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Cross sections for atomic K-shell ionization by ion impact in the single-particle Glauber approximation*

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Total cross sections have been computed for K-shell ionization in selected multielectron atoms by proton impact using the single-particle Glauber approximation with hydrogenic wave functions. Our single-particle Glauber approximation corresponds to an independent-particle model where explicit coupling with target electrons not directly involved in the interaction is omitted. In principle, the Glauber approximation is valid over a wider region of scattering parameters than is the Born approximation. However, our Glauber results are not in significantly better agreement with observation than simpler Born predictions. For all targets considered at projectile velocities near the peak of the cross section, single-particle Glauber results tend to lie beneath observed cross sections by proton impact, in contrast to previous results for electron impact where, as expected, Glauber results are in better agreement with observations than Born results for low-Z_2 targets. Some explanations of the discrepancy and possible extensions of our methods are considered. It is also found that, as the atomic number of the target, Z_2, increases, the relative contribution of Glauber corrections to corresponding Born calculations decreases at projectile velocities near and above the peak of the K-shell ionization cross section. For $Z_2 \gtrsim 5$, the Glauber scattering corrections to Born results for K-shell ionization at projectile velocities near and above the peak of the cross section are less than a few percent, e.g., less than errors due to our use of hydrogenic target wave functions. For $O^{+8} + Ne$, unlike $p^+ + Ne$, significant differences are apparent between Glauber and Born predictions for direct Coulomb ionization.

I. INTRODUCTION

The Born approximation[1,2] has been useful in predicting and analyzing K-shell ionization cross sections in multielectron atoms. An approximation supposedly more complete than the Born approximation is the Glauber approximation,[3,4] which is relatively effective in predicting cross sections for excitation and ionization by electron impact at projectile velocities near and above the peak of the cross section. In this paper some Glauber cross sections for atomic K-shell ionization by proton impact are presented.

Total cross sections for the ionization of atomic hydrogen by proton impact have been presented[5] in an earlier paper. For the case of atomic hydrogen the Glauber results fall below the data near the peak of the cross section, whereas the Born results lie above. This circumstance is unlike the case for the ionization by electron impact[6,7] where the Glauber results are in better agreement with observations than Born as expected.[3,4] In the present paper, single-particle Glauber calculations are used to further investigate possible differences in K-shell ionization of multielectron atoms by the impact of protons and electrons.

There have been a number of attempts[1,8-12] to improve standard Born calculations for ion-atom collisions. In some of these attempts,[8-11] the independent-electron picture using hydrogenic target wave functions is retained, and scattering corrections are sought, ignoring or approximating interactions with target electrons not directly involved. The single-particle Glauber approximation which we employ includes some of these single-electron scattering corrections in an approximate way. Another approach[12] is to concentrate on the effects of using accurate many-body target wave functions, such as Hartree-Fock wave functions,[13] rather than hydrogenic wave functions. In this paper some comparison is made between estimated effects of using relatively accurate many-body target wave functions and the magnitudes of single-particle Glauber scattering corrections to the Born approximation which we compute.

II. THEORETICAL DISCUSSION

A. Full Glauber approximation

The Glauber approximation has been used extensively[3,4,14] in nuclear and high-energy physics. Since its first application[15] in atomic physics in 1968, it has been largely used to compute cross sections for elastic scattering and excitation in hydrogen and helium. The approximation itself[3,4] is a form of the eikonal approximation where the eikonal phase is integrated along a mathematically convenient path. It is sometimes conceptually convenient to view the approximation as a distorted-wave Born approximation whose distortion is given by the eikonal phase term. Also it is interesting to note that the Glauber approximation may be derived[16,17] from closed-coupling formulas where all channels are included in an eikonal approximation. At high velocities, with the standard choice of phase integration path, the Glauber approximation reduces to the Born approximation.

The Glauber scattering amplitude may be mathematically expressed in atomic units as

$$f_G(\vec{q})=\frac{-\mu}{2\pi}\int \psi_{iG}(\vec{R},\vec{r}_1\cdots\vec{r}_n)V(\vec{R},\vec{r}_1\cdots\vec{r}_n)\times\Phi_f^*(\vec{R},\vec{r}_1\cdots\vec{r}_n)\,d^3R\,d^3r_1\cdots d^3r_n\,,$$

where μ is the reduced mass, $\vec{R}$ and $\vec{r}$ the coordinates of the projectile and target electrons respectively, and ψ_{iG} is the approximate Glauber wave function given[3,4] by

$$\psi_{iG}=\Phi_i(\vec{R},\vec{r}_1\cdots\vec{r}_n)\exp\left(i\eta\int_{-\infty}^{Z}V(\vec{B}+\vec{Z}',\vec{r}_1\cdots\vec{r}_n)\,dZ'\right),$$

where $\vec{R}=\vec{B}+\vec{Z}$ and $\eta=-Z_1/v_0$, i.e., the ratio of projectile charge to projectile velocity. The exponential term on the right is the eikonal phase; $\Phi_i(\vec{R},\vec{r}_1\cdots\vec{r}_n)$ is a plane wave multiplied by the bound-state wave function of the target, $\phi_i(\vec{r}_1\cdots\vec{r}_n)$ With the conventional[18,19] choice of taking $\vec{Z}$ perpendicular to the momentum transfer $\vec{q}$, the above equation may be integrated to obtain the standard expression[3,4] for the scattering amplitude in the Glauber approximation

$$f_G(\vec{q})=\frac{-i\mu v_0}{2\pi}\int e^{i\vec{q}\cdot\vec{B}}\phi_i(\vec{r}_1\cdots\vec{r}_n)\phi_f(\vec{r}_1\cdots\vec{r}_n)\times\{1-\exp[i\Delta(\vec{B},\vec{r}_1\cdots\vec{r}_n)]\}\,d^2B\,d^3r_1\cdots d^3r_n\,,$$

where for Coulomb interactions,

$$\Delta(\vec{B},\vec{r}_1\cdots\vec{r}_n)=\sum_{i=1}^{n}\eta\int_{-\infty}^{\infty}\left(\frac{1}{R}-\frac{1}{|\vec{R}-\vec{r}_i|}\right)dZ=\sum_{i=1}^{n}\Delta_i\,.$$

In the limit as η becomes small, the leading term in η is the usual Born approximation.

It is instructive to rearrange the term $1-e^{i\Delta}$ according to

$$\begin{aligned}\Gamma\equiv 1-e^{i\Delta}&=1-\exp\left(\sum_{i=1}^{n}\Delta_i\right)\\&=(1-e^{i\Delta_1})+(1-e^{i\Delta_2})+\cdots(1-e^{i\Delta_n})-(1-e^{i\Delta_1})(1-e^{i\Delta_2})-\cdots(1-e^{i\Delta_{n-1}})(e^{i\Delta_n})\\&\quad+(1-e^{i\Delta_1})(1-e^{i\Delta_2})(1-e^{i\Delta_3})+\cdots+(-1)^n(1-e^{i\Delta_1})(1-e^{i\Delta_2})\cdots(1-e^{i\Delta_n})\\&=\Gamma_1+\Gamma_2+\cdots\Gamma_n-\Gamma_1\Gamma_2-\cdots\Gamma_{n-1}\Gamma_n+\Gamma_1\Gamma_2\Gamma_3+\cdots+(-1)^n\Gamma_1\Gamma_2\cdots\Gamma_n\,.\end{aligned}$$

The Γ_i terms involve only interactions between the projectile and the ith target electron. The terms involving products of the $\Gamma_i\Gamma_j$ involve multiple scattering with more than one electron which lead to scattering amplitudes which do not appear to be factorable as a simple product of single-electron terms even when the target wave functions are expressed as a product of single-particle wave functions. Thus the full Glauber scattering amplitude includes well defined, although approximate, terms which couple together more than one of the target electrons with the projectile.

In the case of atomic excitation to bound state, more rigorous calculations now exist. One example is a multichannel eikonal treatment,[17] using a more complete set of set of coupled channels which reduces to the Glauber approximation as a certain phase contribution goes to zero. Another[18] adds some second-order perturbation terms to a Glauber amplitude expanded through three orders in η. Still others include alternate eikonal[20] and semiclassical[21] approximations. In general, as the rigor is increased, so is the computational difficulty.

Atomic ionization is more tedious than excitation since it is necessary to integrate over additional final-state variables corresponding to the continuum states, $\vec{k}$, of the ejected electron; i.e., in ionization

$$\sigma(v_0)=(\pi\mu^2v_0^2)^{-1}\int|f(\vec{q},\vec{k})|^2\,d\vec{q}\,d\vec{k}\quad(\pi a_0^2)\,.$$

Primarily for this reason, there have been relatively few ionization[6,7,22-24] calculations performed in the Glauber approximation. And, with at least one exception,[25] little has been done at this time past simple Glauber calculations, such as we present. On the other hand, it should be noted that extension to ionization of other excitation and elastic scattering calculations[16-19] more rigorous than Glauber is possible.

B. Single-particle Glauber approximation

In the single-particle Glauber approximation[7] only the terms linear in Γ_j are retained. If the initial and final states, $\phi_i(\vec{r}_1\cdots\vec{r}_n)$ and $\phi_f(\vec{r}_1\cdots\vec{r}_n)$ are represented by a product of distinguishable electron wave functions,

$$\phi_i(\vec{r}_1\cdots\vec{r}_n)=\prod_{j=1}^{n}\phi_i(\vec{r}_j)$$

which are orthonormal, then the single particle Glauber scattering amplitude for ionization of the jth electron becomes[5]

$$f_G(\vec{q},\vec{k}) = \frac{-\mu v_0}{2\pi} \int e^{i\vec{q}\cdot\vec{B}} \phi_i(\vec{r}_j)\phi^*_{\vec{k}}(\vec{r}_j) \times \left[1 - \left(\frac{\vec{B}-\vec{S}_j}{B}\right)^{2i\eta}\right] d^2B\, d^2S_j\, dz_j\,,$$

where

$$\vec{r}_j = \vec{S}_j + \hat{\xi} z_j \quad \text{and} \quad \hat{\xi}\cdot\vec{q} = 0$$

and $\phi^*_{\vec{k}}(\vec{r}_j)$ represents a continuum state with wave vector $\vec{k}$ of the target electron. Antisymmetrization or our wave function corresponding to target electron indistinguishability does not alter the expression[7] for the cross sections.

If the single-particle target wave functions, $\phi(\vec{r}_j)$, are represented by $\phi(r_j)Y_l^m(\hat{r}_j)$ with arbitrary radial wave functions $\phi(r_j)$, the Glauber amplitude may be analytically reduced to a two-dimensional integral. In our calculations we have used less accurate hydrogenic wave functions and reduced[5,26] the amplitude to a one-dimensional integral. For K-shell ionization dropping the subscript j, we choose

$$\phi_i(\vec{r}) = (\lambda^{3/2}/\sqrt{\pi})e^{-\lambda r}\,,$$

where λ is the effective charge of the bound-state wave function. The continuum final-state wave functions are also chosen as hydrogenic corresponding to

$$\phi^*_{\vec{k}}(\vec{r}) = (2\pi)^{-3/2} e^{-1/2\gamma\pi}\Gamma(1+i\gamma) \times e^{-i\vec{k}\cdot\vec{r}}\ {}_1F_1(-i\gamma, 1, i(kr+\vec{k}\cdot\vec{r}))$$

with $\gamma = -Z_2^*/k$ where Z_2^* is the effective nuclear charge seen by the ejected electron.

Expanding the continuum target electron in states of angular momentum designated by l, m about the target nucleus, the single-particle Glauber scattering amplitude may be reduced[5,26] to the form,

$$f(\vec{q},\vec{k}) = \frac{4\pi\mu\lambda^{3/2}Z_1}{(2\pi)^{3/2}q^2} \sum_{l=0}^{\infty} k^l C_l \sum_{m=-l}^{l} (-1)^{(l+m)/2} \frac{\Gamma(m-i\eta)}{m!\,\Gamma(1-i\eta)} e^{-im\phi_q} \sum_{p=0}^{l+2} I^p_{lm} Y_l^m(\hat{k})\,,$$

where $l+m$ is even and

$$C_l = \frac{2^l e^{-\pi\gamma/2}\Gamma(l+1+i\gamma)}{(2l+1)!}\,.$$

Here

$$I^p_{lm} = \int_0^\infty G(q/b)\left[B^p_{lm} c^{-p-4}(c/b)^p\ {}_2F_1(l+1+i\gamma, l+4-p, 2l+2, -2ik/c) + (-1)^{m+p+1} B^p_{lm} d^{-l-4}(d/b)^p\ {}_2F_1(l+1+i\gamma, l+4-p, 2l+2, -2ik/d)\right] db$$

with

$$G(z) = \begin{cases} z^m\ {}_2F_1(-i\eta, m-i\eta; m+1; z^2)\,, & z \le 1 \\ z^{-m+2i\eta}\ {}_2F_1(-i\eta, m-i\eta; m+1; z^{-2})\,, & z \ge 1 \end{cases}$$

and

$$c = a - iqb\,, \quad d = a + iqb\,, \quad a = \lambda - ik$$

and B^p_{lm} are simple complex numbers which have been tabulated[27] for $l \le 4$.

Total ionization cross sections may be evaluated by computing two additional numerical integrations over q and k. In our calculations we require that the numerical error be less than 1% and truncate the expression in l past $l=4$. Evaluation of the total cross section at one projectile energy consumed a few minutes on an IBM 370/158 at a cost of about $40.

It has already recently been pointed out[28] that the $\Gamma_1\Gamma_2$ cross scattering term may be evaluated in a manner which requires one additional integration, somewhat similar to the integration over modified Lommel functions used in helium for elastic scattering[29] and for excitation[30] to the $2p$ level. In the excitation of helium by proton impact inclusion of this multiple scattering term affects the differential cross sections $d\sigma/dq$ more strongly than the total cross section where the cross term lowers the total cross section by about 5% or less near and above the peak of the cross section. On the average, this is roughly comparable to the overall numerical error in our calculation, estimated at 3% or less, due primarily to truncation of the outgoing electron partial waves past $l=4$.

Perhaps surprisingly, there is an advantage to dropping the approximate Glauber cross scattering terms. By working within the framework of an independent-particle model, one may implicitly sum[31] all contributions from processes in outer atomic shells. It is this summed result which corresponds to most experimental observations.

III. RESULTS

A. Helium

Total cross sections for the ionization of helium by proton impact are presented in Fig. 1[32] and

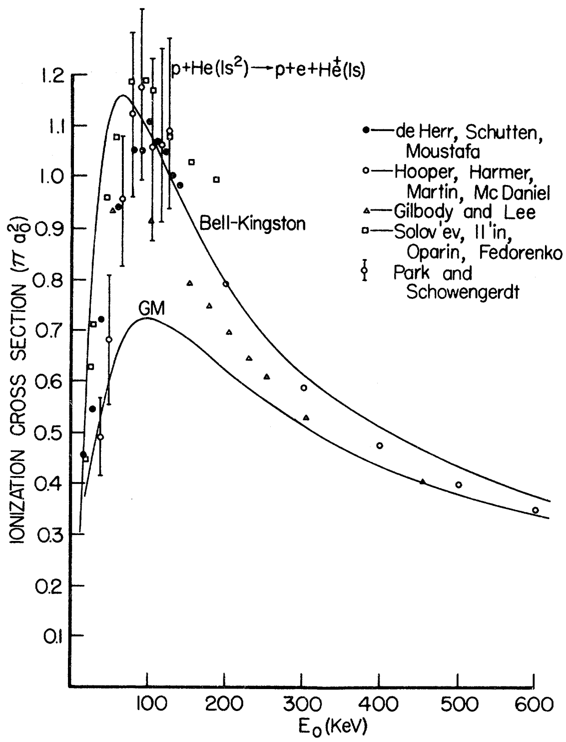

FIG. 1. Total cross sections for the ionization of helium by proton impact vs the projectile energy. Data were extracted from Ref. 35. The Born results are those of Bell and Kingston from Ref. 36. The present result is labeled GM ($\lambda = 1.687$, $Z_2^* = 1.0$).

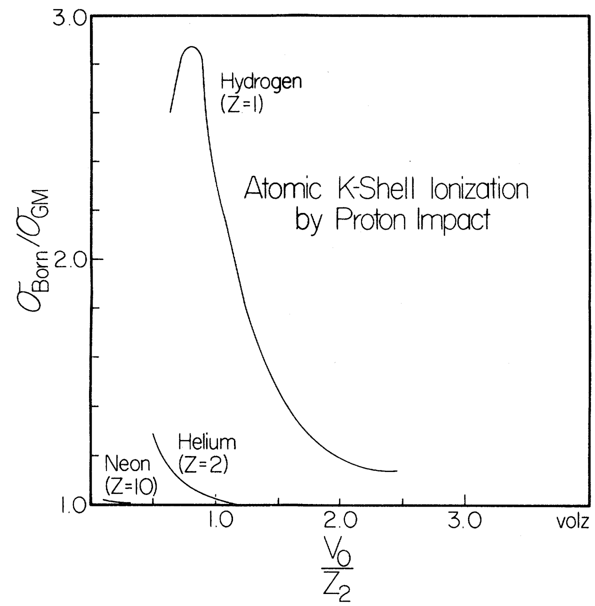

FIG. 2. Ratio of Born to single-particle Glauber cross sections vs a scaled velocity. In both calculations $Z_2^* = \lambda$. The peak of the absolute inoization cross sections occurs near $v_0/Z_2 = 1$.

Table I. In our single-particle Glauber calculations (GM) the effective charge used to characterize the ground state is $\lambda = 1.687$. This value may be obtained by considering λ as the variation parameter[33] using hydrogenic wave functions in a variational calculation of binding energies. In the final-state continuum wave function, we choose $Z_2^* = 1.0$ in all partial waves except $l = 0$ where $Z_2^* = \lambda$. In this manner we attempt to account for screening of the nucleus by the remaining target electron except in $l = 0$ where we choose $Z_2^* = \lambda$ so that the initial and final states are orthogonal. This choice of charge parameters gives agreement within 5% of the asymptotic energy form[34] of Inokuti and Kim. Furthermore, with this procedure single-particle Glauber calculations are in agreement with data for ionization of helium by electron impact[7] near and above the peak of the cross section.

TABLE I. Total single-particle Glauber cross sections for the ionization of helium by proton impact in units of πa_0^2.

E_0 (keV)	GM
10	0.28
20	0.37
30	0.45
40	0.53
50	0.60
70	0.69
90	0.72
110	0.72
130	0.71
150	0.69
500	0.38
1000	0.23

Discrepancy of our single-particle Glauber results with observed results[35] for ionization of helium by proton impact near the peak of the cross section is quite apparent. Indeed the results of Bell and Kingston[36] using a form of the simpler Born approximation are in apparent agreement with experiment. This situation is reminiscent of the ionization of atomic hydrogen, where Glauber predictions are in significantly better agreement with observations for ionization by electron impact than by proton impact.[5] Some explanations for this discord are presented in the last section. First, however, let us consider differences between single-particle Glauber and Born predictions.

B. Target charge dependence

In this section single-particle Glauber corrections to the Born approximation are considered for K-shell ionization in various atomic targets. In the results presented in Fig. 2, we have taken $Z_2^* = \lambda$ in both our Glauber and Born calculations since this choice is widely used[37] and because with this choice it is unnecessary to expand the Born amplitude in partial waves. Furthermore, by choosing Z_2^* and λ in the same way in both approximations, the single-particle Glauber results reduce[38] to Born results at high velocities.

In Fig. 2 we plot the ratio of the Born cross section to the single-particle Glauber cross section as a function of a scaled velocity, v_0/Z_2 where v_0 is the projectile speed and Z_2 the atomic number of the target. The peak of the absolute ionization cross sections[39] (not plotted in Fig. 2) occurs when v_0/Z_2 is about unity. Glauber corrections to the Born approximation may be theoretically justified for $v_0 \gtrsim Z_1$ (where $Z_1 = 1$ for protons), but have not been justified at small values of v_0. Our attention in this paper is primarily limited to projectile speeds comparable to or somewhat greater than Z_2, where the static and possibly the screening approximations[40] may be valid.

Except for low Z_2, single-particle Glauber cross sections are within a few percent of Born cross sections for K-shell ionization by proton impact near and above the peak of the ionization cross section. As we shall later demonstrate it is likely that uncertainties in ionization calculations owing to the choice of target wave functions (especially continuum wave functions) are likely to be greater than single particle Glauber scattering corrections[7,27] for $Z_2 \gtrsim 5$ in K-shell ionization.

The decreasing contribution of Glauber corrections to the Born approximation as Z_2 increases may be simply explained. Expanding the full Glauber term $(1 - e^{i\eta\Delta})$ in powers of $\eta = -Z_1/v_0$, the leading term is the Born approximation and all Glauber corrections are $O(\eta^2)$ at most. As Z_2 increases, the projectile velocity required to reach the peak of the cross section increases, and the Glauber corrections decrease.

When $|\eta| = Z_1/v_0$ is not small compared to Z_2^*, then differences between Glauber and Born may be large. This is the case for outer shell ionization, or when Z_1 is large. Also there are likely to be significant differences between Glauber and Born predictions of differential cross sections, e.g., for large momentum transfer or large ejected electron momenta, regions which contribute little to total cross sections.

C. Neon and argon

Calculations of cross sections for K-shell ionization by proton impact in neon and argon using the single-particle Glauber approximation, the plane-wave Born approximation[37] and the binary-encounter model[41] are compared to recent observations[42,43] at projectile velocities near and above the peak of the ionization cross section in Figs. 3 and 4. In contrast to helium and hydrogen, the shape of the cross section at energies near and above the peak of the cross section is well represented by both the Glauber and Born predictions for neon and argon.

According to Sec. III B, differences between Glauber and Born calculations using the same atomic parameters (not shown) should be within numerical error of 3%. In fact they are. The differences between the single-particle Glauber and Born cross sections apparent in Figs. 3 and 4 are entirely due to differences in the atomic wave functions. Our single-particle Glauber results use the screening parameters of Fisher[13] based on fits of hydrogenic wave functions to Hartree-Fock wave functions corresponding to $\lambda = 9.516$ in neon and $\lambda = 17.431$ in argon. In the final state, $Z_2^* = Z_2 - 1$ except[44] in $l = 0$ where $Z_2^* = \lambda$. In the Born calculations $Z_2^* = \lambda = Z_2 - 0.3$ in both cases. Setting $Z_2^* = \lambda$ in all partial waves lowers our Glauber cross sections typically by about 15% at energies above the peak. In the Born calculation shown[37] the minimum energy transfer is taken to be the observed K-

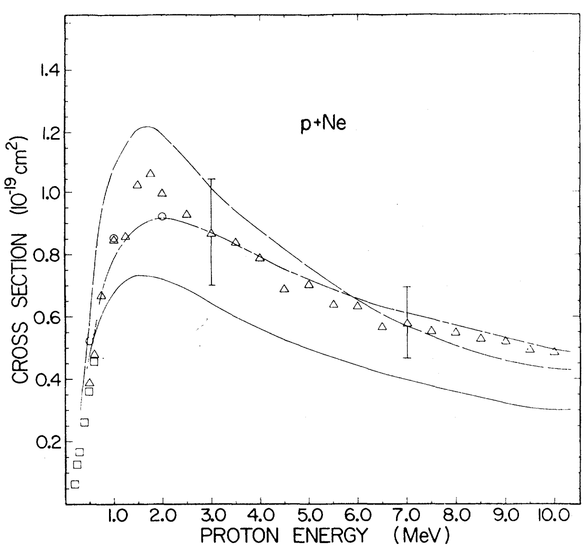

FIG. 3. K-shell ionization in neon by proton impact. Data were extracted from Woods *et al*. (Ref. 42). The solid curve represents our single particle Glauber results; — – — corresponds to a Born calculation (Ref. 45) using target charge parameters differently than in the Glauber results; and — — corresponds to the binary-encounter model (Ref. 41). Differences in this figure between these Glauber and Born results are due to differences in the choice of target charge parameters.

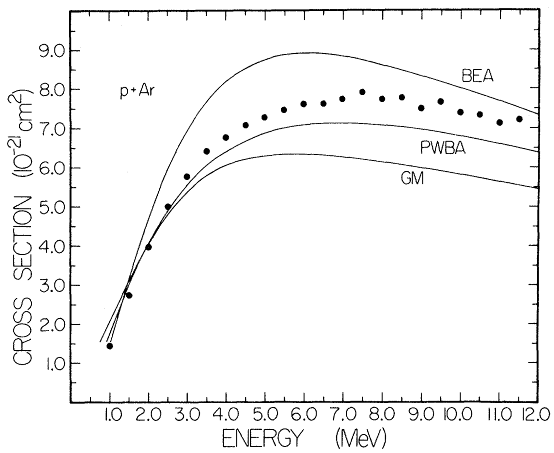

FIG. 4. K-shell ionization in argon by proton impact. The data came from Macdonald *et al*. (Ref. 43). GM corresponds to our single-particle Glauber results which employ target charge parameters different than in the PWBA Born results (Ref. 45). BEA represents the binary-encounter model (Ref. 41). Differences in this figure between these Glauber and Born results are due to differences in the choice of target parameters.

shell binding energy, I_K. This necessitates integration over imaginary momenta[45] of the ejected electron with arbitrary normalization for the wave function. Alternatively[46,47] we choose a minimum energy transfer of Z_2^{*2} to avoid this region of imaginary integration. These discrepancies due to the use of simple hydrogenic wave functions may be reduced by using more rigorous numerical wave functions, such as Hartree-Fock wave functions, in place of the hydrogenic wave functions. Of course the calculations then become more tedious to perform, and less easy to tabulate.

Reading *et al.*[9] have developed a version of the Glauber approximation which differs from that which we present. In the Reading version, the Glauber cross section σ_G is simply related to the Born cross section σ_B by

$$\sigma_G = |\Gamma(1+i\eta)|^2 e^{\eta\pi}\sigma_B$$
$$= -\frac{2\pi\eta}{e^{-2\pi\eta}-1}\sigma_B \equiv R\sigma_B\,.$$

Reading's expression for σ_G converges to the Born approximation more slowly than do our Glauber calculations. At 25 keV, corresponding to the peak of the cross section for $p+\mathrm{H}$, $R\simeq 10^{-2}$, whereas our Glauber results[5] are about a factor of 2 beneath both Born predictions and observed results. At higher velocities, R is smaller. In Fig. 3 and 4, Reading predictions are 0.58, 0.77, and 0.83 times GM and PWBA at 1, 4, and 8 MeV respectively (noting that our GM results have converged to the Born results at these velocities).

It is difficult to make detailed comparison to the binary-encounter model since further theoretical justification is needed[48] for this particular model.

Our results for neon and argon indicate that differences in our cases of typically 30% or so in total cross sections due to inadequacies in atomic wave functions, particularly continuum were functions where charge screening is a difficult problem,[7] are larger than single-particle Glauber corrections to the Born approximation.

While differences between Born and Glauber scattering approximations are small if the projectile charge Z_1 is small compared to the effective target Z_2^*, when Z_1 is comparable to or greater than Z_2^* the differences may be large as illustrated in Fig. 5. Based on prior results,[7,24] we expect that the differences shown are primarily due to differences in the Glauber and Born approximation rather than static differences due to $\lambda \neq Z_2^*$.

IV. DISCUSSION

There is an apparent trend for single-particle Glauber calculations to fall beneath observed data for K-shell ionization proton impact in contrast to electron impact results. Indeed the simpler Born approximation appears to give better agreement with proton-atom observations than our Glauber results. Let us consider some possible explanations, assuming that the Glauber results are more complete[3] than Born results, and leaving aside the interesting question of the region of validity of the Born approximation. Standard Glauber calculations are invariant under sign change of the projectile[16] and depend, of course, primarily on the speed rather than the mass of the projectile. Using an alternative integration path for the eikonal phase term, Byron[16] finds electron excita-

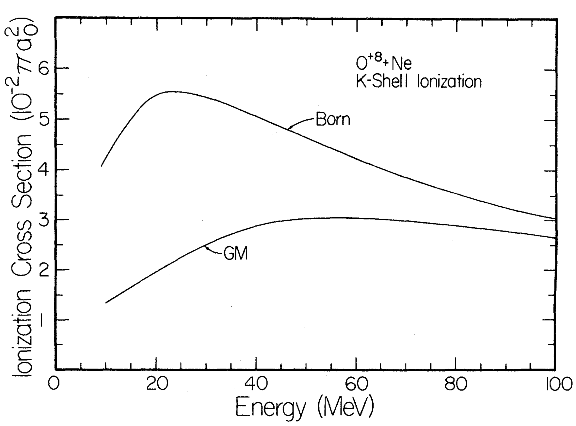

FIG. 5. K-shell ionization in neon by O^{+8} impact. Here $\lambda = 9.516$ and $Z_2^* = 9.0$ for Glauber and $Z_2^* = \lambda = 9.516$ for Born.

tion cross sections in agreement with standard Glauber results. However Byron's positron cross sections lay above standard Glauber results. Alternatively there are some binding energy and recoil corrections to the Glauber approximation developed by Reading,[49] although no numerical result currently exists. Furthermore, Thomas[50] has recently suggested that the expansion in angular momentum states, l, of the ejected electron may converge more slowly than we expect, and it has also been pointed out[50,51] that the mathematical selection rule requiring that $f_G(\vec{q},\vec{k})$ be zero if $l+m$ is odd is approximate and that error could accumulate in our sum over l and m.

A particularly interesting idea is associated with certain charge transfer effects. The $p+$ H data of Fite *et al.*[52] show that an incident proton energies near the peak of the vacancy production, the charge-transfer cross section to bound states is larger than the ionization cross section. It is possible that rather than being captured to a bound state of the projectile the electron lies in the continuum of eigenstates associated with the projectile. Physically this might correspond to the projectile and the ejected electron leaving the collision rapidly with respect to the nucleus but in approximately the same direction and with small relative velocity with respect to each other. It is quite unlikely that such effects are accurately included in the present Glauber calculation or in the Born approximation. Macek,[11] using a first-order solution to the Faddeev equations as well as certain additional approximations, including use of the Brinkman-Kramers approximation, has made partial cross-section calculations differential in the energy and angle of ejection of the ejected electron which have been compared to the data of Rudd *et al.*[53] for He and H_2. It is found that the relative cross section for electron ejection toward the forward direction is considerably enhanced over the standard Born prediction. Recently Park *et al.*[54] have observed the distribution of energies of ejected electrons in the ionization of atomic hydrogen by protons. Their observations are consistent with the idea of charge transfer to the continuum. Extension of Glauber calculations to include charge transfer to the continuum is difficult. Alternatively, it would be interesting, although tedious, to analyze a thorough classical calculation.[55]

The shape of our single-particle Glauber results agrees with the observed cross sections for neon and argon (high Z_2), but not for hydrogen and helium (low Z_2). This result is not inconsistent with the suggestion that charge transfer to the continuum may contribute to total ionization cross sections when $Z_1 \gtrsim Z_2$ since charge transfer cross sections fall off more rapidly than direct Coulomb ionization as Z_1/Z_2 decreases from unity. Of course, our single-particle Glauber and corresponding Born cross sections (not shown) tend to lie below the observed cross sections for neon and argon. This may be due to the normalization of the continuum wave functions which we have used. It is difficult for us to justify the use of one-electron Coulomb wave functions using a single charge parameter in the final state, since the variation with the electron coordinate may be dominated by the effective target charge near the K-shell radius with the normalization determined by the effective charge at larger distances. A decent fit of a hydrogenic continuum function to a more exact, e.g. Hartree-Fock, wave function may require two charge parameters: one corresponding to the structure of the wave function where scattering predominates, and the other for the normalization. The question of the final-state continuum wave function, in our opinion, merits further consideration.

If the discrepancy between Glauber theory and observation of total absolute ionization cross sections by proton impact can be resolved, then the Glauber approximation might provide an interesting tool to study the projectile-charge (Z_1) dependence[8-11] of these cross sections. At high velocities the Glauber approximation is expected[3] to approximately satisfy constraints of unitarity, unlike the Born approximation which scales as Z_1^2. While it is clear that except as Z_1/v_0 tends to zero, the Glauber approximation does not follow a Z_1^2 scaling law, we have been unable to analytically establish a simple dependence on Z_1. Specific deviations from the Born Z_1^2 scaling law k-shell ionization in neon are evident from a comparison of Fig. 3 and 5. However, for $O^{+8}+$Ne direct charge capture is quite likely to play an important role in vacancy production, and should be taken into account. For example a Brinkman-Krammers calculation[56] of $1s$-$1s$ charge transfer to O^{+8} yields cross sections of 0.32 and 0.10 (πa_0^2) at 20 and 40 MeV respectively, i.e., larger than the ionization cross sections in Fig. 5. Experimental data[57] for O^{+8} +Ne lie above the results in Fig. 5 qualitatively in agreement with this picture.

In summary, we conclude that there are evident differences between electron and proton impact K-shell ionization in atoms. While results of single-particle Glauber calculations for electron impact are in better agreement than Born results for low-Z_2 target data at projectile velocities near and above the peak of the cross section, for proton impact single-particle Glauber results tend to fall beneath experiment. It is also apparent that Glauber corrections to the Born approximation fall off monotonically as the target charge Z_2 increases. For $Z_2 \gtrsim 5$, the single-particle Glauber scattering corrections to the corresponding Born approximation are less than a few percent for K-shell ionization by proton impact near and above the peak of the cross section. In cases where $\eta = Z_1/v_0$ is small compared to Z_2, corrections to simple target wave functions are larger than single-particle Glauber scattering corrections to the Born approximation. For $\eta \gtrsim Z_2$ Glauber and Born approximations appear to give different results.

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