiplying these three factors together gives σ_{BK} proportional to $1/v^{12+2l+2l'}$.

There are many other approximations for treating electron capture besides the ones mentioned above. The last comprehensive review was given by Bransden (1972). Since that review a number of interesting papers have been written. In particular, Kramer (1972) has evaluated the second Born terms essentially exactly by numerical integration, and Briggs (1977) has resolved a longstanding discrepancy between the asymptotic forms of the cross section obtained in the impulse and second Born approximations. Some other approximations are discussed by Chen *et al.* (1971), Chen and Kramer (1972), Shastry *et al.* (1972), Kleber and Nagarajan (1975), Das (1976), Dewangan (1977), and Belkić (1977). A combined use of the Brinkman–Kramers and the Drisko second Born approximation in the analysis of the production of inner shell vacancies via capture was recently made by Lapicki and Losonsky (1977).

REFERENCES

Aaron, R., R. D. Amado, and B. W. Lee, 1961, Phys. Rev. **121**, 319.

Abramowitz, M., and I. Stegun, 1970, *Handbook of Mathematical Functions* (Dover, New York).

Abrines, R., and I. C. Percival, 1966, Proc. Phys. Soc. Lond. **88**, 861.

Bates, D. R., and R. McCarroll, 1958, Proc. R. Soc. A **245**, 175.

Bates, D. R., C. J. Cook, and F. J. Smith, 1964, Proc. Phys. Soc. Lond. **83**, 49.

Bates, D. R., and R. A. Mapleton, 1965, Proc. Phys. Soc. Lond. **85**, 605.

Bates, D. R., and R. A. Mapleton, 1966, Proc. Phys. Soc. Lond. **87**, 657.

Belkić Dž., 1977, J. Phys. B **10**, 3491.

Bethe, H. A., and E. E. Salpeter, 1957, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic, New York), p. 322.

Bohr, N., 1948, K. Dan Vidensk. Selsk. Mat.-Fys. Medd. **18**.

Bonham, R. A., 1972, J. Chem. Phys. **57**, 1604.

Bransden, B. H., 1972, Rep. Prog. Phys. **35**, 949.

Briggs, J. S., 1977, J. Phys. B **10**, 3075.

Briggs, J. S., and K. Dettmann, 1974, Phys. Rev. Lett. **33**, 1123.

Briggs, J. S., and K. Dettmann, 1977, J. Phys. B **10**, 1113.

Briggs, J. S., and L. Dube, 1978, J. Phys. B, to be published.

Brinkman, H. C., and H. A. Kramers, 1930, Proc. K. Ned. Akad. Wet. **33**, 973.

Bussard, R. W., R. Ramaty, and K. Omidvar, 1978, Astrophys. J. **220**, 353.
Chen, J. C. Y., A. C. Chen, and P. J. Kramer, 1971, Phys. Rev. A **4**, 1982.
Chen, J. C. Y., and P. J. Kramer, 1972, Phys. Rev. A **5**, 1207.
Cheshire, I. M., 1964, Proc. Phys. Soc. Lond. **84**, 89.
Corbett, J. F., 1968, J. Math. Phys. **9**, 891.
Das, J. N., 1976, J. Phys. B **9**, L539.
Dettmann, K., 1971, Springer Tracts Mod. Phys. **58**, 119.
Dettmann, K., K. G. Harrison, and M. W. Lucas, 1974, J. Phys. B **7**, 269.
Dettmann, K., and G. Leibfried, 1966, Phys. Rev. **148**, 1271.
Dettmann, K., and G. Leibfried, 1969, Z. Phys. **218**, 1.
Dewangan, D. P., 1977, J. Phys. B **10**, 1083.
Dirac, P. A. M., 1958, *The Principles of Quantum Mechanics* (Clarendon, Oxford), 4th edition, p. 244.
Drisko, R. M., 1955, Ph.D. thesis, Carnegie Institute of Technology, unpublished.
Gardner, L. D., 1978, Ph.D. thesis, Yale University, unpublished.
Gradshteyn, I. S., and I. W. Ryzhik, 1965, *Tables of Integrals, Series, and Products*, translated by Scripta Technica Inc., edited by A. Jeffrey (Academic, New York), 4th edition.
Halpern, A. M., and J. Law, 1973, Phys. Rev. Lett. **31**, 4.
Heitler, W., 1954, *The Quantum Theory of Radiation* (Clarendon, Oxford), 3rd edition.
Hills, J. G., 1975, Astron. J. **80**, 809.
Hills, J. G., 1976, Mon. Not. R. Astr. Soc. **175**, p. 1.
Hills, J. G., 1977, Astron. J. **82**, 626.
Jackson, J. D., and H. Schiff, 1953, Phys. Rev. **89**, 359.
Joachain, C. J., 1977, Comments At. Mol. Phys. **6**, 69.
Kleber, M., and D. Jakubassa, 1975, Nucl. Phys. A **252**, 152.
Kleber, M., and M. A. Nagarajan, 1975, J. Phys. B **8**, 643.
Kramer, P. J., 1972, Phys. Rev. A **6**, 2125.
Lapicki, G., and W. Losonsky, 1977, Phys. Rev. A **15**, 896.
LeBellac, M., and J. M. Levy-LeBlond, 1973, Nuovo Cimento B **14**, 217.
Macek, J., 1970, Phys. Rev. A **1**, 235.
Mapleton, R. A., 1964, Proc. Phys. Soc. Lond. **83**, 895.
Mapleton, R. A., 1966, Proc. Phys. Soc. Lond. **87**, 219.
Mapleton, R. A., 1972, *Theory of Charge Exchange* (Wiley, New York).
May, R. M., 1964, Phys. Rev. A **136**, 669.
McDowell, M. R. C., and J. P. Coleman, 1970, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam).
McGuire, J. H., 1973, Phys. Rev. A **8**, 2760.
Mittleman, M. H., 1964, Proc. Phys. Soc. Lond. **84**, 453.
Oppenheimer, J. R., 1928, Phys. Rev. **31**, 349.
Percival, I. C., and D. Richards, 1975, in *Advances in Atomic and Molecular Physics*, edited by D. R. Bates and B. Bederson (Academic, New York), Vol. II, p. 1.
Potapov, V. S., 1972, Zh. Eksp. Teor. Fiz. **63**, 2094 [Sov. Phys.-JETP **36**, 1105 (1973)].
Raisbeck, G., and F. Yiou, 1971, Phys. Rev. A **4**, 1858.
Rosenberg, L., 1963, Phys. Rev. **129**, 968.
Rudd, M. E., C. A. Sautter, and C. L. Bailey, 1966, Phys. Rev. **151**, 20.
Salin, A., 1969, J. Phys. B **2**, 631.
Saslaw, W. C., M. J. Valtonen, and S. J. Aarseth, 1974, Astrophys. J. **190**, 253.
Schiff, L. I., 1968, *Quantum Mechanics* (McGraw-Hill, New York), 3rd edition, p. 292.
Schnopper, H. W., H. D. Betz, J. P. Delvaille, K. Kalata, A. R. Sohval, K. W. Jones, and H. E. Wegner, 1972, Phys. Rev. Lett. **29**, 898.
Shakeshaft, R., 1974a, J. Phys. B **7**, 1059.
Shakeshaft, R., 1974b, Phys. Rev. A **10**, 1906.
Shakeshaft, R., 1974c, J. Phys. B **7**, 1734.
Shakeshaft, R., 1977, Phys. Rev. A **16**, 1458.
Shakeshaft, R., 1978a, Phys. Rev. A **18**, 2047.
Shakeshaft, R., 1978b, Phys. Rev. A **17**, 1011.
Shakeshaft, R., and L. Spruch, 1973, Phys. Rev. A **8**, 206.
Shakeshaft, R., and L. Spruch, 1977, Phys. Rev. Lett. **38**, 175.
Shakeshaft, R., and L. Spruch, 1978a, J. Phys. B **11**, L621.
Shakeshaft, R., and L. Spruch, 1978b, J. Phys. B **11**, L457.
Shakeshaft, R., and L. Spruch, 1978c, Phys. Rev. Lett. **41**, 1037.
Shastry, C. S., A. K. Rajagopal, and J. Callaway, 1972, Phys. Rev. A **6**, 268.
Slater, J. C., 1960, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York), Vol. 1, p. 368.
Sohval, A. R., 1975, Ph.D. thesis, Massachusetts Institute of Technology, unpublished.
Sohval, A. R., J. P. Delvaille, K. Kalata, K. Kirby-Docken, and H. W. Schnopper, 1976, J. Phys. B **9**, L25.
Spindler, E., H.-D. Betz, and F. Bell, 1977, J. Phys. B **10**, L561.
Spruch, L., 1969, in *Lectures in Theoretical Physics—Atomic Collisions*, edited by S. Geltman, K. T. Mahanthappa, and W. E. Britten (Gordon and Breach, New York), Vol. XIC, p. 77.
Spruch, L., 1978, Phys. Rev. A **18**, 2016.
Spruch, L., and R. Shakeshaft, 1979, Phys. Rev. A **19**, 1023.
Suter, M., C. R. Vane, I. A. Sellin, S. B. Elston, G. D. Alton, R. S. Thoe, and R. Laubert, 1978, Phys. Rev. Lett. **41**, 399.
Thomas, L. H., 1927, Proc. R. Soc. **114**, 561.
Tuan, T. F., and E. Gerjuoy, 1960, Phys. Rev. **117**, 756.
Vane, C. R., I. A. Sellin, M. Suter, G. D. Alton, S. B. Elston, P. M. Griffin, and R. S. Thoe, 1978, Phys. Rev. Lett. **40**, 1020.
Wilets, L., and S. J. Wallace, 1968, Phys. Rev. **169**, 84.