Simple heuristic derivation of some charge-transfer probabilities at asymptotically high incident velocities

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For asymptotically high incident velocities we provide simple, heuristic, almost classical, derivations of the cross section for forward charge transfer, and of the ratio of the cross section for capture to the elastic-scattering cross section for the projectile scattered through an angle close to $\pi/3$.

I. INTRODUCTION

The cross section for forward charge transfer for a projectile P incident with asymptotically high velocity $\vec{v}_i = v\hat{u}_z$ on a target nucleus T to which is bound one electron e^- is conceptually of great interest in quantum theory since the *second* Born term gives the dominant contribution. Using a model in which the e^- is initially uniformly distributed over the surface of a sphere of radius a, that is, in which the e^- has an initial (normalized) distribution

$$\rho_a(\vec{r}) = \delta(r-a)/4\pi r^2 \ , \tag{1.1}$$

the cross section was first calculated, classically, by Thomas.[1] After a long period of confusion occasioned by the fact that the classical result did not agree at all with the first-Born-term contribution, it was shown by Drisko[2] that for capture from the $1s$ state Thomas's result and the *second*-Born-term contribution agreed to within a constant. The precise connection between classical and quantum theory was clarified only quite recently; it was shown[3] that for capture from a high Rydberg state (with $l \approx n$)— capture which will occur primarily to final states which are themselves high Rydberg states—the classical and second-Born contributions approach one another exactly as $n \sim \infty$. This is not too surprising a result since high Rydberg states can be described classically. A detailed discussion can be found in Ref. 3 and in a relatively recent review.[4]

The calculation of the second Born term is quite complicated even in the domain of present interest, that is, even for v asymptotically high. We present here a quite simple derivation. The derivation can surely be made rigorous, but the proof that the derivation is rigorous would itself be expected to be very complicated, in which case it would serve no purpose, and we present no such proof. We will consider the paper to be a success if the reader is convinced, as we are, that the conceptually simple derivation is very believable.

Before analyzing the forward-charge-transfer process commented on above, we examine charge transfer at large projectile scattering angles, a process which has received some attention recently.[5–7] Thus we consider a projectile P which captures an outer electron from a heavy atom and scatters elastically through a large angle θ from the heavy-target nucleus T. It turns out that the probability for capture peaks at $\theta = \pi/3$. In Sec. II we give a conceptually simple derivation of the ratio of the cross section for capture to the cross section for elastic scattering. This derivation facilitates the analysis, in Sec. III, of the forward-charge-transfer process.

A preliminary insight into the validity of classical theory for high-energy charge transfer is obtained by considering the consequences of the uncertainty principle with regard to the initial state, an electron bound to a target. The requirement that the initial spatial distribution be known implies that the initial velocity distribution cannot be known exactly, but the enormous speed imparted to the electron by the projectile renders the relatively small uncertainty in the initial velocity distribution irrelevant.

II. CHARGE TRANSFER AT SCATTERING ANGLES CLOSE TO $\pi/3$

The projectile P, with atomic number Z_p and mass $M_p >> m$, is incident with a velocity $\vec{v}_i = v\hat{u}_z$, where $v >> e^2/\hbar$ (a characteristic speed for an outer electron e^- of mass m). T is taken to have a mass $>> M_p$ so that the recoil of T can be neglected. P undergoes two binary collisions, the first with e^- and the second with T. (If the collisions were to occur in the reverse order, e^- and P could not emerge with the same velocity and capture could not occur.) Since P scatters from T through a large angle θ the impact parameter of P relative to T must be very small and we can assume that P is incident along the negative z axis. It follows that *the P-e^- collision occurs effectively at $x=0$, $y=0$, $z<0$*. Note that if $\vec{v}_f$ is the final velocity of P we must have $|\vec{v}_f| = v$ since the P-T collision is elastic and recoiless. Note also that it follows from the kinematics, and from the condition that e^- emerge with a velocity close to $\vec{v}_f$, that $\theta \approx \pi/3$.

The probability $P_{\rm CA}(\theta)$ is the probability, calculated in the classical approximation, that P, scattered through an angle θ with a final velocity $\vec{v}_f$, will capture the e^-. For a given location of the e^- on the sphere of radius a centered at T, we can calculate the velocity $\vec{v}'$ of the emergent e^-. $P_{\rm CA}(\theta)$ is the ratio of the "appropriate" area of the sphere to the total area $4\pi a^2$ of the sphere. The appropriate area is the area for which $|\vec{v}' - \vec{v}_f|$ is less than or equal to the escape velo-

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city immediately after the P-T collision. Integrating over θ gives the total probability $P_{\rm CA}$ of capture. One finds,[5] using the fact that $P_{\rm CA}(\theta)$ peaks at $\theta=\pi/3$,

$$P_{\rm CA}(a \rightarrow bd)=\frac{2\pi}{3}\left[\frac{Z_P e^2}{mv^2/2}\right]^{7/2}\frac{1}{a^{7/2}}\equiv\frac{C}{a^{7/2}} \quad . \tag{2.1}$$

The argument $a \rightarrow bd$ of $P_{\rm CA}$ has been inserted to make it clear that the initial state was characterized by a, with the spatial distribution $\rho_a(\vec{r})$ of Eq. (1.1), and that the final state was any bound (bd) state. We could proceed by a similar analysis to determine $P_{\rm CA}$ for an arbitrary initial distribution $\rho_i(\vec{r})$ rather than for $\rho_a(\vec{r})$, but it will prove convenient instead to rewrite $P_{\rm CA}(a\rightarrow bd)$ in a different form, one which makes the extension to $\rho_i(\vec{r})$ obvious. Thus, we rewrite $P_{\rm CA}(a\rightarrow bd)$ in a form which contains $\rho_a(\vec{r})$ and which contains all of the essential "physics," namely,

$$P_{\rm CA}(a\rightarrow bd)=\int P_{\rm CA}(r\rightarrow bd)\rho_a(\vec{r})4\pi r^2 \times[\delta(x)\delta(y)\Sigma(-z)]\,d\vec{r} \quad , \tag{2.2}$$

where in the integrand we replaced a by the variable r. This equation is an identity, no matter what the form of $P_{\rm CA}(r\rightarrow bd)$ is. The factor $\Sigma(-z)$ in the integrand [here $\Sigma(z)$ is the Heaviside step function] has no effect on the identity; the square bracket in the integrand represents the physical fact that the electron must initially lie on the negative z axis to be struck by P. To obtain $P_{\rm CA}(i\rightarrow bd)$, the probability of capture from an arbitrary initial distribution, we need merely replace $\rho_a(\vec{r})$ in Eq. (2.2) by $\rho_i(\vec{r})$. Using Eq. (2.1) for $P_{\rm CA}(r\rightarrow bd)$, with a replaced by r, we find

$$P_{\rm CA}(i\rightarrow bd)=4\pi C\int\frac{\rho_i(\vec{r})}{r^{3/2}}\delta(x)\delta(y)\Sigma(-z)\,d\vec{r} \quad . \tag{2.3}$$

By time-reversal invariance we expect $P_{\rm CA}(i\rightarrow f)$, the probability of capture from a specified initial distribution $\rho_i(\vec{r})$ to a specified final distribution $\rho_f(\vec{r})$, to contain a factor $\rho_f(\vec{r})$. [Consider capture of an e^- by T for $(P+e^-)$ incident on T; the initial distribution would be $\rho_f(\vec{r})$.] We therefore expect $P_{\rm CA}(i\rightarrow bd)$ to contain

$$\rho_{bd}(\vec{r})=\Sigma_f\rho_f(\vec{r}) \quad , \tag{2.4}$$

where the sum is over all bound states. [The presence of the factor $r^{-3/2}$ in the integrand also suggests the introduction of the factor $\rho_{bd}(r)$, for as is well known, and as we shall see in a moment, $\rho_{bd}(\vec{r})$ is proportional to $r^{-3/2}$.] In a semiclassical approximation we can use a simple version of Thomas-Fermi theory to give

$$\rho_{bd}(\vec{r})=\frac{(4\pi/3)p_F^3(r)}{(2\pi\hbar)^3} \quad ,$$

where the Fermi momentum $p_F(r)$ is given by

$$\frac{p_F^2(r)}{2m}=-V(r)=\frac{Z_P e^2}{r} \quad .$$

[We do not need a self-consistent approach to determine $V(r)$, as in the usual Thomas-Fermi theory, since we are not concerned here with interacting electrons filling up all of available phase space at a given point $\vec{r}$; we have only one e^- and it sees a potential $-Z_P e^2/r$.] We therefore have

$$1=C'\rho_{bd}(\vec{r})r^{3/2} \quad , \tag{2.5a}$$

$$C'=6\pi^2\hbar^3/(2mZ_P e^2)^{3/2} \quad . \tag{2.5b}$$

Introducing the right-hand side of Eq. (2.5a) as a factor in the integrand in Eq. (2.3), we obtain

$$P_{\rm CA}(i\rightarrow bd)=4\pi CC'\int\rho_i(\vec{r})\delta(x)\delta(y)\Sigma(-z)\rho_{bd}(\vec{r})\,d\vec{r} = C''\int_0^\infty\rho_i(-s\hat{u}_z)\rho_{bd}(-s\hat{u}_z)\,ds \quad , \tag{2.6a}$$

where we have integrated over x and y and set $s=-z$, and where

$$C''=16\pi^4(\hbar/mv)^3(Z_P e^2/[mv^2/2])^2 \quad . \tag{2.6b}$$

Writing $\rho_{bd}(-s\hat{u}_z)$ as the sum given in Eq. (2.4), $P_{\rm CA}(i\rightarrow f)$ is obtained from $P_{\rm CA}(i\rightarrow bd)$ by simply replacing $\rho_{bd}(-s\hat{u}_z)$ by just one term in its sum, $\rho_f(-s\hat{u}_z)$. Interpreting $\rho_\alpha(-s\hat{u}_z)$ as $|\phi_\alpha(-s\hat{u}_z)|^2$, for $\alpha=i$ or f, where ϕ_α is a normalized wave function, we obtain exactly the same result as was recently obtained[5] in a semiclassical approximation (SCA).

To understand more thoroughly the basis of the above approach, note firstly that P can be treated classically since the wavelength of P is very much smaller than any relevant length. Note further that the use of the classical distribution $\rho_a(\vec{r})$ for the initial state of the electron is reasonable if $a \gg a_0=\hbar^2/me^2$, that is, if the initial state is a high Rydberg state. Thus the replacement of $\rho_a(\vec{r})$ by $\rho_i(\vec{r})$ is reasonable if $\rho_i(\vec{r})$ is the quantum spatial distribution of a high Rydberg state. Now if i is a high Rydberg state, capture will occur predominantly into high Rydberg states, and the main contribution to the sum $\rho_{bd}(\vec{r})$ will come from states f that are high Rydberg states. In this case it is reasonable to evaluate $\rho_{bd}(\vec{r})$ using Thomas-Fermi theory. Finally, this leads to the above quantum expression for the probability of capture from state i to state f. This expression was derived only for states i and f that are high Rydberg states, but since the expression has a general form it is not unreasonable to conclude that it is valid for all states i and f, and this is borne out by comparison with the exact result.

III. FORWARD CHARGE TRANSFER

We will be concerned with the cross section $\sigma_{\rm ds}$ for forward charge transfer via double scattering (ds). Our objective is to obtain the quantum expression for $\sigma_{\rm ds}$ starting from the classical approximation for $\sigma_{\rm ds}$, found by Thomas[1,4] to be

$$\sigma_{\rm ds}(a\rightarrow bd)=C^*/a^{7/2} \quad , \tag{3.1}$$

where

$$C^*=(\pi/3)2^{13/2}Z_P^{7/2}Z_T^2(e^2/mv^2)^{11/2} \quad ; \tag{3.2}$$

we have assumed an initial distribution $\rho_a(\vec{r})$ defined by Eq. (1.1). The e^- when struck by P emerges at an angle very close to $\pi/3$ with respect to the incident direction $\hat{u}_z$ of P. Thereby e^- attains a speed very close to v. It is then elastically scattered from T through an angle very close to $\pi/3$, emerging with a velocity very close to $\vec{v}_i$. Therefore e^- can be, initially, at any distance r from T, but it must be at a polar angle very close to $2\pi/3$ with respect to $\hat{u}_z$ so that it will pass close by T after being scattered by P. We therefore write our identity—the factor $\delta(\theta-2\pi/3)$ guarantees that the electron has the appropriate initial position and the factor $2/\sin\theta$ is introduced so that we do indeed have an identity—as

$$\sigma_{\rm ds}(a \to bd) = \int \sigma_{\rm ds}(r \to bd)\rho_a(r)\left[\frac{2\delta(\theta-2\pi/3)}{\sin\theta}\right]d\vec{r} \ . \tag{3.3}$$

We now replace $\rho_a(\vec{r})$ by $\rho_i(\vec{r})$, introduce $\rho_{bd}(\vec{r})$ as above, use Eqs. (2.5), and substitute for $\sigma_{\rm ds}(r \to bd)$ from Eq. (3.1) to arrive at

$$\sigma_{\rm ds}(i \to bd) = 2C^*C' \int \rho_i(\vec{r})\delta(\theta-2\pi/3) \times \rho_{bd}(\vec{r})dr\, d\theta\, d\phi \ . \tag{3.4}$$

We replace, in this last equation, $\rho_{bd}(\vec{r})$ by $\rho_f(\vec{r})$ on the right-hand side, and therefore $\sigma_{\rm ds}(i \to bd)$ by $\sigma_{\rm ds}(i \to f)$ on the left-hand side. Assuming that i and f have specified angular momentum quantum numbers, with the z axis the angular momentum quantization axis, $\rho_i(\vec{r})$ and $\rho_f(\vec{r})$ are each independent of ϕ since the angular dependences are given by the absolute squares of spherical harmonics. Therefore integration over ϕ gives 2π and we obtain

$$\sigma_{\rm ds}(i \to f) = \tilde{C} \int_0^\infty \rho_i(r, \tfrac{1}{3}2\pi, 0)\rho_f(r, 2\pi/3, 0)dr \ , \tag{3.5}$$

where

$$\tilde{C} = 4\pi C^*C' = 2^8\pi^4 Z_P^2 Z_T^2 \left[\frac{e^2}{mv^2}\right]^4 \left[\frac{\hbar}{mv}\right]^3 \ , \tag{3.6}$$

in exact agreement with the (quantum) second Born term, Eq. (5.14) of Ref. 4. The transition from the classical to the quantum cross sections, for the two processes considered above, is possible because the classical expressions contain charge densities which can be replaced by probability *densities,* so that interference effects associated with the wave function do not arise.

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[1]L. H. Thomas, Proc. R. Soc. London 114, 561 (1927).
[2]R. M. Drisko, thesis, Carnegie Institute of Technology, 1955 (unpublished).
[3]L. Spruch, Phys. Rev. A 18, 2016 (1978).
[4]R. Shakeshaft and L. Spruch, Rev. Mod. Phys. 51, 369 (1979).
[5]R. Shakeshaft and L. Spruch, Phys. Rev. A 29, 605 (1984).
[6]L. Kocbach and J. S. Briggs, in Abstracts of the Proceedings of the Thirteenth International Conference on the Physics of Electronic and Atomic Collisions, Berlin, 1983 edited by J. Eichler *et al.* (ICPEAC, Berlin, 1983), p. 498.
[7]P. A. Amundsen and D. H. Jakubassa-Amundsen, in Ref. 6, p. 508.