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CONF - 8008120 - - 1

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CONTINUUM CAPTURE IN THE THREE-BODY PROBLEM*

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THE THREE-BODY REARRANGEMENT PROBLEM

The hydrogen atom is often referred to as the Rosetta Stone of atomic physics. It occupies this role as the most readily accessible quantum mechanical realization of the Kepler two-body problem. In the quantum domain only the solution to the static, stationary state Kepler problem, suitably modified by the theories of relativity and quantum electrodynamics, is known to high accuracy. Knowledge of the dynamical two-body problem nonetheless represents a triumph of mathematical understanding compared to the relatively primitive present-day comprehension of the scattering theory appropriate to the three-body problem. Again, the stationary version of the three-body problem is quantitatively far better understood than the dynamical version, even though the analytical history of the problem is a long and distinguished one. In his well-known book entitled Men of Mathematics, E. T. Bell refers to Sir Isaac Newton's work on the particular three-body problem central to Newton's thinking: the motion of the moon. Though Newton regarded this work as a "diversion" from his alchemical and theological studies, Bell notes that "these 'diversions' occasionally cost him more incessant thought than his professed labors, as when he made himself seriously ill by thinking day and night about the motion of the Moon, the only problem, he says, that ever made his head ache."¹

The present paper mainly concerns electron capture to the continuum. One can argue that electron capture in heavy particle collisions is the simplest dynamical quantum mechanical version of the three-body rearrangement problem. Following the notation of an excellent review article published recently by Robin Shakeshaft and

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Larry Spruch concerning mechanisms for charge transfers at asymptotically high impact velocities,² one may in either case envision capture of an object of mass m by a much larger object of mass M_B , where m had initially been bound to a large object of mass M_A . Fig. 1 shows a coordinate diagram.

A suitable Newtonian astronomical analogy to the electron capture phenomenon is the problem of the capture of a gravitationally bound astronomical object by an incident gravitating projectile. Though Ref. 2, to be heavily quoted in the present discussion, deals almost exclusively with quantum atomic scattering problems, there is a brief classical digression on the question of how a neutron star, believed to be the result of a violent collapse, can appear as a binary. It is, of course, possible that the star which collapsed had been the component of a binary, though then the collapse must be sufficiently gentle to preserve the binary bond. A possible alternative explanation, since an appreciable fraction of the known neutron stars is thought to be binary, is attributed to Hills.³ The idea is that a neutron star, born in isolation after breaking any previous bonds, becomes a binary by capturing one of a binary pair of ordinary stars. The analogy to electron capture by a bare nucleus colliding with a hydrogenic system (or one which can be treated within a hydrogenic approximation, perhaps helium) is evident. In a classical calculation, the small size of the electron mass relative to the mass of the nucleon provides some kinematic calculational conveniences,

Fig. 1. Diagram showing the relative coordinates. In the laboratory frame, M_B has an initial velocity $v = v\hat{u}_z$ and M_A is initially at rest. From Ref. 2.

but is not essential to characterizing three-body scattering results in principle. In the quantum mechanical problem, however, there is great simplification in treating the heavy particle motion classically, permitting the electron to be endowed with almost all of the quantum-mechanical aspects of the three-body scattering problem.

Our main topic - electron capture to the continuum (as opposed to a bound state) - has both quantum and classical aspects and analogs. What is meant in the quantum domain is capture to projectile-centered continuum states, where the capture proceeds in analogy to electron transfer to bound states, but the wave function which describes the motion of m after the collision is instead a projectile-centered continuum wave function. The phenomenon therefore represents a form of ionization, but one in which, for example, a plane wave description of the captured electron is completely inappropriate. Rather, Coulomb waves centered on the projectile become a much more appropriate description.

Joseph Macek, in a series of publications on this subject dating back to 1970,⁴ makes the following analogy. Ionization can be thought of as the natural continuation of excitation to a sequence of orbits of ever-increasing principal quantum number into the continuum. The excitation cross sections continue smoothly right through the ionization limit, provided an appropriate normalization of continuum states vis-a-vis excitation to high n Rydberg states per unit bandwidth Δn is considered. In like fashion, one may envision electron capture events accompanying an ion-atom encounter into a sequence of orbits of ever-increasing principal quantum number n , whose production rate also continues smoothly from the region of high Rydberg states just below the continuum into the continuum. Somehow, this process went experimentally undiscovered and theoretically neglected during the 50-odd years which have elapsed since the initial development of the quantum theory. Although quantum mechanical theories of excitation, ionization, and capture to bound states were worked out in the 1920's and 1930's by names so eminent that they need not be referenced here, the electron capture contribution to the ionization channel was somehow ignored. That it can sometimes be extremely important is illustrated by a recent paper by Shakeshaft,⁵ who finds that for certain energies (~ 40 keV), more than half the total cross section for ionization of hydrogen by protons is accounted for by this process. Fig. 2 presents an interesting pictorial account of how the excitation, ionization, electron capture, and capture to continuum phenomena are interrelated. Comprehension of the important interactions characterizing ion-atom, ion-molecule, and ion-solid encounters is sometimes thereby changed significantly. For example, in work which I shall not have time to discuss here,⁶ there is evidence that penetration of highly charged nuclei in condensed matter is accompanied by production of significant numbers of so-called "convoy" electrons, which accompany the ion as it passes through the medium, matched in

Fig. 2. Development of the charge distribution in p-H scattering with time in the lab frame. The incident proton has a lab energy of 40 keV and an impact parameter of 1.5 au. The two protons are represented by black dots. The shading represents the relative electron density. The plane of the paper is the scattering plane of the collision, and the electron charge density has been integrated in the direction perpendicular to the scattering plane. Distances are measured in atomic units. From Ref. 5.

velocity and in direction to the incident ion, the mechanism for production of which is still being debated. Electron capture to the continuum is an oft-discussed possible convoy production mode.

The first observations of such forward-peaked electron production were made for proton-helium scattering by Crooks and Rudd,⁷ and nearly at the same time by Harrison and Lucas⁸ for the ion-solid collision case. The work of our laboratory is distinguished from that of several others⁹ currently active in the study of electron capture to the continuum by virtue of its use of faster, more highly ionized, frequently bare nuclear projectiles. Entry into the regime of asymptotically high velocities is thus made possible, and an additional degree of freedom - the point nuclear charge of an incident, structureless projectile - can be exploited.

While the characterization of collision phenomena such as excitation, ionization, and charge transfer has great practical importance in many fields of applied physics and technology, the funda-

mental interest in the study of electron capture to the continuum, particularly in the high velocity limit, relates to tests of scattering theory. Atomic physics is justly renowned for its role as a fundamental testing ground for principles of scattering theory, thereby guiding subsequent applications to other fields of science, a role which we shall again find emphasized.

SECOND BORN-INDUCED ASYMMETRY IN ELECTRON CAPTURE TO THE CONTINUUM

The detailed technical issue of central concern to this paper is the shape of the velocity spectrum of the continuum electrons captured by incident bare nuclei into continuum states subsequent to their impact at velocities on the order of 5-20 au on simple atoms (helium, neon, argon). The reason for this focus stems from a conjecture of Shakeshaft and Spruch¹⁰ concerning the origin of an experimentally observed asymmetry in the velocity spectrum of such electrons. Fig. 3 displays typical asymmetries observed for O^{8+} and Si^{14+} ions incident on Ar. In the Shakeshaft-Spruch (SS) model the entire asymmetry of the forward electron distribution may result from the second Born contribution to the scattering amplitude, rather than from the first Born term, with the important caveat that a hydrogenic target approximation has been used. A measurement leverage advantage

Fig. 3. Normalized spectra for electron capture and loss to continuum states in the forward direction for 2.5 MeV/A O^{q+} and Si^{q+} on Ar. Zero-count base lines are shown for each spectrum. Statistical errors are about 2% at the peaks.

therefore arises: A highly specific second Born-induced asymmetry may thus appear at a velocity well below that required to assure dominance of the second Born term in, for example, the total continuum electron production cross section. Of the several experiments under way in our laboratory concerning forward electron production in ion-atom and ion-solid collisions, an eventual quantitative check of the validity of the Shakeshaft-Spruch conjecture represents the most fundamental with respect to tests of basic scattering theory.

HISTORICAL CONTEXT; LINKS TO OTHER TESTS OF ATOMIC SCATTERING THEORY

Before proceeding to this central but detailed issue, I prefer to place it in its interesting historical context, and to link it to other present or proposed tests of atomic scattering theory. The latter include high-velocity electron elastic scattering and excitation experiments, high Rydberg state capture phenomena, and proposed atom capture and positronium formation experiments. It turns out that electron capture to the continuum at high velocities has distinctly classical aspects. Further discussion of these links will follow the discussion of experimental electron capture to continuum (ECC) results.

The historical context has been beautifully summarized in Ref. 2, which we paraphrase here. Ref. 2 discusses three different mechanisms for the capture of a light particle bound to a bare nucleus by a projectile nucleus, incident at a very high relative velocity compared to the orbital velocity of the light particle in question. The first mechanism is knock-on capture, where the two nuclei are of equal mass and simply exchange places. This mechanism is not of current experimental interest, since the capture produces a system essentially at rest in the laboratory frame. The second mechanism is radiative capture, which is accompanied by the emission of a photon. Here the target nucleus plays an almost inconsequential role. The process can be thought of simply as the inverse photoelectric effect, in which the subsystem $m + M_B$ emits a photon and becomes bound. Surprisingly, this process also went experimentally undiscovered for nearly 50 years after its initial 1928 discussion by Oppenheimer.¹¹ Only through the work of Raisbeck and Yiou¹² and of Schnopper et al.¹³ did the importance of this mechanism as an increasingly dominant component of the electron capture process at high velocities become evident.

Thomas Double Scattering

The third and most interesting mechanism is double scattering, first suggested and calculated using classical mechanics by L. H.

Thomas* in 1927.¹⁴ In this mechanism the light particle is first struck by the incident nucleus, and then undergoes a second collision with a target nucleus, in such a way that the light particle emerges from the second binary collision at nearly the same speed and in the same direction as that of the incident nucleus and therefore has significant probability of being captured. The non-radiative capture integrated over the forward direction is thought to be dominated by the second Born contribution. (At high, though still only mildly relativistic, velocities, radiative capture overtakes non-radiative capture.) Not only do the first and second Born contributions to the non-radiative scattering amplitude have different asymptotic velocity dependences, but under some circumstances the second Born term is larger than the first. Furthermore, the velocity dependences of the various Born terms do not always coincide with the asymptotic velocity dependences found, for example, in some approximate approaches to Faddeev-Watson scattering theory calculations.¹⁵

Other Classical Analogs; High Rydberg State Capture; Super-Rydberg States

Additionally, for the capture of an electron bound in one high Rydberg state into another, Shakeshaft and Spruch find that the double scattering mechanism is describable classically, and that Thomas' description becomes exact! Not only does the second Born term once again dominate the first, but it produces a classical result applicable at much lower velocities, as the ratio of projectile to bound electron velocity becomes very large. As will be seen, because electron capture to bound states is thought to proceed smoothly through the ionization limit, measurements of the absolute cross section for production of continuum electrons by the continuum capture process is tantamount to measuring the absolute capture cross section to high Rydberg states. We can make such measurements routinely. The term Super-Rydberg states suggests itself.

Simple physical pictures aid in making plausible the above assertions. It turns out that two of the mechanisms discussed, the knock-on and the double-scattering processes, have close classical analogs. Radiative capture, however, involves a coupling to the radiation field, and therefore is not classically describable. Similarly, the familiar first Born approximation approach to electron capture theory,

* The American Physical Society was honored to receive Professor Thomas himself at a session of papers at its 1980 spring meeting in Washington. Papers presented there concerned what grew out of his work on the Thomas precession, the Thomas-Fermi atom, the Thomas cyclotron, the contributions that Thomas subsequently made to hydrodynamics, and the atomic scattering work discussed here. He is currently active in the fields of gravitation theory and cosmology.

the most venerable of which was performed by Brinkman and Kramers,¹⁶ also lacks any classical analog. According to Ref. 2, any attempt to construct one lacks foundation. The first Born approximation contribution is thus intrinsically quantal in nature, but the second and higher Born contributions have both quantal and classical aspects. In particular, the double-scattering part of the second Born amplitude has the strong classical analog noted.

High and Low Target Electron Momentum Components

Following Ref. 2, we think about a two-particle subsystem, consisting of the electron and the projectile nucleus. At high velocities, this subsystem must lose a very large internal kinetic energy in order for capture to occur. In accounting for this large internal kinetic energy loss, the temptation to assume dominance of a single (first Born) scattering mechanism, where the perturbation is the interaction between the projectile nucleus and the electron, must be resisted. The fact that the first Born term does *not* dominate is related to the inability of a bare nucleus incident on a free electron to capture it. The capture is instead mediated exclusively by the high momentum components of the target atom wave function, components which decrease very rapidly with the magnitude of the incident velocity.

The two mechanisms which do not require the central role of high momentum components of the target atom wave function are the knock-on mechanism already discussed and the Thomas double-scattering mechanism, whose close relationship to the second Born approximation seems first to have been realized by Drisko in 1955.¹⁷ It is surprising to find that the high velocity limit corresponds to a two-step as opposed to a one-step process. Pictorially, the electron is scattered first from the projectile nucleus and then scattered by the target nucleus in such a way that the electron emerges with nearly the same vector velocity as that of the incident projectile. The velocity of the target nucleus is negligibly changed during the collision. The net effect of the double scattering is that the subsystem loses nearly all of its internal energy, so that the projectile and electron can become bound through their Coulomb interaction. The same argument should apply to capture into (slightly unbound) continuum states, since there is a continuous transition in cross section right across the ionization limit. Because the second interaction is between the target nucleus and a fast electron, and not between particles of comparable mass, the energy transferred between the projectile electron subsystem and the target nucleus is negligibly small. In effect, the electron second scatters elastically from the target nucleus, which merely serves to convert the internal kinetic energy of the projectile-electron subsystem into external kinetic energy of the center of mass of this subsystem. Common to each mechanism is an effective means of reducing the initially large internal kinetic

energy of the projectile-electron subsystem. Each mechanism corresponds to a different means of achieving this objective, and to a different asymptotic velocity dependence on the cross section for each.

Figures 1 and 4 present schematic diagrams of the collision geometry, the latter specialized to the double-scattering case. The occurrence of the impact parameter b tacitly assumes the validity of the classical trajectory approximation for the heavy particle motion. The double-scattering mechanism further tacitly assumes the division of either bound or continuum capture by the double-scattering mechanism into two distinct events. The adequacy of these approximations receives comment later.

Fig. 4. Schematic diagram depicting the motion of m and M_B in the lab frame for the double scattering process. M_A remains effectively at rest, and M_B moves with effectively constant velocity 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 $r_A \equiv (r_A, \theta_A, \phi_A)$ with the polar axis parallel to v . The value of r_A for the initial collision is roughly $r_{A1} = (2b/\sqrt{3}, 2\pi/3, \phi_A)$. The position vector of m with respect to M_B , also indicated by a dashed line, is $r_B \equiv (r_B, \theta_B, \phi_B)$ with the polar axis again parallel to v . At the time of the second collision m is very close to M_A - roughly at the break in the thin line - and $r_B \approx r_{B2} = (2b/\sqrt{3}, 2\pi/3, \phi_A)$, setting $\phi_B = \phi_A$. The velocities of m after the first and second collisions are v_1 and v_2 , respectively. The uncertainty principle prevents specification of whether the trajectory of m passes above or below M_A . From Ref. 2.

A Fictitious Quantum Conflict

As already noted, the double scattering mechanism was put forward by Thomas 53 years ago as the dominant mechanism controlling forward electron capture at high impact velocities. His classical calculation went roughly as follows. Thoms conjectured that m must acquire a velocity very close to the velocity of the incident nucleus M_B to be captured. For m much less than M_A , M_B , the heavy particle motion is essentially rectilinear with constant velocity. From consideration of conservation of energy and momentum (see Fig. 4), in the laboratory frame m must first be scattered toward the target nucleus M_A with a speed very close to v and in a direction making an angle of almost exactly 60 deg to the direction of motion of the incident projectile mass. m then scatters from M_A through a second angle of almost exactly 60 deg without changing speed, so that it can then emerge with velocity very close to v . For bound-state capture, the mutual attraction between m and M_B then provides the atomic binding. For capture to the continuum, the physics is nearly the same, but the system is then slightly unbound. Using a purely classical calculation, where quantum mechanics only enters in describing the initial effective value of the orbital radius a at which the struck electron moves, Thomas predicted that the cross section for forward capture by protons from hydrogen atoms should scale as v^{-11} for asymptotically high velocities. Three years later (1930), the initial first Born approximation calculation for the capture process was performed by Brinkman and Kramers.¹⁶ While their calculation omitted some finer details incorporated into what is currently referred to as Bates-Born calculations, and also omitted the nuclear-nuclear repulsion terms, their calculation remains the prototypical first Born calculation. Brinkman and Kramers predicted that the cross section for forward capture by protons from hydrogen atoms should instead behave as v^{-12} for asymptotically high velocities, in serious disagreement with Thomas' result. Since the quantum theory was new and had scored many spectacular successes, the Brinkman-Kramers result was awarded yet another kudo in explaining phenomena that classical mechanics could not. Apparently Niels Bohr and others were nonetheless very puzzled by the difference in the asymptotic velocity dependence predicted in the Thomas calculation vis-a-vis that in the Brinkman-Kramers calculation. Since in the Thomas model a light electron of mass m is scattered through large angles and at high speed, and yet the classical Rutherford cross section turns out to coincide with the prediction of the first Born approximation, the inability of the results to agree was extremely disturbing. Shakeshaft and Spruch assert that for many years it was incorrectly thought that the classical treatment failed to yield the v^{-12} dependence because it neglected subtle wave interference phenomena. Quoting Bohr's classic 1948 article on the penetration of charged particles in matter:

"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 center. 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 field may be decisive."¹⁸

Not until the realization by Drisko¹⁷ that classical double scattering is the two-step process which should correspond to second Born terms in the quantum mechanical treatment did the history of the problem materially change. Drisko's calculation of the Born term in the forward capture scattering amplitude found that for proton-H atom scattering, the asymptotic velocity dependence is v^{-11} . Apart from the issue of the accuracy of the numerical coefficient, the puzzling discrepancy between the classical and quantum results thereby was resolved.

Many features of the double-scattering process are predicted to be essentially classical² for high velocities. The argument goes that because each collision involves a momentum transfer to m of order mv , a large quantity even for a particle of small mass at sufficiently high velocities, each collision is a close one. The wave length of m between the two collisions will be of the order of h/mv , which is very much smaller than the separation of the nuclei for almost all important impact parameters. Thus the motion of m between collisions is nearly classical because each collision is very nearly binary, and interference effects between the two collisions are presumably small.

EXPERIMENTS CHARACTERIZING THE VELOCITY DISTRIBUTION OF ECC ELECTRONS

We now turn to a specialized discussion of how continuum electron capture experiments relate to the theoretically predicted first Born and second Born contributions to electron capture, emphasizing high collision velocities. Little theoretical work has been done in this field concerning targets other than atomic hydrogen, so in discussion of other atomic targets it is implicitly assumed (with unknown accuracy) that the target electrons can be treated in a hydrogenic approximation, shell by shell. As will be seen subsequently, there is experimental evidence in favor of this point of view for He, Ne, and Ar targets.

To characterize the velocity distribution of capture to continuum (ECC) electrons, various properties of the differential cross section for their production near the forward direction, $d\sigma/dv_e$ near 0 deg, are measured.

It is instructive to examine the structure of certain simple formulas initially developed by Dettmann et al., who made the first calculation¹⁹ of $d\sigma/dv_e$ within a first Born, Brinkman-Kramers approximation (also, apparently with some errors,² a second Born calculation).

Because the Brinkman-Kramers cross section decreases² as $1/v^{12+2\ell+2\ell'}$, where ℓ and ℓ' are the orbital angular momentum quantum numbers of the initial and final states, only the s-wave component of the continuum eigenfunctions is important. This circumstance leads to isotropy of electron emission in the projectile rest frame. Letting $\vec{v}$ denote the velocity of the emergent electron in the laboratory frame, the projectile rest frame velocity $\vec{k}/m$ is related to $(\vec{v}, \vec{v}_e)$ by $\hbar\vec{k} = m(\vec{v}_e - \vec{v})$.

To leading order in $1/v$, the Brinkman-Kramers contribution is thus isotropic in the vector $(\vec{v}_e - \vec{v})$, in contrast to the prediction² that for Thomas double scattering $d\sigma/dv_e$ contains components of many different ℓ' whose weights are *independent of v* to leading order in $1/v$, which could in principle interfere with one another. The principal experimental goal is thus the measurement of the degree of anisotropy of $d\sigma/dv_e$ under the reflection $\vec{k} \rightarrow -\vec{k}$, or equivalently $(\vec{v}_e - \vec{v}) \rightarrow -(\vec{v}_e - \vec{v})$.

The experimentally desired quantity thus becomes the differential cross section for the electron to emerge in a narrow forward cone of specified half-angle θ_0 with a speed v_e close to v , that is $d\sigma/dv_e$ averaged over θ_0 (typically ~ 1 deg). The degree of asymmetry in $d\sigma/dv_e$ for $v_e \geq v$ with respect to $v_e \leq v$ directly tests the adequacy of the first Born description vis-a-vis higher Born terms.

The average is experimentally tricky because $d\sigma/dv_e$ is predicted to *diverge* at exactly 0 deg. Averaging over θ_0 produces a cusp-shaped measured differential cross section. In the form provided in Ref. 2, the Brinkman-Kramers result for $d\sigma/dv_e$ becomes

$$\frac{d\sigma_{BK}}{dv_e} (ls \rightarrow cont) \sim \frac{2^{17}}{5} Z_A^5 Z_B^3 \left(\frac{e^2}{\hbar v} \right)^{10} \frac{1}{v^2} \times \{[(v_e - v)^2 + (v\theta_0)^2]^{1/2} - |v_e - v|\} (\pi a_0^2). \quad (1)$$

The divergent cross section in exactly the forward direction arises from an approximation to the Coulomb wave normalization factor (to be discussed later) appropriate to the case where the emergent electron is moving relative to the projectile nucleus with an energy $\hbar^2 k^2 / 2m$ that is small compared to the ionization energy of the electron-projectile subsystem.

The divergence of the differential cross section at $k = 0$ can be made more transparent through use of an argument made originally by J. Macek²⁰ and applied more recently by C. Bottcher²⁰ to electron loss to continuum processes. We let the spherical polar angles of $\vec{v}_e$ be (θ, ϕ) and those of $\vec{k}$ be (β, α) . In the two frames $E = 1/2 v_e^2$ and $E = k^2/2m$ (in atomic units). Let the triply differential cross section for production of electrons with momentum k in the moving frame be

$$I_{\text{proj}}(\epsilon, \beta, \alpha) \equiv \frac{d^3\sigma}{d\epsilon d\cos\beta d\alpha} = \frac{k d^3\sigma}{d^3k} \quad (2)$$

Because the Coulomb potential scales as $E_n = -1/2n^2$, and, under the assumption (to be questioned later) that the s-wave scattering is dominant, as predicted by the well-known $\sigma_n \sim n^{-3}$ rule of Oppenheimer, $d\sigma/d\Omega \sim dn/n^3 \sim dE$ and continues smoothly across the ionization limit. One is therefore able to relate the laboratory frame differential cross section to I_{proj} by

$$I_{\text{lab}}(E, \theta, \phi) = \frac{v_e}{k} \frac{d^3k}{d^3v_e} I_{\text{proj}}(\epsilon, \beta, \alpha) \quad (3)$$

Because $\vec{v}_e$ and $\vec{k}/m$ are related by a pure translation $\vec{v}$, $d^3k = d^3v_e$, so that

$$I_{\text{lab}}(E, \theta, \phi) = \frac{v_e}{k} I_{\text{proj}}(\epsilon, \beta, \alpha) \rightarrow \infty \text{ as } k \rightarrow 0. \quad (4)$$

Energy intervals in the laboratory and projectile frames are similarly related by the potentially large expansion factor

$$dE/d\epsilon = v/(k \cos \beta). \quad (5)$$

Important properties of Eq. (1) include: the cubic dependence on Z_B ; the fifth power dependence on Z_A ; the v^{-12} dependence on the fore-factor of the quantity in curly brackets; the cusp-shaped behavior of the quantity within curly brackets; the symmetry in velocity with respect to change of sign of the quantity $(\vec{v}_e - \vec{v})$ - i.e., the cusp is predicted to be *symmetric* about the ion velocity; and the scaling of the full-width half maximum of the cusp-shaped distribution with ion velocity. This scaling is given by $\Gamma = (3/2) v \theta_0$, where Γ denotes the full-width half maximum of the measured velocity distribution.

As we have already seen from Fig. 3, experimental electron capture to continuum spectra exhibit significant asymmetry skewed toward electron velocities below the ion velocity, though we are quick to note the observed cusps do not correspond to hydrogenic targets. It turns out, however, that similar cusp-shaped distributions are observed for all gaseous targets we have tried to date, and these include helium, neon, and argon. The yield - the number of observed

electrons per incident ion, integrated over a suitable velocity interval $(1 \pm \alpha)v$ about the ion velocity - does, of course, depend on the choice of target system ($\alpha \sim 4\%$ is convenient). In general, the Z and v dependences of our observed yields are weaker than given in Eq. (1), though this is to be expected for ion velocities in the range 5-20 au for relatively heavy targets such as argon, which moreover possesses several shells. Fig. 5 provides some representative results. As is seen, the velocity dependence for some very recent data on He obtained in collaboration with our LBL colleagues, C. R. Vane, H. Gould, and R. Marrus at the Berkeley Super-HILAC, is much nearer that predicted by Eq. (1) - $\sim v^{-10}$ - for the highest velocities used (15-18 au). There is therefore considerable hope that helium, at least, can be treated in a hydrogenic target approximation. Cusp shape evidence also favoring this point of view will be presented shortly.

Generally speaking, for all incident projectiles used ($Z_B = 1-18$), all incident velocities used ($v = 5-18$ au), and all targets used ($Z_A = 2, 10, 18$), the observed electron velocity distribution has never been seen to correspond to the symmetric distribution predicted by the Brinkman-Kramers calculation for electron capture to the continuum by bare ions. It was perhaps this observation that led Shakeshaft and Spruch to their interesting conjecture that the origin of the observed asymmetry at high velocities may arise from the Thomas double scattering contributions. We note in passing that for electron

Fig. 5. Differential cross section for production of ECC electrons by a variety of bare nuclear projectiles C^{6+} , O^{8+} , Si^{14+} and Ar^{18+} in He, Ne, and Ar, as a function of v . The $Z_B^{2.2}$ scaling has been incorporated in the ordinate scale. Data from C. R. Vane.

loss processes, which arise when projectile ions possessing electrons initially undergo ionizing collisions, the observed cusps are narrower and more nearly symmetric (see Fig. 3, where rich low-energy Auger structure²¹ is also visible superposed on the cusps for these more symmetric peaks).

Another property of the data inconsistent with Eq. (1) is the behavior of the FWHM, $\Gamma \approx 3/2 v\theta_0$. While we find that Γ in most cases scales roughly as v , only the total FWHM does so. If divided into left-right FWHM's corresponding to $v_e \leq v$, $v_e \geq v$, Γ_R turns out always to be of the order expected from consideration of analyzer resolution (typically $\lambda \approx 1\%$), while Γ_L accounts for the bulk of the growth of Γ with v . Furthermore, there are significant shell effects, as can be seen very clearly in Fig. 6. There Γ_L is seen to rise significantly just as the beam velocity is varied through the range $v \approx v_K$, where v_K represents the K-shell electron velocity in Ne. Similar K-shell effects, though less well resolved, are seen in Ar. Ar possesses three shells whose contributions overlap. Theory has yet to fold in the internal velocity distribution of ECC electrons in explicit quantitative calculations, as the approximation $v \gg Z_A v_B$ is normally made. The onset of the rise in Γ_L occurs just where the Bohr velocity matching criterion¹⁸ would predict.

Fig. 6. Half widths-half maximum for the lower (Γ_L) and higher (Γ_R) energy sides of the continuum capture peaks for O^{8+} in He, Ne, Ar. Note the large shell effect in Ne as the condition $v > v_K \sim 10$ au. A similar effect is seen in Ar for $v \sim v_K \sim 18$ au.

Experimental Techniques

Two different methods of measuring $d\sigma/dv_e$ have been used, one relying on a spherical sector electrostatic analyzer for the velocity range below 15 au, and the other a magnetic sector analyzer for higher velocities. The choice of a magnetic analyzer for higher velocities not only is technically simpler (~ 4 keV electrons), but permits use of virtual rather than physical entrance slits through use of suitable non-magnetic apertures located within the analyzer. Suppression of neutron and gamma-ray backgrounds at the higher velocities proves crucial.

A schematic diagram of the electrostatic variant is shown in Fig. 7. Projectile ions from the ORNL or BNL tandem accelerator traverse a thin gas or interchangeable solid target over a velocity range corresponding to 0.7 - 5 MeV/u. All beams are typically collimated to a 1/3 mm diameter and $\pm 0.025^\circ$ angular spread, and then traverse a 4 mm-thick target cell terminated by ~ 2 mm apertures (or a foil target centered at the same location). The beam and accompanying electrons then enter along the central ray of a 180° spherical-sector analyzer of mean radius 3.8 cm, whose $\Delta E/E$ of 1.4% full width at half-maximum is set by a 0.71 mm analyzer exit aperture and the source dimensions at the center of the cell. The minimally deflected ion beam passes through an aperture in the larger-radius plate of the analyzer and into a Faraday cup used for beam normalization. Typical

Fig. 7. Schematic diagram of the forward peak electron spectrometric apparatus. (1) 0.71 mm aperture; (2) 0.33 mm aperture; (3) 4 mm long gas cell, 2 mm exit aperture; (4), (5) inner, outer spherical sector plates; (6) 0.7 exit aperture; (7) negative biased electron multiplier cone; (8) 7.9 mm Faraday cup shielding aperture; (9) bias ring for adjacent Faraday cup; (11) analyzer housing; (12) variable entrance aperture; (13) electron multiplier output.

gas pressures of ~ 15 mTorr are established by a standard feedback-controlled capacitance-manometer system. Single-collision conditions and negligible charge changing are established by linear plots of integrated cusp cross sections versus pressure for the various ions and energies. The plot intercepts typically coincide precisely with very small residual cusp cross sections measured at zero pressure. Spurious signals from electron loss by contaminant beams were ruled out, as deliberate changes in the accelerator vacuum by a decade in pressure produced no noticeable effect on pressure linearity. The fine collimation guarantees that the beam never encounters any aperture or surface in the gas cell or spectrometer regions, as verified by very low spurious signals obtained at zero pressure. Magnetic fields are reduced to $< 3 \times 10^{-6}$ T over the spectrometer volume by three orthogonal external coils. Changes in coil current of $\leq 20\%$ produce negligible changes in cusp shape and integrated production cross sections.

A schematic diagram of the magnetic variant is shown in Fig. 8. The need for the previously noted nuclear radiation background suppression is in this case exacerbated by the large beam diameter (~ 1 cm) characteristic of linear accelerators such as the Super-HILAC accelerator at LBL. Consideration of this background and conservative projections of the small electron count rates anticipated for light targets such as He at high velocities led to correspondingly conservative choices of resolution determining parameters, in the interest of high collection efficiency. Otherwise, the techniques and dimensions are comparable to those for the electrostatic case. As we shall see, the initial ECC asymmetry data obtained with this instrument are so encouraging and the feared background and intensity problems sufficiently under control that in the future better resolution at the expense of gathering power can be used. A photograph of the instrument is provided in Fig. 9.

Briefly, 15 and 18 au beams of bare Ar ions obtained from the LBL Super-HILAC accelerator pass through a ~ 2 cm long gas cell containing He, Ne, or Ar at pressures well within single collision conditions. The cell is situated at the entrance focus of a double focusing, 90 deg magnetic sector analyzer set to record electron spectra for ejection with a cone of half-angle $\theta_0 = 1.7^\circ$, centered on the forward direction. The momentum resolution is 1.7% FWHM. This instrument, capably designed and executed by a very able graduate student, Scott Berry, follows the high resolution, low aberration design principles (as low as 2 ppm) of an electron microscope analyzer designed originally by Crewe and Isaacson.²² The source volume of dimensions ~ 2 cm in length and 4.0 mm in diameter was defined by graphite collimators of diameters 6.4 mm and 3.2 mm situated upstream of the entrance focus by 2.5 m and 0.2 m, respectively. The resolution was determined by the source size and by an aperture of diameter 3 mm situated at the exit focus of the magnetic analyzer. The electron flight path within the analyzer was about 37 cm in length. The

Fig. 8. Schematic diagram of magnetic sector spectrometer. Ion beam enters spectrometer (1) and exits to Faraday cup (or CEM) (2). Electrons follow curved path (3) through pole pieces (4). Mirror pieces (5) shape field edges for improved focusing. Shield pieces (6) minimize magnetic fields along electron path, house gas cell (7) defined by apertures (8), angle defining aperture (9), and exit aperture (10). Channel electron multiplier (CEM) detector has negatively biased cone (11).

The collection geometry for electrons near $v_e \approx v$ ejected within a cone of half-angle $\theta_0 \sim 1$ deg near the forward direction is schematically illustrated in the lower figure.

Fig. 9. Photograph of Oak Ridge Magnetic Sector Analyzer (ORMS Analyzer). Courtesy of Scott Berry and Sven Huldt. See Ref. 22 for design principles.

acceptance angle θ_0 was determined by the field of view of the exit aperture and a second aperture of diameter 6.4 mm situated 10.7 cm upstream. Stray electrons generated upstream of the experiment were rejected by repeller electrodes mounted just prior to the gas cell. The radiation backgrounds, believed to result from neutron and gamma rays generated at upstream collimators and in the beam dump, proved to be far less severe than originally feared (typically less than 20%). In any event, these backgrounds could be easily removed from the data by subtracting so-called "gas dump" spectra acquired when an unaltered amount of gas was fed directly into the vacuum system through a simple high-conductance by-pass valve, leaving all other experimental conditions fixed.

Initial Tests of the Second Born-Induced Asymmetry Conjecture for
15-18 au Ar^{18+} Traversing He, Ne, Ar

The outcome of the first tests of the predicted second Born asymmetry conjecture - for Ar^{18+} on He - is the principal subject of this section. These experiments were performed at the LBL Super-HILAC accelerator, in collaboration with Richard Marrus, Harvey Gould, and Randy Vane. Asymmetries have very recently been measured for higher velocities (15-18 au) and for a heavier bare projectile (Ar^{18+}) than used heretofore, for ECC in He, Ne, and Ar. The results provide guidance to and stimulus for further quantitative calculations, especially for He. Strictly, the theoretical results apply to hydrogenic targets and may need modification for He.²³ A second issue is the conflicting need for $Z_B \gg 1$ projectiles, because the second Born asymmetry is highly Z-dependent, while simultaneously requiring $\sqrt{Z_A Z_B} \times e^2/\hbar v, \ll 1$. For $Z_B \sim 1$ the asymmetry is predicted to be small. But for large v the highly asymmetric second Born contribution has small yield. Because v should lie below the range where radiative capture dominates, the ideal Z and v parameter ranges are narrow. The obvious desirability of obtaining data for atomic H targets at slightly higher impact velocities presents fierce unsolved experimental problems.

A counter-conjecture concerning the origin of the observed asymmetry is provided by Chan and Eichler,²⁴ who note that retention of terms linear in $\Delta v_e/v = (|\vec{v}_e - \vec{v}|)/v$ beyond those incorporated in the first Born-Brinkman-Kramers (BK) approach originally used by Dettmann, et al.,¹⁹ produces a similar asymmetry when compared^{10, 24} to earlier Ar target data at $v = 9$ au.⁹ However, predictions of Refs. 10 and 24 concerning the projectile Z and v dependence are very different, as is the predicted shape of the corresponding cusps (note the extremely sheer drop of the high velocity edge for the second Born cusp depicted in Fig. 10, curve B). These differing dependences enable experiment to distinguish between the various theories. For example, it is predicted¹⁰ that ECC for high velocity projectiles $Z_B \sim 1$ is dominated by the first Born asymmetry, but that for $Z_B \gg 1$, the second Born term dominates.

Typical data for Ar^{18+} on He are displayed in Fig. 10, overlaid with the best fits to the data obtained with a convoluted Shakeshaft-Spruch (SS) line shape (curve A), and a convoluted Chan-Eichler (CE) line shape (curve D). Data were acquired over a wider velocity range, but since detailed line shape predictions apply only very near $v = v_e$, only the corresponding region is displayed. Convolution of the best fits to parameterized theoretical line shapes (curves B and E) with the 1.7% FWHM, nearly triangular apparatus function shown in curve H (from electron gun calibration data) produced A, D. That the asymmetries observed are valid is demonstrated in curve G, which depicts the narrower, much more symmetric line shape (with Auger structure superposed) obtained for forward electron loss⁹ from 8.5 MeV/u Ar^{18+}

Fig. 10. Comparison of the central portion of ECC cusps obtained for 18.1 au Ar^{18+} on He with the overlaid best fit line shapes from Ref. 10 (A) and Ref. 24 (B). The respective best fit theoretical shapes (B and E), when convoluted with the measured apparatus function (curve H), produce fits (A) and (B). A narrower, more symmetric ELC spectrum for 18.1 au Ar^{18+} on He is shown in (G).

on Ar. Here only the incident beam was switched, with all other conditions unaltered.

Possible target contamination was a serious worry owing to small ECC cross sections in He. Results for both low and high (six 9's) purity He were compared. Leaks and contamination in the gas feed and transfer lines were ruled out by examining backgrounds with the He tank valve closed and the leak valve to the cell open. Data with and without LN trapping of the feed gas were compared. Final data were acquired with a high purity tank unopened prior to evacuation of baked and LN trapped gas feed lines.

Because the theoretical curves B and E apply to $Z = 6$ at 9 au in a hydrogenic target, our comparisons are only partially appropri-

ate. However, these comparisons are so successful that a quantitative calculation for $v = 15-20$ au in He is strongly indicated. The characteristic feature of the SS shape is the sheer drop on the high-velocity side of the peak. When convoluted with the instrument function, a drop is expected whose slope and width are essentially determined by the analyzer resolution function - a feature displayed by every ECC cusp we have ever observed for C^{6+} , O^{8+} , Si^{14+} , and Ar^{18+} in He, Ne, and Ar at all velocities (5-18 au)! This property is *not* shared by the CE shape. Second, the SS shape is predicted to persist with increasing ion velocity, whereas that of the CE model is predicted to become symmetric at high v as $\sim 1/v$. There is *no* evidence in our data for any decline in asymmetry. On the contrary, for He the asymmetry (as defined below) is found to rise very slightly in the range 15 to 18 au (consistent with v independence within errors). For C^{6+} , O^{8+} , and Si^{14+} on Ne, the asymmetry is a strongly increasing function of v in the range 7-18 au, rising sharply as the neon K-velocity matching condition is reached (see Fig. 6). Third, the ECC asymptotic velocity dependence of $d\sigma/dv_e$ predicted by Dettmann et al.,¹⁹ when integrated over an appropriately scaled velocity region (e.g., $(1 - \alpha)v$ to $(1 + \alpha)v$, with $\alpha = 0.04$) is $\sim v^{-10}$. This dependence coincides with our experimental results for Ar^{18+} in He, which (over the range $v = 15 \rightarrow 18$ au) scale as $\sim v^{-9.9}$, suggesting that the anticipated asymptotic dependence has been reached (not so for either Ne or Ar targets, which scale as $\sim v^{-7}$ over the same range).

Standard reduced χ^2 tests, in addition to a deviation test to be described, exhibit a marked preference for the SS as opposed to the CE shapes. For the data of Fig. 1, the fitted SS line shape yields $\chi^2 = 1.2 \pm 0.2$, whereas the CE shape yields 1.8 ± 0.4 (a value from 0.5 to 1.5 is "respectable"). At the same velocity, the analogous values are $\chi^2 = 6.5$ and 10 for Ne, and 8.9 and 10.8 for Ar, values which demonstrate the inappropriateness of a single cusp fit to data we expect to be characterized by overlapping cusps of somewhat different width for each shell. Curves C and F are derived from the deviation spectrum ($y_i - y_{FIT}$, vs. i) corresponding to A and B. To extract trends from the large statistical scatter in the deviation spectrum, we have appropriated the moving average technique routinely used by Wall Street chartists when confronted with similar scatter in financial market averages. Curves C and F represent ten-channel moving averages, smaller than but of the same order as the analyzer resolution (16 channels). The clear preference for the SS vs. the CE fit is exhibited by the large dip in curve F, which shows that the CE shape simply lacks the drop-off characterizing both the SS line shape and - by this test - the data. A moving average over fewer channels *enhances* the valley in the deviation spectrum (at the expense of scatter). In dozens of spectra acquired for He, Ne, and Ar, similar valleys were invariably absent for SS fits and invariably present for CE fits.

Spontaneous evidence that the drop-off is real arose in the fitting procedure. The CE shape was simulated by multiplying a symmetric Dettmann cusp shape (Eq. (1)) $A[(v_e - v)^2 + v^2 \theta_0^2]^{1/2} - |v_e - v|$ by the asymmetric function $[1 - a(v_e - v)]$, with a starting value of the fitted parameter $a \approx 0.73$, read from Ref. 24. A very similar multiplicative factor $\{[1 - a(v_e - v)]$ for $v_e \leq v$ and $[b - a(v_e - v)]$ for $v_e \geq v\}$ simulated the SS shape, where the values $(a, b) = (0.73, 1)$ characterize the CE shape, and $(0.73, 0.63)$ characterize the SS shape read from Ref. 10. A key point is that the *starting* values of (a, b) in the SS case were chosen to be $(0.73, 1)$, deliberately biasing the iterative, gradient search, least squares fitting routine in favor of the CE shape. The fitting routine spontaneously introduced an SS step! The best fit values for 18 au Ar¹⁸⁺ on He gave $(a, b) = (0.12 \pm 0.02, b = 0.44 \pm 0.04)$ for the SS fit ($\chi^2 = 1.2 \pm 0.2$), and $a = 0.69 \pm 0.1$ ($\chi^2 = 1.8 \pm 0.02$) for the CE fit. Direct deconvolution of the data yielded results entirely consistent with those just given. However, the discontinuity in derivative at the tip of the cusp renders the deconvoluted fit exceedingly sensitive to variations in peak channel amplitude, making conclusions about, for example, full-width half maximum and left-right asymmetry subject to considerable uncertainty.

One experimental, model-independent measure of the asymmetry is the ratio $(\Gamma_L - \Gamma_R)/(\Gamma_L + \Gamma_R)$, where Γ_L and Γ_R are the half widths (half maximum) of the cusp to the left and right of the peak. At 15 au, the measured values in He, Ne, and Ar are 0.28, 0.45, and 0.35, respectively. At 18 au, they are 0.35, 0.39, and 0.44, respectively. The uncertainties are ± 0.07 in each case. The Ne asymmetry results are dominated by ECC of the Ne-1s electrons (v is appreciably greater than the Ne K-shell electron velocity). A measurable increase in the observed asymmetry for Ar targets is ascribed to the approach to K-shell velocity matching taking place in the velocity region 15-18 au.

Though the present shape and velocity dependence data are much better in accord with Ref. 10 than with Ref. 24, other predictions of Ref. 10 are not observed. For example, the asymmetries observed in Ne, Ar are very similar for all bare projectiles ranging from $Z = 6$ -18, a finding not in accord with a predicted strongly Z -dependent asymmetry. Also, the yields scale as $\sim 1:200:500$ for 18 au Ar¹⁸⁺ on He, Ne, and Ar, respectively, a dependence much weaker than a simple Z_A^5 dependence.¹⁰ (For a multi-electron target, no simple Z_A dependence is anticipated).

Confirmation of a drop-off at $v = v_e$ at least as steep as the analyzer resolution function permits is thus the most encouraging evidence in favor of the SS asymmetry conjecture provided by our data. An attractive experimental goal we intend to pursue is to better quantify the size of the drop-off by improving the instrument resolution at the expense of intensity. We recommend a theoretical goal:

a serious quantitative calculation of the predicted second Born-induced asymmetry for several bare nuclei traversing He in the present velocity range. Present results both demonstrate the feasibility of future quantitative experiments of this type and suggest that the two electrons of He do not introduce appreciable additional complications (e.g., interference structure, additional electron-electron scattering complications).

Source of the Asymmetry

The source of the asymmetry depicted in Fig. 10 has been described in detail in Ref. 10, and in a somewhat simplified manner in Ref. 2. Here we follow the discussion of Ref. 2, which treats only the v^{-11} contributions to the differential cross section explicitly. The asymmetry arises in the context of a specific application of a more general result derived by Shakeshaft and Spruch for the differential cross section for double scattering. The final SS result for the differential cross section for double scattering per unit impact parameter is given by the following equation:

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

where

$$\vec{r}^* = (2b/\sqrt{3}, 2\pi/3, \phi). \quad (6)$$

Here $W_A(r)$ and $W_B(r)$ denote the interactions between m and M_A and between m and M_B , and $\tilde{W}_A(mv)$ and $\tilde{W}_B(mv)$ refer to the Fourier transforms of these distributions with respect to the argument $p = mv$. $\psi_f(r)$ refers to the electronic wave function of the final state f and ψ_i refers to the initial atomic state wave function.

The term "capture to the continuum" refers to the situation in which the electron emerges slightly unbound, in a continuum state just above the highest Rydberg states possible, i.e., just above the ionization limit. The adaptation of Eq. (6) to this case is undertaken in Ref. 2 under the assumption that the emergent electron moves relative to the projectile nucleus with a positive energy that is small compared to the ionization energy of the electron-projectile subsystem. The wave function ψ_f is replaced² by $\psi_k^{\rightarrow}(\vec{r}^*)$, where $\vec{k}$ then denotes a continuum Coulomb wave function:

$$\begin{aligned} \psi_k^{\rightarrow}(\vec{r}^*) &= (2\pi)^{-3/2} e^{i\pi/2} \Gamma(1 + in) e^{i\vec{k} \cdot \vec{r}} \\ &\times {}_1F_1[-in, 1, -i(kr + \vec{k} \cdot \vec{r})], \end{aligned}$$

where

$$k = |\vec{k}| \text{ and } \eta = Z_B/(a_0 k). \quad (7)$$

After a number of additional approximations, Shakeshaft and Spruch derive the following equation to describe the differential cross section for electron capture from a hydrogenic 1s orbit to the continuum, in the asymptotic velocity limit:

$$\frac{d\sigma}{dv_e} (1s \rightarrow \text{cont}) \sim 2^5 Z_A^4 Z_B^3 \left(\frac{e^2}{\hbar v} \right)^9 (\pi a_0^2) I(v_e),$$

where

$$I(v_e) = \int d\Omega_e \frac{1}{|\vec{v} - \vec{v}|} J_0 \left[i \left(\frac{Z_B}{Z_A} \right) \chi \right] \exp \left[- \left(\frac{Z_B}{Z_A} \right) \chi \right], \text{ and}$$

$$\chi = 1 + \hat{k} \cdot \hat{r}^*. \quad (8)$$

Among the most important of these approximations is one already noted, $\eta \gg 1$; r^* is effectively restricted by the initial wave function to satisfy $r^* \lesssim a_0/Z_A$.

The factor $\chi = 1 + \hat{k} \cdot \hat{r}^*$ is for obvious reasons referred to as the "asymmetry source factor." Eq. (8) lacks the transparent analytic form available for the BK cusp described by Eq. (1) and requires an explicit numerical evaluation on a case-by-case basis. However, $I(v_e)$ has some simple properties² whose identification assists interpretation of Eq. (8). Because $I(v_e)$ scales as v^{-2} , the v dependence of Eq. (8) is v^{-11} (as in the Thomas calculation). Because $I(v_e)$ has a cusp at $v = v_e$, Eq. (8) also displays one, just as does Eq. (1). Experiment thus seeks to test the modifications to Eq. (1) brought about by the asymmetry source factor $\chi = 1 + \hat{k} \cdot \hat{r}^*$.

OTHER ATOMIC PHYSICS TESTS OF HIGH VELOCITY BORN EXPANSIONS

A primary assertion of Ref. 2 is that in a variety of high velocity collision situations, the double scattering mechanism is thought to be the dominant non-relativistic mechanism for radiationless capture into the forward direction, even if the Born scattering series does not converge. It has often been suggested that the Born series for an exchange amplitude which includes charge transfer diverges. What is less clear is the significance of this result for a calculation which stops at the second Born term. Because the Born series may be an asymptotic series, the question of which term(s) are dominant at high velocities becomes important.

Appropriateness of Approximations Used for Heavy Particle Collisions

Some comment on the appropriateness of the impact parameter and other approximations is in order. The appeal of constructing classical approaches to heavy particle collision phenomena arises in part from the remarkable circumstance that the differential cross section for non-relativistic Rutherford scattering between two charged particles is identical whether calculated classically or alternatively by means of the first Born approximation. Though much attention has been paid to use of such approximations to describe charge transfer phenomena, substantially more has been paid to those used to describe charged particle ionization phenomena. As calculated in the first Born approximation, heavy particle ionization cross sections for inner electrons are similarly sensitive to the high momentum parts of the momentum distribution of the electrons to be ionized, in contrast to the situation prevailing for electron impact ionization and the photoelectric effect. The exact correspondence between the Rutherford cross section for scattering of two heavy charged particles, whether calculated by the first Born approximation or classically, has stimulated development of classical binary encounter models of the ionization phenomenon. The so-called binary encounter approximation postulates a classical collision between the projectile and the atomic electron, where, because the projectile and target nuclear systems both have heavy masses, it is reasonable to describe the relative heavy particle motion in terms of curvilinear classical trajectories. The electron is of course viewed as a quantum object, but most of the quantum behavior is determined by the static electronic wave function of the electron prior to the collision interaction. When more than one target electron exists, it is customary to treat the collision between the projectile and the target system in terms of a binary encounter between the projectile and a particular active electron. The rest of the target electrons (if any) are regarded as spectators in the collision, becoming available for secondary or tertiary scattering at high collision velocities. The accuracy and legitimacy of the classical trajectory approach to heavy particle-atom collisions has been broadly described in a general review article by Madison and Merzbacher,²⁵ to which the reader is referred for justification of similar approximations. In the preceding discussion, we assumed that any electron which undergoes a large change of momentum in a double scattering or backward scattering process does so through a binary collision. It is asserted² that the Coulomb potential is sufficiently singular to make this assumption an accurate one. Thus, phenomena such as close nuclear collisions and sequential close electron-nucleus collisions, as in double scattering, can be treated in this approximation. For high v , $\hbar k/mv$ is so small that even the electron motion can be described classically between collisions.

Electron Impact Elastic Scattering and Excitation at High Velocities

There is, of course, an enormous literature concerning the accuracy of the first Born series in accounting for scattering cross sections in many different subfields of physics. Within atomic physics, for example, one can trace a long history of tests of the first and higher Born terms in electron-atom elastic scattering and excitation. For example, a helpful capsule review published by Joachain²⁶ appeared in 1977. In particular, Byron and Joachain have looked into details of elastic scattering from the ground states of atomic hydrogen and helium. The dominant contribution to the direct elastic scattering amplitude is thought to be given by the first Born approximation at most momentum transfers. According to Joachain, appreciable contributions from the first, second and third Born approximation amplitudes are required to give reasonably good agreement at small angles.

The situation is different for direct inelastic collisions, in which the target atom is excited from the ground state to some final excited state. For s-s transitions, it is found that, although the first Born term still dominates at momentum transfers less than or on the order of one au, the situation is different for high momentum transfers. When the momentum transfer is large the Born series is thought to be dominated by the second Born term. This situation arises because the electron-nucleus "Rutherford" cross section becomes relatively important, with the additional electronic excitation playing a parasitic role. Given that an excitation exists, it is likely to arise as secondary in a double-scattering event. Because the first Born term for inelastic scattering is found to fall off very rapidly with increasing momentum transfer compared to that for the elastic amplitude, Joachain's interpretation is that the most effective way for the system to undergo a large-angle inelastic transition is by means of a two-step process, beginning with a small-angle inelastic collision combined with a large-angle elastic scattering through a virtual intermediate state. The situation is similar for s-p transitions, though the relationship among the various order contributions to the scattering amplitude is said to be much more angle-dependent than for s-s scattering.

Comparison is made by Joachain to the results of two elastic scattering experiments²⁷ for electrons in atomic hydrogen at 50 eV, where a serious deficiency of the Born approximation amplitude is noted at angles in the range 10-40 deg. In comparing theory with several different experiments²⁸ concerning inelastic scattering to the 2^1S state in He at 200 eV, the striking failure of the first Born approximation to account for the differential cross section at angles larger than 40 deg is demonstrated. Impressive success in accounting for these large-angle data by means of inclusion of higher Born terms is claimed.

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Fig. 11. Contour maps of the electron density in a head-on H^+-H collision at 20 keV. The collision is shown in the center-of-mass frame. Because of the rotational symmetry about the z axis the electron density is drawn only in the z - p plane. The positions of the nuclei are indicated by crosses. The elapsed times for each frame are given on the upper left in units of 10^{-17} sec. From one contour line to the next the density changes by a factor of 10, indicated by the numbers for the negative exponents in the figure. From Ref. 29.

quantum feature introduced is the choice of a . In Ref. 2, an exposition of the exactitude of Thomas' result for high Rydberg state atoms is given. It has already been noted that the double-scattering capture mechanism does not depend on the high momentum components of the bound state wave functions, whereas both the radiative and the Brinkman-Kramers amplitudes do. When an atom is in a high Rydberg state, the electron moves in a fairly well-defined orbit and has a narrow momentum spectrum. It is reasonable to anticipate that the double-scattering capture cross section for a projectile incident on a high Rydberg atom should be very large compared to the non-classical radiative and Brinkman-Kramers cross sections, and that owing to the low velocity in the Rydberg electrons, the approach of the cross section to the asymptotic regime should occur at substantially lower velocity. Thomas' classical result for double scattering is quoted in the following equation:

$$\sigma_{ds} (a \rightarrow bd) \sim \frac{2^{13/2} \pi Z_A^2 Z_B^{7/2}}{3} \left(\frac{e^2}{mv^2} \right)^{11/2} \frac{1}{a^{7/2}}. \quad (9)$$

Quantum physics enters only in the choice of a , for which Thomas chose the value a_0 . Spruch finds that a very good estimate for

double-scattering capture to a bound state from a high Rydberg state emerges³⁰ from an appropriate quantum mechanical choice of a , for which choice the Thomas result becomes exact. (The adequacy of the classical description of the entire process for high Rydberg states depends on the circumstance that capture to a bound state *from* a high Rydberg state occurs predominantly *to* a high Rydberg state. Theory predicts this to be the case.) The appropriate choice of a appears to be $a = n^2 a_0 / Z_A$.

ATOM CAPTURE

In electron capture to bound states or to the continuum, the magic angle of 60 deg arises owing to the small ratio of electron to heavy particle mass. Because of the small electron-to-nucleon mass ratio, the incident nucleus is scattered forward through a very narrow range of angles close to 0 deg, with negligible change in speed. When the projectile and electron masses are equal, as prevails for the case of positron-electron scattering, the analogous angle is very close to 45 deg for each of the light particles, in the laboratory frame. Another interesting case of equal masses arises in a recent discussion of a process called "atom" capture by protons incident on a hydrogenated molecule³¹ containing a single heavy atom. In the approximation that the heavy constituent in the molecule is infinitely massive, a condition, for example, approximately met by the carbon atom in methane, the p-H laboratory frame scattering angle is nearly 90 deg. The second scattering occurs with the heavy nucleus, so that the fragments emerge together at a 45 deg angle. Because of the identity of the protons, the proton-proton cross section is zero if the two protons collide in a triplet spin state. If, however, the two protons collide in a singlet spin state, the proton-proton cross section becomes equal to the Rutherford cross section. Application of the Pauli principle to a scattered H_2^+ ion, formed by "atom capture" by the incident proton, requires the occurrence of only even J rotational states in the molecule thus formed, since the spatial part of the H_2^+ eigenfunction must then be symmetric. Hence only even J states will be formed in the atom-capture process, with the emergent H_2^+ ions formed at approximately 45 deg with respect to the incident beam direction. A search for H_2^+ continuum capture events is being undertaken by our colleague Marianne Breinig. The asymptotic velocity region is reached at energies of ~ 100 eV, however, since the relevant velocity ratio is that of the incident beam compared to the *molecular* vibrational speeds of the atom in the initial and final molecules. Owing to the finite carbon mass, for a methane target the scattering angle of the molecule is closer to 47 deg, and the restriction on J states is correspondingly relaxed.

CAPTURE BY POSITRONS

The interesting problem of positronium formation through electron capture by a positron incident on, for example, a hydrogen atom leads instead to the production of *odd* angular momentum states of the positronium system formed. Here there is no problem of particle identity, but the positronium system formed must result from the coherent addition of paths wherein the positron is scattered first and the electron second, and the complementary process wherein the positron is scattered second and the electron first. The second scattering matrix element changes sign for positrons vis-a-vis electrons ($-Ze^2/r \rightarrow Ze^2/r$). Simultaneous consideration of this matrix element sign switch, together with the $(-1)^l$ parity of the positronium system formed, gives an overall scattering amplitude sign of $-1 \times (-1)^l$, leading to vanishing probability when two paths corresponding to even l are superposed; hence only odd l positronium states are predicted to be formed by this means. Fig. 12 provides a schematic diagram which illustrates this point. Pictorially, as is seen in Fig. 12, the effect arises because the relative position vector of the electron relative to the positron subsequent to the second scattering has the same magnitude but opposite directions in the two cases considered.

Fig. 12. Two mechanisms for positronium formation at high-impact speeds. The thick and thin lines, respectively, describe the paths of the positron and electron. The vertical dashed line is the position vector of the electron relative to the positron immediately after the second collision. From R. Shakeshaft, to be published.

PION CAPTURE TO THE CONTINUUM

In a remarkable example of parallel, nearly simultaneous developments in different subfields of physics, it appears that a large peak in the π^-/π^+ ratio for production of low-energy forward pions has recently been found³² in heavy-ion pion production experiments carried out from 125 to 400 MeV/u. The peak is observed at a pion velocity very nearly equal to that of the projectile. Though Benenson et al.³² seem to have been unaware of the previous theoretical and experimental study of the type of Coulomb-final state interaction encountered here in the electron capture to continuum context, there can be little doubt that very similar underlying physical principles apply. Fig. 1 of Ref. 32, which depicts a large peak in the ratio of π^- to π^+ production in Ne + NaF as a function of the pion projectile frame velocity, has been analyzed in terms of a first-order Coulomb distortion of the pion wave function in the vicinity of the projectile charge. In the data displayed, there may even be the hint of asymmetry toward velocities lower than that of the projectile, as in the electron capture to continuum work that I have described. One can only speculate about what features of the electron problem may be instructive in the pion production case. Fig. 13 shows the ratio of π^- to π^+ production as a function of incident ion energy.

Fig. 13. Ratio, R , of π^- to π^+ cross sections in Ne + NaF (0°) as a function of pion energy in the projectile frame. From Ref. 32.

ACKNOWLEDGEMENTS

A number of colleagues have contributed greatly to the carrying out of the experiments described, ably aided by generous help from staff at ORNL, LBL, and BNL. The most substantial contributions - also those sustained over the longest period of time - have been provided by Charles R. Vane (with whose able colleagues Professor Richard Marrus and Dr. Harvey Gould a joint collaboration at LBL has been possible) and by my faculty colleague Stuart B. Elston. Marianne Breinig has played the leading role in recent analysis and interpretation of the Ar^{18+} data obtained at LBL, as did Martin Suter (ETH-Zürich) for earlier data obtained at ORNL and LBL. Substantial contributions have also been made by my other UT-ORNL colleagues Gerald Alton, Leif Liljeby, and Robert Thoe. Thoe's design and fabrication of our most recent electrostatic analyzer (replacing one kindly lent us by M. O. Krause), together with Scott Berry's design and fabrication of our magnetic analyzer, have been essential to the work. Finally, the continued collaboration of our well-appreciated colleague from East Carolina University, Roman Laubert (who leads the solid target aspects of our work) has been aided by the East Carolina University Research Foundation and by Oak Ridge Associated Universities.

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* This work was partially supported by the National Science Foundation; by the Office of Naval Research; and by the Fundamental Interactions Branch, Division of Chemical Sciences, Office of Basic Energy Sciences, U. S. Department of Energy, under contract W-7405-eng-26.