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Impact-parameter dependence for collisions of atoms with projectiles carrying electrons

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A method is proposed for studying collisions between two atoms or ions with one or more electrons each. An effective charge density as a function of a physically unobservable impact parameter $\vec{b}'$ is introduced to describe the spatial nonlocalization of the electron cloud of the projectile atom. It is shown that the probability amplitude at a given (real) impact parameter may be reduced to a convolution over $\vec{b}'$ of the effective charge density with target excitation amplitude per unit charge. This method, which we call the virtual-impact-parameter method, enables one to identify in a physical way in impact-parameter space the contribution of the electron-electron interaction as well as that of the electron-nucleus interaction. A node structure in the target excitation probability amplitude is found due to the electron-electron interaction. Generalization of the method to the description of many-electron transitions is discussed within the independent-electron approximation.

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I. INTRODUCTION

Many interactions that occur in nature involve at least two atoms with one or more electrons each. The evaluation of cross sections and transition rates for such processes requires a method for dealing with at least four interacting bodies. If multiple electron transitions occur on any of the atomic centers, then some form of even higher-order many-body theory is required. In general such a many-body description is difficult.

In this paper we present a method for evaluating the transition probability in the impact-parameter representation for two quickly interacting atoms (or ions). The target atom may have an arbitrary number of active electrons, but the projectile is restricted to one active electron at most due to our particular use of first-order perturbation theory. We introduce a method of virtual impact parameters in which the electron carried by the projectile is not localized at a definite classical impact parameter $\vec{b}$, but is spread out over a range of virtual, physically unobservable, impact parameters $\vec{b}'$. In our first-order theory the influence of the projectile electron in the target excitation is described by a surface charge density, denoted by $\varsigma(\vec{b}' - \vec{b})$. This surface charge density is the effective projectile charge per area $d^2\vec{b}'$. This projectile charge density per $d^2\vec{b}'$ is convoluted with the probability amplitude per unit projectile charge for the transition of target electrons by integrating over cylindrical Gaussian surfaces of radii $\vec{b}' - \vec{b}$. This yields the transition probability amplitude for any specified transition of electrons on both the projectile and the target at a given impact parameter $\vec{b}$. If there is no projectile electron, then our $\varsigma(\vec{b}' - \vec{b})$ reduces to $\delta(\vec{b}' - \vec{b})$ as expected. Our first-order formulation, together with the physical interpretation, is valid for both screening processes where there is no transition of the projectile electron and the antiscreening process where there is a transition of the projectile electron (caused by its interaction with a target electron). Our method may be used when independent multiple-electron transitions occur in the target since this method provides a rigorous way to evaluate probability amplitudes to first order within the independent-electron approximation.

The first description of such processes was the first-order theory of Bates and Griffing [1] in 1955 which correctly describes ionization cross section for H + H collisions at high collision velocities v in the momentum transfer representation. This first-order theory was extended to other atomic systems about 15 years ago by various authors [2–6]. Stolterfoht [7] has brought forth appealing physical pictures of the effects due to the projectile electron and established a connection to the dynamics of electron correlation and to dielectronic processes in general. Improvement by Anholt [8] of a closure approximation led to the understanding of the threshold of the antiscreening effect. Higher-order methods for the screening contribution have been fruitfully developed by Jakubassa-Amundsen [9] and Wang *et al.* [10], while an appealing impulselike model for the antiscreening contribution was developed by Zouros *et al.* [11,12]. The theory of interactions between atoms and projectiles carrying electrons has been recently reviewed by Montenegro *et al.* [13].

Various experiments [14–16] have generally established the validity of the theory. The impact-parameter representation has been discussed recently by Montenegro and Meyerhof [17,18], Ricz *et al.* [19], and Kabachnik [20]. Our paper develops the first-order theory in the impact-parameter representation for both screening and

antiscreening on an equal footing and presents a physical picture of the nature of the quantum spreading of the projectile electron.

II. THEORY

A. Formulation

We consider a collision system consisting of a projectile carrying a single electron incident on a single-electron target. For simplicity, we assume both the projectile and the target to be hydrogenic with effective nuclear charges of Z_P and Z_T, respectively. Furthermore, we work within the semiclassical approximation in which the internuclear motion is assumed to be classical with a given classical trajectory specified by $\vec{R}(t)$. In general $\vec{R}(t)$ is arbitrary and may be calculated using the actual interacting potential [21]. Sometimes the actual trajectory can be specified to a good degree of approximation as a straight line $\vec{R}(t) = \vec{b} + \vec{v}t$ where $\vec{b}$ is the impact parameter and $\vec{v}$ the collision speed. The straight-line path will be used in our treatment below. Since we are only interested in the electronic transitions, the replacement of the actual trajectory by a straight line has no significant effect on the transition probabilities because of the small electron-nucleon momentum ratio at high v where our theory is valid.

The total Hamiltonian of the system is

$$H = H_P + H_T - \frac{Z_P}{|\vec{R} - \vec{r}_T|} - \frac{Z_T}{|\vec{R} + \vec{r}_P|} + \frac{1}{r_{12}} + \frac{Z_P Z_T}{R}, \tag{1}$$

where H_P (H_T) is the Hamiltonian of the projectile (target), $\vec{r}_P$ ($\vec{r}_T$) are the coordinates of the projectile (target) electron with respect to its parent nucleus, and $r_{12} = |\vec{R} + \vec{r}_P - \vec{r}_T|$ is the distance between the electrons. With the use of the classical trajectory [22], we can drop the internuclear potential $Z_P Z_T / R$ from the total Hamiltonian. Then the total Hamiltonian H may be replaced [21] by the electronic Hamiltonian H_e given by

$$H_e = H_P + H_T + V,$$

$$V = -\frac{Z_P}{|\vec{R} - \vec{r}_T|} - \frac{Z_T}{|\vec{R} + \vec{r}_P|} + \frac{1}{r_{12}}. \tag{2}$$

Here $-\frac{Z_P}{|\vec{R}-\vec{r}_T|}$ is the interaction between the projectile nucleus and the target electron, $-\frac{Z_T}{|\vec{R}+\vec{r}_P|}$ the interaction between the target nucleus and the projectile electron, and $\frac{1}{r_{12}}$ the interaction between the projectile electron and the target electron. This electronic Hamiltonian H_e may be used to find the full electronic wave function $\psi_i(t)$ satisfying

$$i\frac{\partial \psi_i}{\partial t} = H_e \psi_i. \tag{3}$$

The exact transition probability amplitude describing the change of states $i \to f$ under the influence of the interaction V is [23]

$$a_{f_T, f_P}(\vec{b}) = \lim_{t \to \infty} \langle f | \psi_i(t) \rangle = -i \int dt \langle f | V | \psi_i \rangle,$$

where $\psi_i(t)$ is the exact wave function (3) at time t propagated from the initial state $|i\rangle$ of the system at $t = -\infty$. Here i and f denote the electronic states on both the target and the projectile. The cross section for the transition of an arbitrary number of electrons on either atomic center is given by

$$\sigma = \int d\vec{b} |a_{f_T, f_P}(\vec{b})|^2, \tag{4}$$

where $|a_{f_T, f_P}(\vec{b})|^2$ is the probability that the transition $i \to f$ has occurred.

B. The first Born approximation

In the following, we consider only cases where at least one transition in the target occurs. For simplicity we regard the target as having a single active electron. Later we shall extend our result to collisions in which more than one transition occurs in the target. Within the first Born approximation, the exact wave function $\psi_i(t)$ is approximated by its zeroth-order unperturbed initial state wave function $|i\rangle$. The transition amplitude in the first Born approximation as a function of impact parameter for target excitation is given by

$$\begin{aligned} a_{f_T, f_P}(\vec{b}) &= -i \int dt \langle f | V | i \rangle \\ &= i \int dt e^{i \Delta E t} \left[\delta_{f_P i_P} \left\langle f_T \left| \frac{Z_P}{|\vec{R} - \vec{r}_T|} \right| i_T \right\rangle \right. \\ &\quad \left. - \left\langle f \left| \frac{1}{r_{12}} \right| i \right\rangle \right], \end{aligned} \tag{5}$$

where $i_{P,T}$ and $f_{P,T}$ denote the initial and final states of the projectile and target, respectively, and i, f represent the initial and final product projectile-target states. Here $\Delta E = \varepsilon_f^P + \varepsilon_f^T - \varepsilon_i^P - \varepsilon_i^T$ is the energy difference of the final and initial states of the projectile and the target. In arriving at (5) it has been assumed that $f_T \neq i_T$. Consequently, the $-\frac{Z_T}{|\vec{R}+\vec{r}_P|}$ term in V of Eq. (2) does not contribute due to orthogonality of $|f_T\rangle$ and $|i_T\rangle$.

The first term in (5) is from the nuclear-electron interaction and the second term from the two-center electron-electron correlation interaction. The nuclear-electron interaction $-\frac{Z_P}{|\vec{R}-\vec{r}_T|}$ contributes only if $f_P = i_P$. In this case, because of the relative negative sign in front of the $1/r_{12}$ term, correlation generally reduces the transition amplitude. This effect of lowering the transition probability has been termed "screening" [4] because the reduction corresponds to a reduction of the interaction strength due to screening of the nuclear projectile charge by the projectile electron.

If $f_P \neq i_P$, then more open channels become available

to target excitation, which cause the transition probabilities to add incoherently. The effect of enhancing the transition rate is called "antiscreening" [4] because the cross section is increased rather than decreased. It immediately becomes clear from (5) that for antiscreening term (i.e., $f_P \neq i_P$), the transition amplitude is identically zero unless the correlation term $1/r_{12}$ is included. This furnishes a direct link between correlation and antiscreening.

Further reduction of $a_{f_T,f_P}(\vec{b})$ can be carried out using Bethe's integral, which expresses the Coulomb potential in momentum space

$$\frac{1}{R} = \frac{1}{2\pi^2}\int d\vec{q}\frac{e^{-i\vec{q}\cdot\vec{R}}}{q^2}.$$

Substitution into (5) of $1/|\vec{R}-\vec{r}_T|$ and $1/r_{12}$ by their momentum representation quickly yields

$$a_{f_T,f_P}(\vec{b}) = i\int dt e^{i\Delta E t}\frac{1}{2\pi^2}\int d\vec{q}\frac{e^{-i\vec{q}\cdot\vec{R}}}{q^2}\left[\delta_{f_P i_P}Z_P - F_{f_P i_P}(-\vec{q})\right]F_{f_T i_T}(\vec{q}), \quad (6)$$

where the atomic form factor F is defined as

$$F_{f_{P,T} i_{P,T}} = \langle f_{P,T}|e^{i\vec{q}\cdot\vec{r}}|i_{P,T}\rangle. \quad (7)$$

The integration over time in (6) may now be carried out explicitly

$$\int dt e^{i\Delta E t}e^{-i\vec{q}\cdot\vec{R}} = e^{-i\vec{q}\cdot\vec{b}}\int dt e^{i(\Delta E-\vec{q}\cdot\vec{v})t} = e^{-i\vec{q}\cdot\vec{b}}2\pi\delta(\vec{q}\cdot\vec{v}-\Delta E)$$

to give

$$a_{f_T,f_P}(\vec{b}) = \frac{i}{\pi}\int d\vec{q}\delta(\vec{q}\cdot\vec{v}-\Delta E)\frac{e^{-i\vec{q}\cdot\vec{b}}}{q^2} \times\left[\delta_{f_P i_P}Z_P - F_{f_P i_P}(-\vec{q})\right]F_{f_T i_T}(\vec{q}). \quad (8)$$

The Dirac δ function in (8) restricts the component of $\vec{q}$ along the beam axis $\hat{v}$ (defined as the z axis) such that $q_z \equiv q_\parallel = \Delta E/v$. Introducing the transverse and parallel momentum transfers, $\vec{q}_\perp$ and $q_\parallel$ such that

$$\vec{q} = \vec{q}_\perp + q_\parallel\hat{v}, \quad \vec{q}_\perp\cdot\hat{v} = 0, \quad q_\parallel = \frac{\Delta E}{v},$$

into (8) and carrying out the integration over q_z, we arrive at

$$a_{f_T,f_P}(\vec{b}) = \frac{i}{\pi v}\int d\vec{q}_\perp\frac{e^{-i\vec{q}_\perp\cdot\vec{b}}}{q^2}\left[\delta_{f_P i_P}Z_P - F_{f_P i_P}(-\vec{q})\right] \times F_{f_T i_T}(\vec{q}). \quad (9)$$

This result holds for both screening ($f_p = i_P$) and antiscreening ($f_p \neq i_p$). This is the usual first Born transition amplitude in the impact-parameter approach. It is expressed here in terms of momentum transfer $\vec{q}$. We note that a finite minimum momentum transfer $q_\parallel$ is required to effect a given transition with a transition energy ΔE.

III. THE VIRTUAL-IMPACT-PARAMETER METHOD

It is conceptually and mathematically advantageous to use the factorization in momentum space of the transition amplitude into a product of projectile and target terms. To that end, we introduce (as has been done before [24], but with slightly different coefficients) the momentum-transfer-dependent projectile effective charge

$$Z^{fi}_{\rm eff}(\vec{q}) = \frac{1}{(2\pi)^2}\left[\delta_{f_P i_P}Z_P - F_{f_P i_P}(-\vec{q})\right]. \quad (10)$$

We also introduce the first-order scattering amplitude as

$$T_{fi}(\vec{q}) = \frac{i4\pi}{v}\frac{F_{f_T i_T}(\vec{q})}{q^2}. \quad (11)$$

Up to a multiplicative factor, the first-order scattering amplitude $T_{fi}(\vec{q})$ consists of the product of the usual atomic form factor $F(\vec{q})$ of Eq. (7) and $1/q^2$. The factor of $1/q^2$ is characteristic of the Coulomb scattering between charged particles. For a given transition, only target quantum numbers are involved in defining $T_{fi}(\vec{q})$ in (11). Therefore $T_{fi}(\vec{q})$ depends only on the properties of the target. Equation (9) may be rewritten in the form

$$a_{f_T,f_P}(\vec{b}) = \int d\vec{q}_\perp e^{-i\vec{q}_\perp\cdot\vec{b}}Z^{fi}_{\rm eff}(\vec{q})T_{fi}(\vec{q}). \quad (12)$$

The effective charge $Z^{fi}_{\rm eff}(\vec{q})$ has been considered previously in q space [24] and some useful limits ($q \to 0$ and $q \to \infty$) have been obtained. However, little attention has been paid to its dependence on the impact parameter. In this section we consider the transition amplitude not in terms of the momentum transfer $\vec{q}$ as in (12), but in terms of virtual impact parameters $\vec{b}'$. The underlying idea is to utilize the intuitive picture that when a projectile carries electrons into the collision, there is a diffused charge cloud rather than a pointlike particle interacting with the target. The overlap of the charge cloud with the target will be determined by the virtual impact parameter, which measures the deviation from the projectile nucleus (the actual impact parameter) as depicted in Fig. 1. In addition to providing a simple physical picture

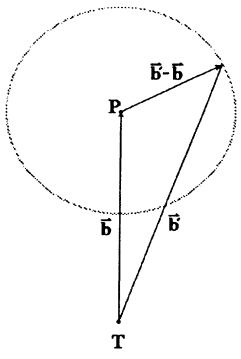

FIG. 1. The end view of the collision showing the real impact parameter $\vec{b}$ and the virtual impact-parameter $\vec{b}'$.

of the collision, it is often advantageous to invoke the impact-parameter approach since the multiple-electron transition amplitude may be approximated by the product of single-electron transition amplitudes. Thus our impact-parameter formulation will enable us to deal with multiple- as well as single-electron transitions, as we detail in Sec. VII.

A. Surface charge density

The separation of projectile and target in terms of the virtual impact parameter may be achieved by introducing an effective surface charge density of the projectile by the Fourier transform of $Z_{\rm eff}^{fi}(\vec{q})$

$$\varsigma_{\rm eff}^{fi}(\vec{b}) = \int d\vec{q}_\perp e^{i\vec{q}_\perp\cdot\vec{b}} Z_{\rm eff}^{fi}(\vec{q}) \tag{13}$$

and by expressing the target excitation probability amplitude in b space as

$$a_{fi}^T(\vec{b}) = \frac{1}{(2\pi)^2}\int d\vec{q}_\perp e^{-i\vec{q}_\perp\cdot\vec{b}} T_{fi}(\vec{q}). \tag{14}$$

Rewriting (14) in its complimentary form

$$T_{fi}(\vec{q}) = \int d\vec{b}' e^{i\vec{q}_\perp\cdot\vec{b}'} a_{fi}^T(\vec{b}')$$

and substituting $T_{fi}(\vec{q})$ into (12) yields

$$\begin{aligned} a_{f_T,f_P}(\vec{b}) &= \int d\vec{q}_\perp e^{-i\vec{q}_\perp\cdot\vec{b}} Z_{\rm eff}^{fi}(\vec{q}) \int d\vec{b}' e^{i\vec{q}_\perp\cdot\vec{b}'} a_{fi}^T(\vec{b}') \\ &= \int d\vec{b}' \left[\int d\vec{q}_\perp e^{i\vec{q}_\perp\cdot(\vec{b}'-\vec{b})} Z_{\rm eff}^{fi}(\vec{q})\right] a_{fi}^T(\vec{b}'). \end{aligned} \tag{15}$$

Recognizing the bracketed term in (15) as the surface charge density $\varsigma_{\rm eff}^{fi}(\vec{b}'-\vec{b})$ defined in (13), Eq. (15) can be simplified as

$$a_{f_T,f_P}(\vec{b}) = \int d\vec{b}' \varsigma_{\rm eff}^{fi}(\vec{b}'-\vec{b}) a_{fi}^T(\vec{b}'). \tag{16}$$

This result (16) reflects the general convolution (or Faltung) theorem for the Fourier transform, namely,

$$\int d\vec{q}_\perp e^{-i\vec{q}_\perp\cdot\vec{b}} A(\vec{q}_\perp) B(\vec{q}_\perp) = \int d\vec{b}' \tilde{A}(\vec{b}'-\vec{b})\tilde{B}(\vec{b}'), \tag{17}$$

where A and B are arbitrary functions and $\tilde{A}$ and $\tilde{B}$ their respective Fourier transforms.

In (16) $a_{fi}^T(\vec{b})$ is the amplitude for an electron transition in the target caused by a particle of unit charge localized on an impact parameter $\vec{b}$. This amplitude may be calculated from the first-order scattering amplitude (11) for any given excited state. Equation (16) is the central result of this paper. It holds for both screening and antiscreening.

B. Virtual impact parameters

Equation (16) describes the transition amplitude as a product of projectile and target terms convoluted over the virtual impact parameter $\vec{b}'$. Under certain conditions [25] it is reasonable to regard the impact parameter $\vec{b}$ as well localized and observable. It is seldom the case that the variable $\vec{b}'$ is observable and so we call it a "virtual" impact parameter. In contrast to the usual expression (9) involving momentum transfers, our result (16) affords an interpretation in terms of the projectile's nonlocalized spatial charge distribution. This interpretation is elaborated in detail in the following two sections.

IV. TARGET EXCITATION AMPLITUDES

To calculate the transition amplitudes from Eq. (16), knowledge of both $\varsigma_{\rm eff}^{fi}(\vec{b}'-\vec{b})$ and $a_{fi}^T(\vec{b}')$ is required. Detailed discussions of the former will be deferred to the next two sections. Here we give the explicit expressions of the latter for target excitation by a point particle of unit positive charge. The target excited states to be considered are $1s$ to $2s$ (dipole forbidden) and $2p+$ (dipole allowed) with $\hat{v}$ as the quantization axis. The transition to $2p0$ is ignored compared to the dominant $2p+$ transition at large v.

Using the well-known atomic form factor in q space (see [22], p. 319), the first-order scattering amplitudes for these two states read, for $1s \to 2s$, as

$$T_{2s,1s}(\vec{q}) = \frac{i4\pi}{v}\frac{4\sqrt{2}Z_T^4}{[(\frac{3}{2}Z_T)^2+q^2]^3}$$

and, for $1s \to 2p+$, as

$$T_{2p+,1s}(\vec{q}) = \frac{i4\pi}{v}\frac{6iZ_T^5 q_\perp}{q^2\left[(\frac{3}{2}Z_T)^2+q^2\right]^3}\exp(i\varphi_{\vec{q}_\perp}).$$

The target excitation amplitudes in b space may be obtained by using the above expressions with the Fourier transform of Eq. (14). Doing this we obtain, for $1s \to 2s$,

$$a_{2s,1s}^T(\vec{b}) = \frac{i\sqrt{2}Z_T^4}{v}\frac{b^2 K_2\left[\sqrt{(\frac{3}{2}Z_T)^2+q_\parallel^2}\,b\right]}{[(\frac{3}{2}Z_T)^2+q_\parallel^2]^3} \tag{18}$$

and, for $1s \to 2p+$,

$$\begin{aligned} a_{2p+,1s}^T(\vec{b}) = &-\frac{i12Z_T^5}{v\alpha^6}e^{i\varphi} \\ &\times\left[|q_\parallel|K_1(|q_\parallel|b) - \beta K_1(\beta b) - \frac{\alpha^2 b}{2}K_0(\beta b)\right. \\ &\left. -\frac{\alpha^4 b^2}{8\beta}K_1(\beta b)\right], \end{aligned} \tag{19}$$

where φ is the azimuthal angle of $\vec{b}$, K_i the modified Bessel function of the second kind, $\alpha = 3Z_T/2$, and $\beta = \sqrt{\alpha^2+q_\parallel^2}$.

V. SCREENING TERMS

To understand the physical pictures presented previously and the meaning of the surface charge density, we discuss in this section the screening contribution to target excitation.

A. Surface charge density for screening

The effective charge in q space for screening may be obtained from (10) by setting $f_P = i_P = 1s$, which after the Fourier transform (13) yields the effective surface charge density for screening term

$$\begin{aligned}\varsigma_{\rm eff}^{\rm sc}(\vec{b}'-\vec{b}) &= Z_P\delta(\vec{b}'-\vec{b}) \\ &\quad -\frac{4Z_P^4}{\pi}\frac{|\vec{b}'-\vec{b}|K_1\left(\sqrt{4Z_P^2+q_\parallel^2}|\vec{b}'-\vec{b}|\right)}{\sqrt{4Z_P^2+q_\parallel^2}} \\ &\equiv \varsigma_{\rm bare}(\vec{b}'-\vec{b}) - \varsigma_{e\text{-}e}(\vec{b}'-\vec{b}), \end{aligned} \tag{20}$$

where we have divided the total charge density into the bare projectile component $\varsigma_{\rm bare}$ and the electron charge cloud part $\varsigma_{e\text{-}e}$. Equation (20) shows three key features. (i) For a point particle such as the projectile nucleus, the charge density $\varsigma_{\rm bare}(\vec{b}'-\vec{b})$ is localized as a Dirac δ function, as expected. (ii) $\varsigma_{e\text{-}e}$ and $\varsigma_{\rm bare}$ are of opposite sign so that $\varsigma_{\rm eff}^{\rm sc} < \varsigma_{\rm bare}$. (iii) The electronic charge cloud $\varsigma_{e\text{-}e}(\vec{b}'-\vec{b})$ is "fuzzy," i.e., smeared out over a range of $\vec{b}'$ around $\vec{b}$.

B. Gaussian-like surfaces

Following directly from (7), (10), and (13), the electronic charge density of (20) may be alternatively expressed as

$$\begin{aligned}\varsigma_{e\text{-}e}(\vec{b}'-\vec{b}) &= \int d\vec{q}_\perp e^{i\vec{q}_\perp\cdot(\vec{b}'-\vec{b})}\frac{1}{(2\pi)^2}\langle 1s|e^{-i\vec{q}_\perp\cdot\vec{r}}|1s\rangle \\ &= \langle 1s|\frac{1}{(2\pi)^2}\int d\vec{q}_\perp e^{i\vec{q}_\perp\cdot(\vec{b}'-\vec{b}-\vec{r}_\perp)}e^{-iq_\parallel z}|1s\rangle \\ &= \langle 1s|\delta(\vec{b}'-\vec{b}-\vec{r}_\perp)e^{-iq_\parallel z}|1s\rangle. \end{aligned} \tag{21}$$

This expression is connected to the static surface charge density, which can be obtained by integrating over z of the volume charge density as

$$\begin{aligned}\varsigma_{\rm static}(\vec{b}'-\vec{b}) &= \int dz|\phi_{1s}(\vec{r})|^2_{\vec{r}_\perp=\vec{b}'-\vec{b}} \\ &= \int d\vec{r}\delta(\vec{b}'-\vec{b}-\vec{r}_\perp)|\phi_{1s}(\vec{r})|^2 \\ &= \langle 1s|\delta(\vec{b}'-\vec{b}-\vec{r}_\perp)|1s\rangle \end{aligned} \tag{22}$$

As pictured in Fig. 2, $\varsigma_{\rm static}$ may be viewed as a surface charge density accumulated on a Gaussian-like cylindrical surface along z direction of a volume charge density. Similarly, $\varsigma_{e\text{-}e}$ is an effective surface charge density differing from the static charge density only by a modulating factor $e^{-iq_\parallel z}$. This factor is related to the fact that a minimum momentum transfer is required, which limits the spatial extent along z that can contribute to the transition. In the limit of large impact speed v, the minimum momentum transfer becomes small $\sim v^{-1}$ and $\varsigma_{e\text{-}e}$ approaches $\varsigma_{\rm static}$ within $O(v^{-2})$. That is, within the accuracy of the first-order perturbation theory,

$$\varsigma_{e\text{-}e}(\vec{b}'-\vec{b}) \simeq \varsigma_{\rm static}(\vec{b}'-\vec{b}). \tag{23}$$

Thus $\varsigma_{e\text{-}e}$ behaves like an effective surface charge density. Referring back to Fig. 1, we may regard a contribution to the transition probability amplitude at a fixed value of $\vec{b}$ and $\vec{b}'$ and a given finite time t. This contribution is the target probability amplitude $a_{fi}^T(\vec{b}')$ weighted with the static projectile charge density per $(\vec{b}'-\vec{b})$, $\varsigma_{\rm static}(\vec{b}'-\vec{b})$, which accumulates over a path $z = vt$ during the collision. Of course, the total transition amplitude must be convoluted over all virtual impact parameters.

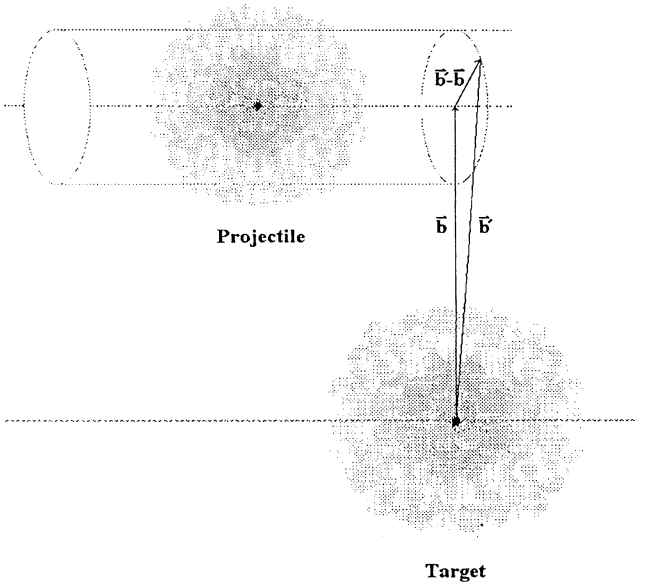

FIG. 2. The cylindrical Gaussian surface along which the surface charge density is defined.

C. 1s-2s target excitation

The convolution process is illustrated for a $1s \to 2s$ transition in Figs. 3(a) and 3(b), for which the transition probability amplitude can be evaluated from (16) and (18), namely,

$$\begin{aligned}a_{2s,\rm sc}(\vec{b}) &= \int d\vec{b}'\varsigma_{\rm eff}^{\rm sc}(\vec{b}'-\vec{b})a_{2s,1s}^T(\vec{b}') \\ &= \int d\vec{b}'\left[Z_P\delta(\vec{b}'-\vec{b}) - \varsigma_{e\text{-}e}(\vec{b}'-\vec{b})\right]a_{2s,1s}^T(\vec{b}'). \end{aligned} \tag{24}$$

Explicit evaluation of the (24) yields a simple analytic result

$$a_{2s,\mathrm{sc}}(\vec{b}) = Z_P \frac{i\sqrt{2}Z_T^4}{v}\frac{b^2K_2(\beta b)}{\beta^2} - \frac{i2^{\frac{15}{2}}Z_P^4Z_T^4}{v\lambda^8}\left[\frac{\lambda^2}{2}\frac{bK_1(\gamma b)}{\gamma} - 3K_0(\gamma b) + 3K_0(\beta b) + \lambda^2\frac{bK_1(\beta b)}{\beta} + \frac{\lambda^4}{8}\frac{b^2K_2(\beta b)}{\beta^2}\right], \tag{25}$$

where $\gamma = \sqrt{4Z_P^2 + q_\parallel^2}$ and $\lambda^2 = \alpha^2 - 4Z_P^2$ [α and β are given earlier following (19)].

The solid curve in Fig. 3(a) is due to the bare projectile nucleus and corresponds to the convolution of the first term in (24). The surface charge density of the nucleus is simply $Z_P\delta(\vec{b}' - \vec{b})$, represented by the dashed curve in Fig. 3(a). Convolution of this surface charge density with the target excitation amplitude (18) yields the first term in (25).

The convolution from the second term in (24) results in the contribution due to the electronic screening [solid curve in Fig. 3(b)] and corresponds to the bracketed term in (25). The broadening of the transition amplitude due to a broad electronic cloud [Fig. 3(b)] is shown clearly by comparing with the transition amplitude due to the bare nucleus [Fig. 3(a)]. The width of $\varsigma_{e\text{-}e}(\vec{b}' - \vec{b})$ is seen to be approximately the size of the electron cloud of the projectile, as would be expected.

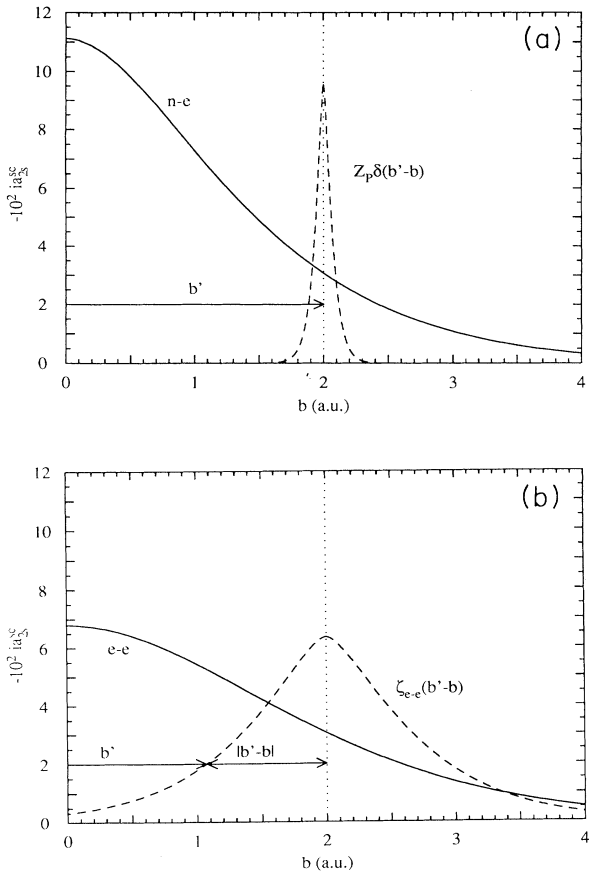

FIG. 3. Screening contribution and the convolution process for target excitation $1s \rightarrow 2s$ in H + H collisions at $v = 5$ a.u. (a) The bare nuclear contribution. Solid curve, transition amplitude; dashed curve, point charge density $\varsigma_{\mathrm{bare}}$. (b) The electronic contribution. Solid curve, transition amplitude; dashed curve, electronic charge density $\varsigma_{e\text{-}e}$.

D. Transition probability for screening

The experimentally measurable transition probability $P(\vec{b}) = |a|^2$, where a is the probability amplitude shown in Figs. 3(a) and 3(b), may be calculated by the square of the coherent sum of the nuclear and the electron contributions shown in Figs. 3(a) and 3(b). In this case $P(\vec{b}) = P(b)$ is isotropic in the azimuthal angle of scattering φ. The result $bP(b)$ is displayed in Fig. 4 for the $1s \rightarrow 2s$ transition. Also shown in Fig. 4 is the $1s \rightarrow 2p+$ transition probability determined numerically in a similar fashion from (16) with (19) and (20). The plotting of the quantity $bP(b)$ rather than $P(b)$ in Fig. 4 is to enhance the node which occurs and also to correspond to the cross section that is measured experimentally.

We note the node structure in the $1s \rightarrow 2s$ transition in Fig. 4 at $b \sim 2$, where the transition probability vanishes. This is a result of the screening. We recall from (24) that the net transition amplitude is determined by subtracting the screening contribution from that of the bare nucleus. Because of the smearing of the convolution process, the screening amplitude [the second term in (24)] becomes larger than the nuclear amplitude [the first term in (24)] from approximately $b \geq 2$. This results in a total cancellation of the net transition amplitude at the point $b = 2$ (thus a node) and a second peak at $b \sim 3$. It is clearly a signature of the electron-electron correlation in the screening term. The second peak is expected to be even larger if the electronic cloud is more delocalized, such as the case of an excited state of the projectile. Our prediction of such a node structure may be tested experimentally.

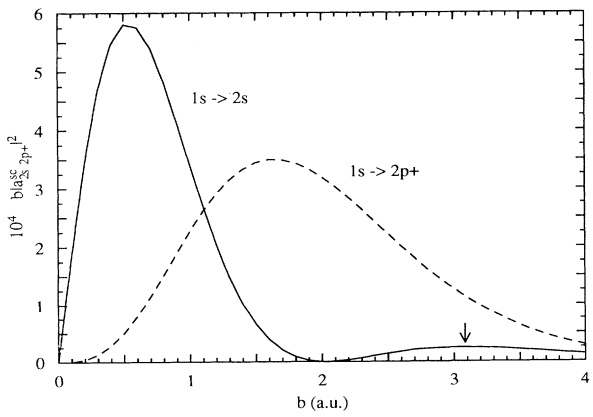

FIG. 4. Screening probabilities to target excitation $1s \rightarrow 2p+$ in H + H collisions at $v = 5$ a.u. The arrow indicates the node structure due to electron screening (see text).

The behavior of the transition probability at small b is also of interest. As $b \to 0$, the quantity $bP(b)$ approaches zero linearly in b [i.e., $P(b \to 0)$ is nonzero] for $1s \to 2s$ and quadratically in b [$P(b) \to b$] for $1s \to 2p+$. Symmetry consideration of the $1s \to 2p+$ transition requires that the transition amplitude vanish for any azimuthally symmetric charge distribution in b space around the target nucleus. This criterion is only satisfied for the special case of $b = 0$ (Figs. 1 and 2), resulting in the different behaviors of the transition probabilities at small impact parameters for $2s$ and $2p+$ states, respectively. These behaviors lead to suppression of large angle scattering of the projectile, or, equivalently, suppression of large transverse momentum transfers, for excitation to $2p+$ compared to $2s$. The difference may be sufficiently large for experimental separation of the relative contribution of the two states.

VI. ANTISCREENING TERMS

Like target excitation, the projectile may also be excited in the collision. This opens up additional channels contributing to target excitation. Proper inclusion of all the channels in antiscreening is relatively difficult even within the first Born approximation.

A. Summing over the excited states of the projectile

It is desirable to study to what degree the intuitive pictures discussed above about screening may also be applied to antiscreening, so that one may still retain some of the advantages of the virtual-impact-parameter approach. A reasonable premise exists which suggests that the antiscreening transition probability may be related to the screening transition probability, for the former is equal to the total (all final projectile states) transition probability less that for screening. In the case of antiscreening, we have not found a general analytic method to calculate the probability amplitude of Eq. (16). Some simplification can be made by considering the transition probability $|a_{f_T,f_P}(\vec{b})|^2$ instead of the transition amplitude $a_{f_T,f_P}(\vec{b})$. The transition probability for antiscreening as an incoherent sum over all final states except the initial state is

$$|a_{f_T,\mathrm{anti}}(\vec{b})|^2 = \sum_{f_P \neq i_P} |a_{f_T,f_P}(\vec{b})|^2 = \int\int d\vec{b}'\,d\vec{b}'' \times \sum_{f_P \neq i_P} a^T_{fi}(\vec{b}')\,a^{T*}_{fi}(\vec{b}'') \times \varsigma^{f_P,1s}_{\mathrm{eff}}(\vec{b}-\vec{b}')\,\varsigma^{f_P,1s*}_{\mathrm{eff}}(\vec{b}-\vec{b}''), \tag{26}$$

where the relation (16) has been used. A useful tool in dealing with the infinite sum presented in (26) is the closure approximation, which uses the properties of a complete basis set. For this purpose, we use the alternative expression for $\varsigma^{fi}_{\mathrm{eff}}(\vec{b})$ in the form we used in (21), namely,

$$\varsigma^{f_P,1s}_{\mathrm{eff}}(\vec{b}) = \langle f_P|\delta(\vec{b}-\vec{r}_\perp)e^{-iq_\parallel z}|1s\rangle, \tag{27}$$

where $f_P \neq 1s$. Substituting (27) into (26) we obtain

$$|a_{f_T,\mathrm{anti}}(\vec{b})|^2 = \int\int d\vec{b}'\,d\vec{b}'' \sum_{f_P \neq i_P} a^T_{fi}(\vec{b}')\,a^{T*}_{fi}(\vec{b}'') \times \langle 1s|\delta(\vec{b}-\vec{b}''-\vec{r}_\perp)e^{iq_\parallel z}|f_P\rangle \times \langle f_P|\delta(\vec{b}-\vec{b}'-\vec{r}_\perp)e^{-iq_\parallel z}|1s\rangle. \tag{28}$$

This expression is the antiscreening transition probability summed over all final excited states of the projectile. It is exact within the first-order perturbation theory. We next simplify (28) using the closure approximation.

B. Closure approximation

In the closure approximation [8], it is assumed that the target excitation amplitude, which is an implicit function of $q_\parallel$ (hence f_P through $q_\parallel = \Delta E/v$ and $\Delta E = \varepsilon^P_f + \varepsilon^T_f - \varepsilon^P_i - \varepsilon^T_i$) may be approximated at some average $\bar{q}_\parallel$. We denote this by $\bar{a}^T_{fi}$ and factor both of the terms outside the sum in (28)

$$|a_{f_T,\mathrm{anti}}(\vec{b})|^2 = \int\int d\vec{b}'\,d\vec{b}''\,\bar{a}^T_{fi}(\vec{b}')\,\bar{a}^{T*}_{fi}(\vec{b}'') \times \sum_{f_P \neq i_P} \langle 1s|\delta(\vec{b}-\vec{b}''-\vec{r}_\perp)e^{i\bar{q}_\parallel z}|f_P\rangle \times \langle f_P|\delta(\vec{b}-\vec{b}'-\vec{r}_\perp)e^{-i\bar{q}_\parallel z}|1s\rangle. \tag{29}$$

Using the exact closure property of a complete basis set

$$\sum_{f_P \neq i_P} |f_P\rangle\langle f_P| = 1 - |i_P\rangle\langle i_P|$$

we obtain, from (29),

$$|a_{f_T,\mathrm{anti}}(\vec{b})|^2 = \int\int d\vec{b}'\,d\vec{b}''\,\bar{a}^T_{fi}(\vec{b}')\,\bar{a}^{T*}_{fi}(\vec{b}'')\langle 1s|\delta(\vec{b}-\vec{b}''-\vec{r}_\perp)e^{i\bar{q}_\parallel z}\,|1-|1s\rangle\langle 1s|\,\delta(\vec{b}-\vec{b}'-\vec{r}_\perp)e^{-i\bar{q}_\parallel z}|1s\rangle, \tag{30}$$

$$|a_{f_T,\mathrm{anti}}(\vec{b})|^2 = \int\int d\vec{b}'\,d\vec{b}''\,\bar{a}^T_{fi}(\vec{b}')\,\bar{a}^{T*}_{fi}(\vec{b}'') \times \left[\delta(\vec{b}'-\vec{b}'')\langle 1s|\delta(\vec{b}-\vec{b}'-\vec{r}_\perp)|1s\rangle - \langle 1s|\delta(\vec{b}-\vec{b}''-\vec{r}_\perp)e^{i\bar{q}_\parallel z}|1s\rangle\langle 1s|\delta(\vec{b}-\vec{b}'-\vec{r}_\perp)e^{-i\bar{q}_\parallel z}|1s\rangle\right] = \int d\vec{b}'\,\varsigma_{\mathrm{static}}(\vec{b}'-\vec{b})\left|\bar{a}^T_{fi}(\vec{b}')\right|^2 - \left|\int d\vec{b}'\,\bar{\varsigma}_{e\text{-}e}(\vec{b}'-\vec{b})\bar{a}^T_{fi}(\vec{b}')\right|^2, \tag{31}$$

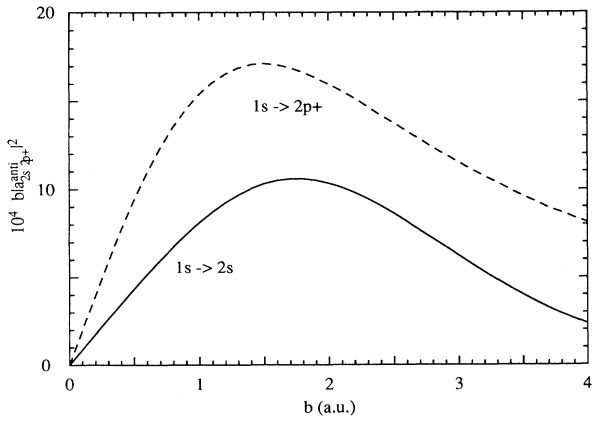

FIG. 5. Antiscreening probabilities to target excitation $1s \rightarrow 2s, 2p+$ in H + H collisions at $v = 5$ a.u.

where $\bar{\varsigma}_{e\text{-}e}$ is understood to be evaluated at an average $\bar{q}_{\|}$ just like $\bar{a}^T_{fi}$ is.

Equation (31) is the final result for antiscreening after using the closure approximation. The validity of this approximation has been well studied and various schemes have been suggested [26–29]. We use a simple rule to determine $\bar{q}_{\|}$

$$\bar{q}_{\|} = \frac{\varepsilon^T_f - \varepsilon^T_i - \varepsilon^P_i}{v} \tag{32}$$

in which it is assumed that the mean energy of the projectile final state is zero. This may be reasonable in view of the bound and continuum contributing states, as well as the observation that most contribution to antiscreening comes from low-lying continuum states of the projectile. Other choices of $\bar{q}_{\|}$ may also be used [26].

C. Transition probability for antiscreening

As an example, the antiscreening contribution to $1s \rightarrow 2s, 2p+$ transitions is displayed in Fig. 5. The transition probabilities are calculated from (31) by their respective target excitation amplitudes. We note that regardless of the details of how $\bar{q}_{\|}$ is chosen, the overall structure in the virtual-impact-parameter method for antiscreening as given by (31) is correct. Comparing Figs. 4 and 5 shows that the antiscreening probabilities are significant in a much broader range of impact parameters than the screening contribution, especially for the $1s \rightarrow 2s$ transition. This is a signature for the antiscreening term. Such a broad distribution has been observed experimentally for the loss process [30]. Naturally this feature is a consequence of the nonlocalized contribution of the projectile electron cloud.

VII. DISCUSSION

In deriving Eq. (16) and in the subsequent application of it to screening and antiscreening, we have shown that a virtual impact parameter $\vec{b}'$ may be introduced to describe the nonlocalization of the projectile electron at a definite (real) impact parameter $\vec{b}$. The influence of the projectile electron is simply given by an effective surface charge density $\varsigma^{fi}_{\text{eff}}(\vec{b}' - \vec{b})$, which may be obtained by integrating over a Gaussian surface of fixed $\vec{b}' - \vec{b}$ of the electronic charge cloud. The surface charge density is convoluted over $\vec{b}'$ with the transition amplitude $T_{f_T}(\vec{b}')$ for the target electrons to yield the two-center transition amplitude $a_{f_T,f_P}(\vec{b})$ in (16).

We have used a first-order theory within the straight-line trajectory approximation for the internuclear motion in obtaining Eq. (16). The first Born approximation for the electronic transitions is restricted to perturbations where both the projectile and the target Massey parameters Z_P/v and Z_T/v are small. The classical description of the internuclear motion, on the other hand, is expected to be valid over a wide range of collision speeds owing to the heavy nuclear mass [21]. Provided that the above conditions are met, our method is expected to yield accurate integral, and in most cases differential, cross sections. We note, however, that there are circumstances where a first-order theory may fail even if these conditions are fulfilled. For instance, when fast electrons are ejected as a result of antiscreening, it has been shown that a second-order theory is required to adequately describe the process [28,31]. In general, whenever antiscreening processes involve large momentum transfers, higher-order interactions may be important. Although higher-order terms in the Born series are difficult to calculate, one may alternatively use the classical approach as has been recently demonstrated [32,33]. The success of the classical approach can be traced to the correspondence principle for large momentum transfers.

Let us briefly consider application of Eq. (16) to reactions in which the target atom undergoes multiple transitions of independent electrons. The independent-electron approximation is valid if electron correlation in the target is neglected [34]. For bare projectiles the probability amplitude a_{f_T} in the independent-electron approximation reduces to a product of single-electron probabilities, i.e., $a_{f_T} = \prod_j a^j_{f_T}$, where $\prod_j a^j_{f_T}$ are the probability amplitudes for the independent (or uncorrelated) electrons [34]. This may be used in Eq. (4) to evaluate total cross sections. In this paper we have extended the case of bare projectiles to projectiles carrying one active electron which may interact with the target electrons. Then for multiple-electron transitions in the independent-electron approximation, the probability amplitude of Eq. (16) becomes

$$a_{f_T,f_P}(\vec{b}) = \prod_j a^j_{f_T,f_P}(\vec{b}),$$

where $a^j_{f_T,f_P}(\vec{b})$ is defined for each electron by Eq. (16). Now two-center correlation (with both screening and antiscreening) for one projectile electron is included. The target electrons are still independent of one another, but not of the electron on the projectile.

We remarked earlier following Eq. (16) that the vir-

tual impact parameter $\vec{b}'$ is seldom a physical observable. There may be cases where the electronic cloud may be relatively localized. For example, in collisions involving Rydberg atoms the active electron is far from the nucleus. The core electrons (if any) may then be regarded as well localized for all practical purposes. In this case, we may assume that the screening of the core electrons may be specified by well-defined $\vec{b}$, yielding an approximate method for treating many-electron projectiles.

VIII. SUMMARY

The screening and antiscreening contributions between structured particle impact have been studied within the virtual-impact-parameter method. In this method, we have achieved the separation of the projectile and the target terms. An effective surface charge density has been introduced to describe the projectile term, which yields a simple and intuitive physical picture for screening. Signatures of the *e-e* correlation are presented as nodes of the transition amplitudes. This picture is extended to antiscreening where we have shown that the overall mathematical structure is preserved. The virtual-impact-parameter method may prove useful to a variety of problems involving interactions of structured particles, particularly to the separation of *e-e* correlation effects from independent-electron effects, single- or multiple-electron transitions, and to the study of nondipole transitions by charged particles in relation to photon impact. This method may be fruitfully used in the analysis of recent experimental determination [35,36] of both transverse and parallel recoil ion momenta, from which the impact-parameter dependence of the screening and antiscreening terms may be extracted separately.

ACKNOWLEDGMENTS

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