Angular-distribution peak at 60° in electron capture from a heavy atom by a fast light ion

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(Received 11 July 1983)

A light ion, incident on a heavy atom with a speed $v \gg e^2/\hbar$, may capture an outer electron as follows: The ion first hits the electron and knocks the electron out of the atom with a speed v. The ion then scatters elastically, through an angle θ, from the target nucleus so as to finally move in the same direction, and with the same speed, as the emergent electron. Kinematics require that $\theta \approx 60°$. This process is analyzed both classically and semiclassically, and it is shown that the angular distribution has a sharp peak about $\theta = 60°$.

I. INTRODUCTION

It is well known that the dominant contribution to forward charge transfer in an ion-atom collision at asymptotically high incident speed v is not the first but the second Born term.[1-3] The target electron e^- is scattered *twice*, first by the projectile P and then by the target nucleus T. In the first collision the e^- acquires the speed v and P is scattered through a very small angle $(\sqrt{3}/2)m/M$, where m and M are the masses of e^- and P, respectively. In the second collision the e^- scatters elastically from T and emerges in almost the same direction and with almost the same speed as P so that capture can occur. This double-scattering mechanism corresponds to a second Born term, and is understandable classically.[4] In contrast to the second Born contribution, the first Born contribution invokes the high-speed components of the initial- and final-electron wave functions and these components are very small. The sharp peak in the angular distribution about the small angle $(\sqrt{3}/2)m/M = 1.6'$, for electron capture by protons from helium atoms, was recently observed.[5]

We will be concerned here with the capture of an outer electron from a heavy atom by a light bare ion P that is incident with an asymptotically high velocity $\vec{v}_i$ and scatters through a *large* angle, emerging with a velocity $\vec{v}_f$. We work in the laboratory frame, in which the target nucleus T remains at rest, and we take the direction of incidence to be the z axis, designated by the unit vector $\hat{u}_z$. The process again involves two collisions, a P-T collision to scatter P through a large angle and a P-e^- collision to give e^- almost the same velocity $\vec{v}_f$ as the emergent P (see Fig. 1). Note that $|\vec{v}_f| = |\vec{v}_i| \equiv v$ since T is regarded as infinitely massive so that P scatters elastically from T. The P-e^- collision cannot follow the P-T collision. If it were to, the P-e^- collision would have to be head-on in order for e^- to emerge in the same direction as P; but then the kinematics would dictate that e^- would emerge with twice the speed of P so that capture could not occur (unless the high-speed components of the initial and final electron wave functions were invoked). Therefore, the P-e^- collision precedes the P-T collision. The speed of e^- after its collision with P is $v' = 2v\cos\theta'$ where θ' is the angle at which e^- emerges relative to the direction $\hat{u}_z$. For e^- to be captured by P we require $v' \approx v$ and $\theta' \approx \theta$. In this classical picture we therefore require $\theta' \approx \theta \approx \pi/3$. In other words, we expect the probability of electron capture as a function of θ, for fixed high incident speed v and for θ large, to be peaked about $\theta = \pi/3$; the high-speed components of the initial- and final-electron wave functions need not be invoked for θ near $\pi/3$. We examine this situation. In our first approach the formal calculation itself is an entirely classical one; quantum theory enters only in the assignment of a value to a characteristic atomic dimension a which enters in the choice of our model of an atom. Our second approach is a semiclassical one. We will find that some of the results obtained are special cases of results previously obtained in a (rough) quantum treatment of "atom capture."[6] The classical kinematics of the atom-capture process was studied previously,[6,7] and the sharp peak in the angular distribution was confirmed experimentally several years ago.[8] We

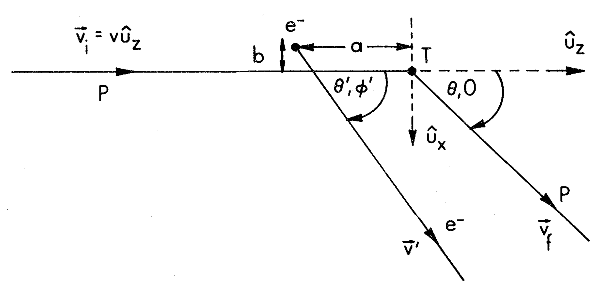

FIG. 1. Diagram, not drawn to scale, showing the projectile P incident with a velocity $\vec{v}_i = v\hat{u}_z$ (speed $v \gg e^2/\hbar$) on the infinitely massive target nucleus T. The electron e^- is at a characteristic distance a from T. The impact parameter of P relative to T is very much smaller than a, and we take it to be zero. The impact parameter of P relative to e^- is rather small compared to a, and is denoted by b. After the collision P emerges with polar angle $\theta \approx 60°$, azimuthal angle 0, and speed $|\vec{v}_f| = v$; e^- emerges with speed $v' \approx v$ at angles $\theta' \approx 60°$ and $\phi' \approx 0$.

hope this paper might stimulate a search for the predicted peak at 60° in the electron-capture angular distribution.

We note that capture of an outer electron involves a fractional loss of energy by P of the order of m/M. Restricting our considerations to incident energies of P up to just a few MeV, the loss of energy by P will be at most a few keV. This loss is rather small, but there can be cases in which it will not be very small compared to the width of a nuclear resonance; for those cases, the very interesting interface between atomic and nuclear physics explored by many authors[9] in the context of K-shell ionization may also be of relevance in the present context. We note further that when P scatters through 60° from T, there is no difficulty in reconciling energy and momentum conservation with the condition that e^- emerge with the same velocity as P; for this reason radiative capture, which dominates over nonradiative capture at forward angles, does not dominate at 60°.

In the large-angle scattering process under consideration, both P and e^- are scattered, so that two collisions *must* occur. This case is therefore less interesting conceptually than the forward scattering case. There the second Born term dominates as $v \sim \infty$ even though the first Born term does *not* vanish.

II. THE CLASSICAL APPROXIMATION

The projectile P, with atomic number Z_P, is incident with a velocity $\vec{v}_i = v\hat{u}_z$. For purposes of simplicity, the target nucleus T, with atomic number Z_T, is taken to be sufficiently massive with respect to the mass of P for the recoil of T to be ignored. The initial and final velocities of P, namely $\vec{v}_i$ and $\vec{v}_f$, define the scattering plane, which is taken to be the x-z plane; we can assume that $v_f = v_i$ $(\equiv v)$. The polar and azimuthal angles of scattering of P are then θ and 0. Since P is scattered through a large angle θ its impact parameter with respect to T will be very small compared to an atomic dimension a, and we can take the impact parameter of P with respect to T to be zero. The electron e^- initially bound to T in an outer shell is struck by P before P is scattered by T. The e^- emerges with a velocity $\vec{v}\,'$, with polar and azimuthal angles θ' and ϕ'. The e^- of mass m is initially uniformly distributed over the surface of a sphere of radius a, which in many cases should not be too bad an approximation for an outer e^-. The initial speed of e^-, which is of order $e^2/\hbar$ for an outer e^-, can be ignored, since $v \gg e^2/\hbar$. If the e^- is to be picked up by P (after P has been scattered) it must emerge with $\vec{v}\,' \approx \vec{v}_f$, that is, with $v' \approx v$, $\theta' \approx \theta$, and $\phi' \approx 0$. As noted above, by simple kinematics the light e^- when scattered through an angle θ' by the heavy P emerges with a speed

$$v' = 2v \cos\theta' , \qquad (2.1)$$

and we must therefore have $\theta' \approx \theta \approx \pi/3$. P is incident along the negative z axis, and its impact parameter with respect to e^- will be taken to be b. Since the speed $v' \approx v$ imparted to e^- by the P-e^- interaction is much larger than $e^2/\hbar$, we must have $b \ll a$. Thus, if θ'' and ϕ'' are the polar and azimuthal angles of e^- before it is struck by P, we must have $\theta'' \approx \pi$. Further, since the P-e^- interaction is attractive, and since therefore $\phi'' = \phi' + \pi$, it follows from $\phi' \approx 0$ that $\phi'' \approx \pi$. We assume, again for simplicity, that P assumes two straight-line orbits of constant speed v. It would probably not be too difficult to build in Coulomb effects—see, for example, the Appendix of Ref. 9—but at least at this stage it does not seem worth doing.

The experiment will consist of two measurements, the differential elastic cross section for P on T, $\sigma_{\rm el}(\theta)$, and the differential cross section for charge transfer (or capture), $\sigma_{\rm cap}(\theta)$. One would seek a peak in the ratio, the relative probability of capture,

$$P(\theta) \equiv \sigma_{\rm cap}(\theta)/\sigma_{\rm el}(\theta) , \qquad (2.2)$$

at an angle near $\pi/3$. To simplify the measurements, one would want $\sigma_{\rm el}(\theta)$ to be large. We therefore probably want the P-T scattering to be primarily Coulombic rather than nuclear, so large Z_T is desirable.

The condition for capture to occur is taken to be that the relative velocity of P and e^- *after* P has been scattered by T be below the escape velocity, that is,

$$\tfrac{1}{2} m (\vec{v}_f - \vec{v}\,')^2 \le Z_P e^2/\bar{a} , \qquad (2.3)$$

where $\bar{a}$ is the P-e^- separation immediately after the P-T collision. One easily finds that $\bar{a} = a$ for all θ. (The relative speed of P and e^- immediately after their collision is v, and it takes P a time a/v from the time of the P-e^- collision to reach T.) Using Eq. (2.1), we can rewrite Eq. (2.3) in terms of the angles which define the directions of $\vec{v}_f$ and $\vec{v}\,'$ as

$$1 + 4\cos^2\theta' - 4\cos\theta'(\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\phi') \le 2/q , \qquad (2.4)$$

where

$$\frac{2}{q} \equiv \frac{Z_P e^2/a}{mv^2/2} . \qquad (2.5)$$

Since we are concerned with Rutherford scattering, the connection between the impact parameter b and θ' is given by

$$\tan\theta' = \frac{mv^2}{Z_P e^2/b} \equiv \tau . \qquad (2.6)$$

The use of Eq. (2.6) in Eq. (2.4) gives

$$\tau^2 + 1 + 8\sin^2\tfrac{1}{2}\theta - 4\tau\sin\theta\cos\phi' \le \frac{2(\tau^2+1)}{q} . \qquad (2.7)$$

The probability of capture is the ratio of the area on the sphere of radius a from which an e^- will emerge with the appropriate velocity to the total area of the sphere. Since $b \ll a$, we can ignore the curvature of the sphere in determining the "appropriate" area; the correction is of order $1/q^2$. We then have as our classical approximation (CA) for capture at a given angle

$$P_{\rm CA}(\theta) = \int\int db\, b\, d\phi' (4\pi a^2)^{-1} ,$$

with the allowable domain of b and ϕ' defined by Eqs.

(2.5)–(2.7). From Eqs. (2.5) and (2.6), we have

$$b=\tau a/q \ . \tag{2.8}$$

It follows that

$$P_{\rm CA}(\theta)=\int\int d\tau\,\tau\,d\phi'(4\pi q^2)^{-1} \ , \tag{2.9}$$

with the domain of τ and ϕ' defined by Eq. (2.7). $P_{\rm CA}(\theta)$ as defined by Eq. (2.9), subject to Eq. (2.7), can be evaluated exactly. Introducing

$$\mu=\cos\theta \ ,$$

one finds (after some tedious algebra which we omit)

$$P_{\rm CA}(\mu)=\frac{-4\mu^2+4\mu-1+(4/q)(3-2\mu)-(4/q^2)}{4(q-2)^2} \tag{2.10}$$

for μ such that the numerator is non-negative and $P_{\rm CA}(\mu)=0$ if the numerator is negative. The total probability of capture is given, in our classical approximation, by

$$P_{\rm CA}=\int P_{\rm CA}(\mu)2\pi\,d\mu \ .$$

This gives

$$P_{\rm CA}=\frac{16\pi}{3q(q-2)^2}\left[\frac{2}{q}\right]^{1/2} . \tag{2.11}$$

There is not much point in using Eqs. (2.10) and (2.11) as they are, for only the leading terms can be expected to have physical significance. (Even apart from quantum effects, we have already ignored $1/q^2$ corrections.) We therefore simplify the above equations to

$$P_{\rm CA}(\mu)=[-(2\mu-1)^2+(8/q)]/(4q^2) \ , \tag{2.12a}$$

$$\tfrac{1}{2}[1-(8/q)^{1/2}]\le\mu\le\tfrac{1}{2}[1+(8/q)^{1/2}] \ , \tag{2.12b}$$

$$P_{\rm CA}(\mu)=0 \ , \quad \text{otherwise} \ , \tag{2.12c}$$

and

$$P_{\rm CA}=\frac{2\pi}{3}\left[\frac{2}{q}\right]^{7/2} . \tag{2.13}$$

In arriving at Eqs. (2.12), we recognized that the $(4/q)(3-2\mu)$ term is only a correction term, and this enabled us to approximate $(4/q)(3-2\mu)$ by $(8/q)$, replacing μ by $\frac{1}{2}$, its value at $\theta=\pi/3$. [We cannot simply drop the term in $P_{\rm CA}(\mu)$ in Eq. (2.10) proportional to $(4/q)$; the remaining expression is negative for all μ other than $\mu=\frac{1}{2}$ and is equal to zero at $\mu=\frac{1}{2}$.]

Rather than derive the full expressions given by Eqs. (2.10) and (2.11), we limit ourselves to a sketch of the derivation of Eqs. (2.12) and (2.13). We begin by noting that the main contribution to $P_{\rm CA}(\theta)$ comes from $\phi'\approx 0$ and $\tau=\tan\theta'\approx\tan(\pi/3)=\sqrt{3}$. The spread in τ and in ϕ' will become vanishingly small as $q\sim\infty$. Neglecting correction terms to $P_{\rm CA}(\theta)$ which vanish as $q\sim\infty$, we can therefore approximate the inequality (2.7) by replacing the term $2(\tau^2+1)/q$ by $8/q$. Further, we can approximate $\cos\phi'$ by $1-\frac{1}{2}\phi'^2$. But for $q\sim\infty$, $P_{\rm CA}(\theta)$ is vanishingly small unless $\theta\approx\pi/3$ and $\tau\approx 3^{1/2}$, so we can make the further replacement—since ϕ'^2 is already very small—of $2\tau\sin\theta\phi'^2$ by $3\phi'^2$.

Equation (2.7) can therefore be rewritten as

$$(\tau-2\sin\theta)^2+(3^{1/2}\phi')^2\le(8/q)-1-8\sin^2\tfrac{1}{2}\theta+4\sin^2\theta$$
$$=(8/q)-(2\mu-1)^2 \ .$$

Introducing $u=\tau-2\sin\theta$, $w=3^{1/2}\phi'$, and $R^2(\mu)=(8/q)-(2\mu-1)^2$, with μ restricted to the region for which $R^2(\mu)\ge 0$, we have

$$u^2+w^2\le R^2(\mu) \ , \quad 8/q\ge(2\mu-1)^2 \ ,$$

and Eq. (2.9) becomes

$$P_{\rm CA}(\mu)\cong 3^{1/2}\int\int d\tau\,d\phi'(4\pi q^2)^{-1}$$
$$=\int\int du\,dw(4\pi q^2)^{-1} \ .$$

But $\int\int du\,dw=\pi R^2(\mu)$, and we thereby obtain Eq. (2.12). Equation (2.13) follows easily.

III. THE SEMICLASSICAL APPROXIMATION

As in the classical approximation, we assume that P moves in straight-line orbits of constant speed, with zero impact parameter relative to T. The P-e^- interaction, which we denote by $V(\vec{x})$ with $\vec{x}$ the P-e^- separation, is treated as a perturbation. [We will ultimately set $V(\vec{x})=-Z_Pe^2/x$, but through Eq. (3.5) the derivation is much more general.] The difference from the classical approximation of Sec. II lies in our treatment of e^-, which is here treated quantum mechanically. The normalized initial- and final-state spatial wave functions are denoted by $\phi_i(\vec{r})$ and $\phi_f(\vec{r})$, respectively; the corresponding energies are denoted by ϵ_i and ϵ_f. It will be convenient to introduce the time-dependent wave functions

$$\psi_i(\vec{r},t)=e^{-i\epsilon_i t/\hbar}\phi_i(\vec{r}) \tag{3.1a}$$

and

$$\psi_f(\vec{r},t)=e^{-i(\epsilon_f+mv^2/2)t/\hbar}e^{im\vec{v}_f\cdot\vec{r}/\hbar}\phi_f(\vec{r}-\vec{v}_ft) \ . \tag{3.1b}$$

The argument of ϕ_f accounts for the fact that P moves with velocity $\vec{v}_f$ after its collision with T; the phase factors other than $-i\epsilon_ft/\hbar$ are other manifestations of that effect. Using first-order time-dependent perturbation theory, the amplitude A for capture is given by

$$A=I_-+I_+ \ , \tag{3.2}$$

where I_- and I_+ give the contributions due to P-e^- collisions before and after the P-T collision, with

$$I_-=-\frac{i}{\hbar}\int_{-\infty}^{0}dt\int d\vec{r}\,\psi_f^*(\vec{r},t)V(\vec{r}-\vec{v}_it)\psi_i(\vec{r},t) \ . \tag{3.3}$$

I_+ differs from I_- in that the range of integration of t is not $-\infty$ to 0 but 0 to ∞, and in the replacement of $V(\vec{r}-\vec{v}_it)$ by $V(\vec{r}-\vec{v}_ft)$. We now introduce the Fourier transform for an arbitrary function $f(\vec{r})$:

$$\tilde{f}(\vec{k}) \equiv (2\pi)^{-3/2}\int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} f(\vec{r}) \ .$$

Expressing $\phi_i(\vec{r})$, $V(\vec{r}-\vec{v}_i t)$, and $\phi_f^*(\vec{r}-\vec{v}_f t)$ in terms of their Fourier transforms, involving $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$, respectively, the integration over $\vec{r}$ is proportional to $\delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_f)$, where

$$\vec{k}_f \equiv m\vec{v}_f/\hbar \ .$$

Integration over $\vec{k}_3$ is then immediate and gives

$$I_- = (-i/\hbar)(2\pi)^{-3/2}\int_{-\infty}^{0} dt \int d\vec{k}_1 \int d\vec{k}_2 e^{i\Lambda t}\tilde{\phi}_f^*(\vec{k}_1+\vec{k}_2-\vec{k}_f)\tilde{V}(\vec{k}_2)\tilde{\phi}_i(\vec{k}_1) \ ,$$

where

$$\Lambda \equiv \omega_{fi} - \tfrac{1}{2}\omega + \vec{k}_1\cdot\vec{v}_f + \vec{k}_2\cdot(\vec{v}_f-\vec{v}_i) \ ,$$

with

$$\omega_{fi} \equiv (\epsilon_f - \epsilon_i)/\hbar \ , \quad \omega \equiv mv^2/\hbar \ .$$

Since $\tilde{\phi}_i(\vec{k}_1)$ is small unless $k_1 \lesssim 1/a_0$, we have $k_1 \ll mv/\hbar = k_f$. The presence of $\tilde{\phi}_f^*(\vec{k}_1+\vec{k}_2-\vec{k}_f)$ then demands that $\vec{k}_2 \approx \vec{k}_f$. We can therefore approximate $\tilde{V}(\vec{k}_2)$ by $\tilde{V}(\vec{k}_f)$, which enables us to remove $\tilde{V}$ from the integral. We now make the transformation

$$\vec{k}_2 \to \vec{k}_2 - \vec{k}_1 + \vec{k}_f \ ,$$

and find

$$I_- = (-i/\hbar)(2\pi)^{-3/2}\tilde{V}(\vec{k}_f)\int_{-\infty}^{0} dt\, e^{i\Sigma t}\int d\vec{k}_1\tilde{\phi}_i(\vec{k}_1)e^{i\vec{k}_1\cdot\vec{v}_i t}\int d\vec{k}_2\tilde{\phi}_f^*(\vec{k}_2)e^{i\vec{k}_2\cdot(\vec{v}_f-\vec{v}_i)t} \ ,$$

where

$$\vec{k}_f\cdot\vec{v}_i = m\vec{v}_f\cdot\vec{v}_i/\hbar \equiv mv^2\cos\theta/\hbar = \omega\cos\theta$$

and

$$\Sigma \equiv \omega_{fi} + (\tfrac{1}{2} - \cos\theta)\omega \ .$$

The integrals over $\vec{k}_1$ and $\vec{k}_2$ are just Fourier transforms. We therefore have

$$I_- = -(i/\hbar)(2\pi)^{3/2}\tilde{V}(\vec{k}_f)J(\theta) \ ,$$

where

$$J(\theta) \equiv \int_{-\infty}^{0} dt\, e^{i(1/2-\cos\theta)\omega t}\phi_f^*(\vec{v}_i t - \vec{v}_f t)\phi_i(\vec{v}_i t) \ ;$$

we have dropped the term $\omega_{fi}t$ from the exponent since $\phi_i(\vec{v}_i t)$ is small for $(v_i t/a_0)$ larger than unity, so the significant range of t is $|t| \lesssim a_0/v$ and therefore $|\omega_{fi}t| \ll 1$. We now make the important observation that the integrand is a rapidly oscillating function of θ except in the neighborhood of $\cos\theta = \frac{1}{2}$. (That the capture probability would peak at $\theta = 60°$ is a result easily anticipated, as noted in the Introduction.)

An analogous analysis of I_+ shows that the integrand of I_+ does not yield any similar maximum as a function of θ, but rather oscillates rapidly over the entire range of integration, and indeed I_+ is negligible compared to I_-. This is simply the statement that the P-e^- collision should occur *before* (or just at) the P-T collision. This too has a simple physical explanation, as discussed in the Introduction.

We now have as our semiclassical approximation (SCA) for the capture probability at an angle θ:

$$P_{\text{SCA}}(\theta) = |A|^2 \approx |I_-|^2 \ .$$

Since the (Born-approximation) differential cross section for the P-e^- collision, in their center-of-mass frame, is

$$\sigma_{Pe}(\theta) = 2\pi(m^2/\hbar^4)\,|\tilde{V}(\vec{k}_f)|^2 \ ,$$

we can write

$$P_{\text{SCA}}(\theta) = (2\pi\hbar/m)^2 d\sigma_{Pe}/d\Omega\,|J(\theta)|^2 \ .$$

Setting $\mu = \cos\theta$, we then have

$$P_{\text{SCA}} = \int_{-1}^{1} P_{\text{SCA}}(\mu)2\pi\, d\mu \ .$$

To evaluate P_{SCA}, we set $\theta = 60°$, that is, $\mu = \frac{1}{2}$, everywhere in $P_{\text{SCA}}(\mu)$ except in the oscillatory exponential; thus, we replace $\vec{v}_f$ by $v\hat{u}_{\pi/3}$, where the unit vector $\hat{u}_{\pi/3}$ is at an angle of 60° with respect to $\hat{u}_z$. We then obtain

$$P_{\text{SCA}} = (2\pi)^3(\hbar/m)^2 d\sigma_{Pe}/d\Omega \int_{-\infty}^{0} dt \int_{-\infty}^{0} dt' K^*(t)K(t')e^{i\omega(t-t')/2}L(t'-t) \ ,$$

where

$$K^*(t) = \phi_f^*[(\hat{u}_z - \hat{u}_{\pi/3})vt]\phi_i(\hat{u}_z vt)$$

and

$$L(t-t') \equiv \int_{-1}^{1} d\mu\, e^{-i\omega(t-t')\mu} \ .$$

Since a characteristic value of $t-t'$ is a_0/v, a characteristic value of $\omega(t-t')$ is $a_0/(\hbar/mv)$, a very large number, and we have

$$L(t-t') \approx (2\pi/\omega)\delta(t'-t) .$$

$P_{\rm SCA}$ then simplifies to

$$P_{\rm SCA} = (2\pi)^4(\hbar/mv)^3 d\sigma_{Pe}/d\Omega Q , \tag{3.4}$$

where

$$Q \equiv \int_0^\infty ds \, |\, \phi_f^*[(\hat{u}_{\pi/3}-\hat{u}_z)s]\phi_i(-s\hat{u}_z)\,|^2 ; \tag{3.5}$$

we have introduced

$$s \equiv -vt .$$

This result agrees with Eq. (3.14) of Ref. 6. The present treatment gives the angular distribution $P_{\rm SCA}(\theta)$, a result not contained in Ref. 6; the situation we have considered here is simpler than that considered there, for we are concerned here with $m \ll M$.

If now we specialize to $V(x) = -Z_P e^2/x$, we have

$$d\sigma_{Pe}/d\Omega = (2Z_P e^2/mv^2)^2 ,$$

and therefore

$$P_{\rm SCA} = (2\pi)^4 \left[\frac{\hbar}{mv} \right]^3 \left[\frac{Z_P e^2}{mv^2/2} \right]^2 Q . \tag{3.6}$$

IV. COMPARISON OF THE CLASSICAL AND SEMICLASSICAL APPROXIMATIONS

The classical approximation (CA) and the semiclassical approximation (SCA) differ in two ways:

(i) In the CA the e^- is initially uniformly distributed over the surface of a sphere of radius a, while in the SCA the e^- initially has a density distribution given by $|\,\phi_i(\vec{r})\,|^2$.

(ii) In the CA, capture is defined by the condition $|\,\vec{v}_f-\vec{v}'\,|$ is less than or equal to the escape velocity, corresponding to capture into *any* bound state, while in the SCA we evaluate capture into a *particular* bound state, with normalized wave function $\phi_f(\vec{r})$.

We will limit our discussion of the connection between the CA and the SCA approximations to the total capture probabilities, ignoring the probabilities for capture at a given angle θ. To emphasize the differences between the CA and SCA derivations of the total capture probabilities, we will no longer use the symbols $P_{\rm CA}$ and $P_{\rm SCA}$ but will use $P_{\rm CA}(a\to bd)$ and $P_{\rm SCA}(i\to f)$ to represent the total capture probabilities for the two approximations.

Turning to $P_{\rm SCA}(i\to f)$, we sum over all bound states f, and using Eqs. (3.6) and (3.5), arrive at

$$P_{\rm SCA}(i\to bd) \equiv \sum_f P_{\rm SCA}(i\to f)$$

$$= 16\pi^4 \left[\frac{\hbar}{mv} \right]^3 \left[\frac{Z_P e^2}{mv^2/2} \right]^2 \times \int_0^\infty |\,\phi_i(-s\hat{u}_z)\,|^2 \rho_{bd}(s) ds , \tag{4.1}$$

where

$$\rho_{bd}(s) \equiv \sum_f |\,\phi_f(s)\,|^2 ;$$

since the sum over all bound states must be a spherically symmetric function, we replaced the argument of ϕ_f, namely $(\hat{u}_{\pi/3}-\hat{u}_z)s$, by its absolute magnitude, which is just s since $|\,\hat{u}_{\pi/3}-\hat{u}_s\,| = 1$. We now assume that the initial state i is one with reasonably large quantum numbers, so that $|\,\phi_i(-s\hat{u}_z)\,|^2$ peaks at reasonably large values of s. It is then a reasonable approximation to replace ρ_{bd} by its WKB approximation since the bulk of the contribution to the integral in Eq. (4.2) comes from states f with reasonably large quantum numbers at relatively large values of s. Sums over a number of particular subsets of bound states were evaluated in the WKB approximation in the course of the analysis of a problem very similar to the present problem, the connection between the classical and quantum treatments of forward charge transfer.[2] The sums evaluated included the sum over all bounds states which we require here, but that sum can be obtained trivially by means of a Thomas-Fermi statistical approach for noninteracting electrons. [We are not summing over the different states of many (interacting) electrons but over all hydrogenic bound states of a single electron.] Thus, since the spin of the electron is of no relevance here so that there is no additional factor of 2, we write

$$\rho_{bd}(s) \approx \frac{(4\pi/3)p_F^3(s)}{(2\pi\hbar)^3} ,$$

where the Fermi momentum $p_F(s)$ is defined by

$$p_F^2(s)/2m = Z_P e^2/s .$$

We therefore have, approximately,

$$\rho_{bd}(s) = \frac{1}{6\pi^2\hbar^3} \left[\frac{2mZ_P e^2}{s} \right]^{3/2} ,$$

and Eq. (4.1) becomes

$$P_{\rm SCA}(i\to bd) = \frac{8\pi^2}{3} \left[\frac{Z_P e^2}{mv^2/2} \right]^{7/2} \int_0^\infty \frac{|\,\phi_i(-s\hat{u}_z)\,|^2}{s^{3/2}} ds . \tag{4.2}$$

Comparison with Eq. (2.13) shows that $P_{\rm CA}(a\to bd)$ and $P_{\rm SCA}(i\to bd)$ become identical on identifying $|\,\phi_i(-s\hat{u}_z)\,|^2$ with

$$\rho_a(s) \equiv \delta(s-a)/4\pi a^2 ,$$

the density for an electron uniformly distributed over the surface of a sphere.

V. DISCUSSION

A necessary condition for the validity of the result for $P_{\rm SCA}(i\to bd)$ given in Eq. (4.2) is that $\hbar/mv$ be very small compared to any other relevant dimension. Assume for simplicity that the effective charge seen by the outer electron in its initial state is of order unity and that P is a proton. Let the initial state have a characteristic dimension a; capture will tend to occur to final states with comparable dimensions. With $\epsilon_i \approx \hbar^2/ma^2$, the condition $\hbar/mv \ll a$ leads to

$$E_P \equiv \tfrac{1}{2}Mv^2 \gg (M/m)\epsilon_i . \tag{5.1}$$

In the derivation of Eq. (2.12a) we dropped corrections of order $1/q$; on using $\epsilon_i \approx e^2/a$, the requirement $1/q \ll 1$ reproduces the condition (5.1).

The restriction imposed on E_P by (5.1) can be very strong. The condition is eased for capture of an electron initially in a high Rydberg state. To be concrete, assume that n is of order 10 and l is of order n. ϵ_i will then be of the order of tenths of an eV, and we demand that E_P be very much larger than hundreds of eV; one would probably require E_P to be at least of the order of some keV's. $\phi_i(\vec{r})$ would be almost hydrogenic, and it would not be difficult to estimate the value of the integral in Eq. (4.2). The situation is rather different for capture from an atom with no electron in a high Rydberg state. ϵ_i (and the significant ϵ_f's) are then of the order of a few eV's, and Eq. (4.2) for $P_{\rm SCA}(i \to bd)$ will probably not become valid until E_P is at least of the order of 500 keV. Further, it is much more difficult than for an atom with one electron in a high Rydberg state to estimate $\phi_i(\vec{r})$ for the most weakly bound electron in an atom in its ground state, say; one could use Hartree-Fock calculations to obtain $\phi_i(\vec{r})$. Finally, the replacement of $\rho_{bd}(r)$ by its WKB approximation would be far less reliable in the non-Rydberg case. The dominant contributions to capture might then well come from a few low-lying states f. One might be interested in capture to a particular final state, but the experiment will be much simpler if one allows capture to any bound state. To determine the probability for capture to any bound state one would probably not want to use Eq. (4.2) for $P_{\rm SCA}(i \to bd)$; it would probably be better to sum $P_{\rm SCA}(i \to f)$, given by Eqs. (3.4) and (3.5), for a few of the low-lying states f.

For a concrete case, one would use the best $\phi_i(\vec{r})$ available—the $\phi_f(\vec{r})$ are hydrogenic and therefore known—and evaluate Eqs. (3.4) and (3.5) for a few states f. We restrict our attention to a crude estimate of capture; one might, for example, be interested in some other process and simply wish to have an order-of-magnitude estimate of the capture process under consideration in order to be able to determine whether or not the capture process need be a matter of concern. Assume then that we have a heavy atom with one electron in its outer shell, and that the shell has an orbital angular momentum quantum number l which is not too small, say 4 or 5. Averaging over its angular momentum projections gives a spherically symmetric density function $\rho_i(r)$ which can be crudely approximated by $\delta(r-a)/4\pi a^2$ (where a is of order a_0). We then return to Eq. (2.13) and have, with $\epsilon \equiv \frac{1}{2}mv^2$,

$$P_{\rm CA}(a \to bd) = \frac{2\pi}{3}\left[\frac{2}{q}\right]^{7/2} = \frac{2\pi}{3}\left[\frac{Z_P e^2/a}{\epsilon}\right]^{7/2} . \tag{5.2}$$

The estimate given by Eq. (5.2) is probably not very accurate until ϵ is at least ten times greater than $Z_P e^2/a$; at that value of ϵ,

$$P_{\rm CA}(a \to bd) \approx \tfrac{2}{3} \times 10^{-3} , \quad q \approx 20 .$$

The estimate of the *form* of the angular distribution given by Eq. (2.12), essentially that in the square brackets in Eq. (2.12a), is probably more reliable than is the estimate of the total capture probability given by Eq. (2.13). Furthermore, the experimental detection of the peak in the angular distribution would be easier to perform than an absolute measurement of the cross section. We note firstly that $P_{\rm CA}(\mu)$ is symmetric about $\mu = \frac{1}{2}$. We note further that as q increases, the width of $P_{\rm CA}(\mu)$ decreases, but that unfortunately the magnitude of the peak, which occurs at $\mu = \frac{1}{2}$, also decreases. More precisely, we have

$$P_{\rm CA}(\mu = \tfrac{1}{2}) = 2/q^3 ,$$

$$\cos(\theta_{\max}) = \mu_{\min} = \tfrac{1}{2}[1 - (8/q)^{1/2}] ,$$

$$\cos(\theta_{\min}) = \mu_{\max} = \tfrac{1}{2}[1 + (8/q)^{1/2}] .$$

Note that $\mu_{\min} + \mu_{\max} = 1$. To give some feeling for numerical values, we evaluate these results for two values of q:

$$q = 16: \quad \theta_{\min} \approx 31^\circ , \quad \theta_{\max} \approx 82^\circ , \quad P_{\rm CA}(\tfrac{1}{2}) \approx 5 \times 10^{-4} ,$$

$$q = 80: \quad \theta_{\min} \approx 49^\circ , \quad \theta_{\max} \approx 70^\circ , \quad P_{\rm CA}(\tfrac{1}{2}) \approx 4 \times 10^{-6} .$$

ACKNOWLEDGMENT

This work was supported in part by the National Science Foundation under Grants Nos. PHY-79-10413 and PHY-81-19010, and by the Office of Naval Research under Contract No. N00014-77-C0553.

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