Asymmetry in the Cusp of the Cross Section for Electron Capture to the Continuum for a Fast Bare Ion on a Hydrogenlike Atom

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It is shown that at a high impact velocity $\vec{v}$ the *second*-order Born term can provide a significant *asymmetric* (skew) contribution to the cusp at $|\vec{v}_e|=|\vec{v}|$ in the differential cross section for "electron capture to the continuum" from a hydrogenlike atom in its 1s state by a bare ion, where $\vec{v}_e \approx \vec{v}$ is the velocity of the emergent electron. The asymmetry in the cusp, heretofore unexplained, has been observed in several recent experiments.

We consider a *bare* ion of atomic number Z_B incident with a very high speed v on a hydrogenlike atom of atomic number Z_A initially in the 1s state. We wish to determine the singly differential cross section, $d\sigma/dv_e$, for "capture to the continuum," in which the electron emerges with a speed between v_e and v_e+dv_e into a cone with semiangle θ_0 and axis parallel to the beam, where $|v_e-v|$ and $v\theta$ are both small so that the emergent electron is moving relative to the projectile nucleus with a (positive) energy that is small compared to the ionization energy of the electron-projectile subsystem.[1] Dettmann *et al.* showed,[2] within the Brinkman-Kramers (BK) approximation, that asymptotically

$$d\sigma_{\rm BK}/dv_e \sim (2^{17}/5)Z_A{}^5 Z_B{}^3(e^2/\hbar v)^{10}v^{-2}\{[(v_e-v)^2+(v\theta_0)^2]^{1/2}-|v_e-v|\}\pi a_0{}^2. \qquad (1)$$

They noted in particular that, because of the quantity in curly brackets, $d\sigma_{\rm BK}/dv_e$ has a cusp at $v_e=v$.

A significant feature of the cusp in $d\sigma_{\rm BK}/dv_e$ is that it is symmetric about $v_e=v$. However, several measurements,[3] most notably the very recent measurements of Suter *et al.*,[4] indicate that for bare projectiles incident at high velocities the actual cusp may be strongly asymmetric about $v_e=v$. Our purpose is to explain that the observed asymmetry is probably due to the contribution from a *second*-order Born term in the Born expansion of the scattering amplitude. This result is physically reasonable since at high impact velocities the BK amplitude, $\mathcal{T}_1$, defined by Eq. (2c) below, for capture into a true bound state is proportional to the high-momentum component of the final bound-state wave function, a component which is very small and diminishes even more rapidly as the orbital angular momentum quantum number, l', of the final state increases. Thus the relative probability for capture into a bound state with $l'\neq 0$ compared to capture into a bound state (including a high Rydberg state) with $l'=0$ decreases as $1/v^{2l'}$. In contrast, the second-order Born term $\mathcal{T}_2$, defined by Eq. (2d) below, does not depend on the high-momentum component of the final-state wave function and the relative probability for capture into states of different l' is therefore independent of v to leading order in $1/v$. Furthermore, at high impact velocities $\mathcal{T}_2$ dominates over $\mathcal{T}_1$.[5] By reason of continuity, one expects these results to remain valid for capture to the continuum. Thus for continuum capture via the BK mechanism, only the s-wave component of the continuum is expected to be important, and $\mathcal{T}_1$ is expected to be isotropic in the vector $\vec{v}_e-\vec{v}$, where $\vec{v}_e$ and $\vec{v}$, respectively, are the emergent electron and projectile velocities in the lab frame. In contrast, many different angular momentum components of the continuum are expected to be important for continuum capture via the second Born mechanism so that $\mathcal{T}_2$ will depend on both the magnitude *and* direction of $\vec{v}_e-\vec{v}$. Thus the contribution to the differential cross section from $\mathcal{T}_2$ is not expected to be invariant under $(\vec{v}_e-\vec{v})\to-(\vec{v}_e-\vec{v})$.

We now proceed to a mathematical analysis. We make use of asymptotic formulas derived previously[6] in the context of electron capture to a true bound state from a hydrogenlike atom by a bare ion incident with a high velocity $\vec{v}$; if corrections of the order of the electron-nucleus mass ratio are neglected, the contribution from the sum of the first- and second-order Born terms to the cross section (denoted by the subscript 2) for capture from a bound state i to a bound state f with wave functions $\psi_i(\vec{r})$ and $\psi_f(\vec{r})$ is, at asymptotically high velocities,

$$\sigma_2 \sim (2\pi\hbar^2 v^2)^{-1} \int |\mathcal{T}|^2 K dK, \tag{2a}$$

where (as throughout this paper) $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2$, K ranges from $\frac{1}{2}q$ to ∞, $q = |\vec{q}|$, and

$$\vec{q} \equiv m\vec{v}/\hbar, \quad \vec{T} \equiv \vec{q} + \vec{K}, \quad D \equiv q^2 - K^2, \tag{2b}$$

$$\mathcal{T}_1 \sim -(4\pi^3\hbar^2 K^2/m)\tilde{\psi}_f^*(\vec{K})\tilde{\psi}_i(\vec{T}), \tag{2c}$$

$$\mathcal{T}_2 \sim -i(2^4\pi^2 Z_A Z_B e^2/K^4 a_0)\int_0^\infty ds e^{iDs/2}\psi_f^*(-s\vec{T})\psi_i(-s\vec{K}), \tag{2d}$$

where a tilde denotes a Fourier transform. $\hbar\vec{K}$ is the difference between the final "average" momentum of the projectile and the initial momentum of the projectile. We need know only that $|\vec{K}| = K$ and $\vec{K} \cdot \hat{q} = -\frac{1}{2}q$, from which it follows that $T \equiv |\vec{T}| = |\vec{q} + \vec{K}| = K$. Note that $\mathcal{T}_1$ and $\mathcal{T}_2$ are the first- and second-order Born amplitudes with the internuclear potential omitted. ($\mathcal{T}_1$ is the BK amplitude).

Turning now to the problem at hand, we assume that initially the electron is in the 1s state and that finally it is moving in a continuum state in the Coulomb field of the projectile with the wave function

$$\psi_{\vec{k}}(\vec{r}) = (2\pi)^{-3/2} N(\eta) e^{i\vec{k}\cdot\vec{r}}\, {}_1F_1(-i\eta, 1, -i(kr + \vec{k}\cdot\vec{r})), \tag{3}$$

where $\hbar\vec{k} = m(\vec{v}_e - \vec{v})$, $k = |\vec{k}|$, and $N(\eta) = \exp(\eta\pi/2)\Gamma(1 + i\eta)$ with $\eta \equiv Z_B/a_0 k \gg 1$. Let θ_e and φ_e denote the polar and azimuthal angles of $\vec{v}_e$ with the polar axis along $\vec{v}$. See Fig. 1. The azimuthal angle of $\vec{T}$ is defined to be zero. To obtain $d\sigma_2/dv_e$ we simply replace ψ_f by $\psi_{\vec{k}}$ and [noting that $d^3k = (m/\hbar)^3 v_e^2 dv_e d\Omega_e$ and that $v_e^2 \approx v^2$] replace Eq. (2a) by

$$d\sigma_2/dv_e \sim (m^3/2\pi\hbar^5)\int d\Omega_e \int |\mathcal{T}|^2 K\, dK, \tag{4}$$

where $d\Omega_e = \sin\theta_e d\theta_e d\varphi_e$ and where $0 \le \theta_e \le \theta_0$ and $0 \le \varphi_e \le 2\pi$. Note that since $\int |\psi_f(\vec{r})|^2 d^3r = 1$ we have normalized $\psi_{\vec{k}}(\vec{r})$ so that $\int \psi_{\vec{k}'}(\vec{r})\psi_{\vec{k}}(\vec{r}) d^3r = \delta(\vec{k}' - \vec{k})$.

Inserting $\tilde{\psi}_{1s}(\vec{T})$ and $\tilde{\psi}_{\vec{k}}^*(\vec{K})$ into Eq. (2c), we obtain[7]

$$\mathcal{T}_1 \sim -2^{7/2} Z_A^{5/2} Z_B e^2 N^*(\eta)/(a_0^{5/2} K^6), \tag{5}$$

in agreement with Dettmann, Harrison, and Lucas.[2] We now evaluate $\mathcal{T}_2$. The presence of $\psi_i = \psi_{1s}(-s\vec{K})$ in Eq. (2d) restricts sK to the region $sK \lesssim a_0/Z_A$. Hence $sT \lesssim a_0/Z_A$. Now if $\hbar^2 k^2/2m \ll Z_B e^2/sT$ for the significant range of sT, that is, if $\eta^2 \gg Z_B/2Z_A$, the energy in the Schrödinger equation for $\psi_{\vec{k}}(-s\vec{T})$ can be neglected and $\psi_{\vec{k}}(-s\vec{T})$ simplifies to[8]

$$\psi_{\vec{k}}(-s\vec{T}) \sim (2\pi)^{-3/2} N(\eta) e^{-i\vec{k}\cdot s\vec{T}} J_0((4Z_B \chi sT/a_0)^{1/2}), \tag{6a}$$

where, with a carat denoting a unit vector, the "asymmetry source factor" $\chi \equiv 1 - \hat{k}\cdot\hat{T}$, so that

$$\chi = 1 - (\cos\theta\cos\theta_T + \sin\theta\sin\theta_T\cos\varphi_e), \tag{6b}$$

$$\theta_T \equiv \cos^{-1}(\hat{v}\cdot\hat{T}) = \cos^{-1}(q/2K), \tag{6c}$$

$$\theta \equiv \cos^{-1}(\hat{v}\cdot\hat{k}) \sim \tan^{-1}\{v\theta_e/(v_e - v)\}. \tag{6d}$$

Note that $0 \le \chi \le 2$ and, since $\frac{1}{2}q \le K \le \infty$, that $0 \le \theta_T \le \frac{1}{2}\pi$.

In Eq. (2d) we use Eq. (6a) to substitute for $\psi_f(-s\mathrm{T})$, we use $\vec{k}\cdot\vec{T} = (1-\chi)kK$, we define

$$1/\alpha \equiv Z_A K a_0 - \tfrac{1}{2}iDa_0^2 + i(1-\chi)kKa_0^2, \tag{7}$$

and we integrate over s; we then obtain[9]

$$\mathcal{T}_2 \sim \tfrac{1}{2}i\mathcal{T}_1 K^2 a_0^2 \alpha \exp(-Z_B \chi K a_0 \alpha). \tag{8}$$

This result differs significantly from the $\mathcal{T}_2$ obtained by Dettmann, Harrison, and Lucas[2]; we believe there is an error in Eq. (4.25) of their paper. Note particularly, from Eqs. (6d) and (6b), that under a change of sign of $\vec{v}_e - \vec{v}$ we have $\theta \to \pi - \theta$; thus χ and therefore $\mathcal{T}_2$ are asymmetric about $v_e = v$.

Combining Eqs. (4), (5), and (8) and noting that $|N(\eta)|^2 \sim 2\pi\eta$, we obtain

$$d\sigma_2/dv_e \sim 2^7 Z_A^5 Z_B^3 a_0^{-8} \int d\Omega_e\, |\vec{v}_e - \vec{v}|^{-1} \int |1 + \tfrac{1}{2}i\alpha K^2 a_0^2 \exp(-Z_B\chi K a_0 \alpha)|^2 K^{-11} dK, \tag{9}$$

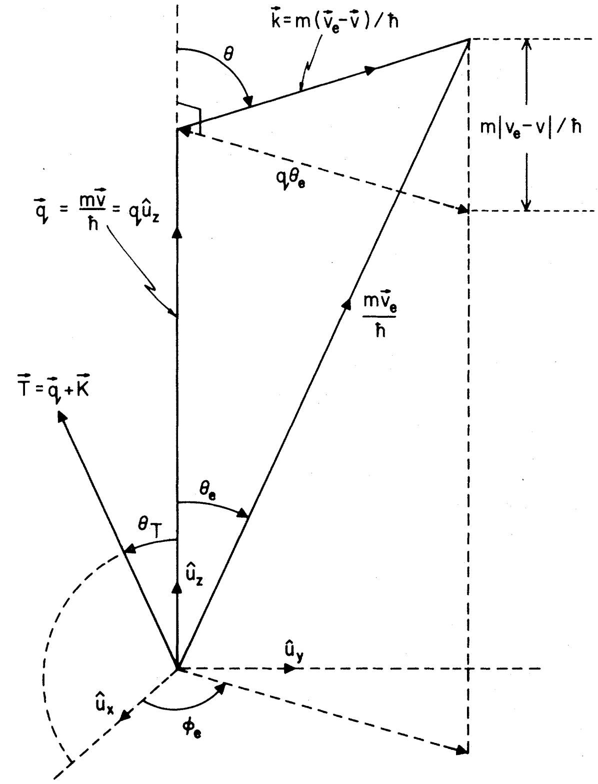

FIG. 1. The coordiante system. (The various vectors are not drawn to scale.) The polar axis is along $\vec{v}$ and the azimuthal angle of $\vec{T}\equiv\vec{q}+\vec{K}$ is defined to be zero.

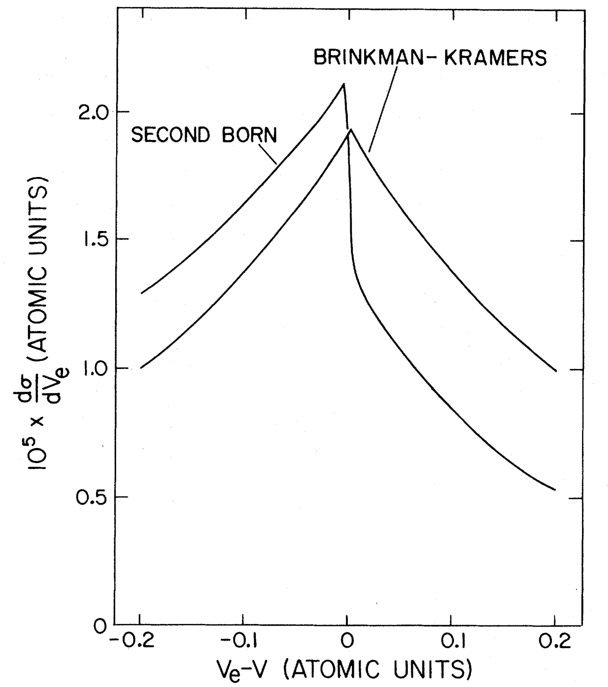

FIG. 2. The singly differential cross section for continuum electron capture from the 1s state of a hydrogen atom by a bare ion of atomic number $Z_B=6$ incident with an energy of 2 MeV per nucleon in the lab frame. The electron emerges into a cone of semiangle $\theta_0=1.85°$. The curve marked "Brinkman-Kramers" is the contribution to the differential cross section from the Brinkman-Kramers amplitude, while the curve marked "second Born" is the contribution from the sum of the first- and second-order Born terms. $d\sigma/dv_e$ is in units of $a_0^2(e^2/\hbar)^{-1}$.

where, we recall, $0\leq\theta_e\leq\theta_0$, $0\leq\varphi_e\leq 2\pi$, and $\frac{1}{2}q\leq K\leq\infty$. This integral must be evaluated numerically. Note that it is the term $2\pi\eta$ in the factor $|N(\eta)|^2$ that gives rise to the cusp, but the asymmetry in the cusp arises from the presence of χ in $\mathcal{T}_2$. Since ka_0 is assumed here to be very small, the last term in Eq. (7) can be neglected (though it was retained in our numerical calculations). Then χ appears only in the exponent in Eq. (9), in the form $\exp(-Z_B\chi\cdots)$. Therefore for Z_B small the asymmetry is negligible while for Z_B large $\mathcal{T}_2$ is highly asymmetric. (However, as Z_B increases, $\mathcal{T}_2$ decreases in magnitude relative to $\mathcal{T}_1$ and the net effect of $\mathcal{T}_2$ on $d\sigma_2/dv_e$ becomes small, though not exponentially small.) We calculated $d\sigma_2/dv_e$ for $Z_B=1$ and 6, respectively, with $Z_A=1$, with $\theta_0=1.85°$, and with the projectile energy equal to 2 MeV/nucleon. We have $|v_e-v|\leq 0.2e^2/\hbar$ and therefore $\eta>5$ ($\eta>30$) when $Z_B=1$ ($Z_B=6$). When $Z_B=1$ the asymmetry is barely noticeable, but when $Z_B=6$ (see Fig. 2) the asymmetry is very clear, and in qualitative agreement with observations.[4] (Unfortunately we cannot compare our results *quantitatively* with existing measurements since the targets used in the experiments were many-electron atoms, such as Ar, for example.) In order to gain a (crude) estimate of the error in the asymptotic approximations used, we evaluated $d\sigma_{BK}/dv_e$ exactly. With $\eta\gg 1$, the relative error in the asymptotic formula, Eq. (1), is $10(Z_Ae^2/\hbar v)^2$. At a projectile energy of 2 MeV/A, this is an error of about 13% when $Z_A=1$. We note that radiative capture to the continuum dominates over nonradiative capture above an energy of about 13 MeV/A when $Z_A=1$.[10]

The Z_B dependence of $d\sigma/dv_e$ is probably not a power-law dependence. In the extreme high-v limit, we can evaluate the integral over K and show that the asymptotic v dependence of $d\sigma_2/dv_e$ is $1/v^{11}$. (This is also shown in Ref. 10 using a semiclassical approximation.) From Eq. (1) we see that the *asymptotic* v dependence of $d\sigma_{BK}/dv_e$ is $1/v^{12}$. (Note that $v\theta_0$ and the range of $|v_e-v|$

must be independent of v asymptotically since we require $\eta \gg 1$, independent of v.)

It follows from our discussion that recent observations of cusp asymmetries[4] may represent the first experimental confirmation of the importance of the second Born contribution at high impact velocities. Other possibilities for detecting this contribution were recently suggested.[11]

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Doppler-Free Stimulated-Emission Spectroscopy and Secondary Frequency Standards Using an Optically Pumped Laser

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A new Doppler-free stimulated-emission technique using an optically pumped laser with applications in spectroscopy and optical frequency standards is reported. An argon-laser–pumped cw I_2 laser is used to demonstrate the technique as well as measure the complete hyperfine structure of the I_2 $B0_u{}^+$-$X^1\Sigma_g{}^+$ (43, 83) P(13) line. Hyperfine coupling strengths obtained for the $X^1\Sigma_g{}^+$ $v''=83$, $J''=13$ level are $eQq''=-1550.1\pm0.5$ MHz and $C''=59\pm5$ kHz. In addition, the I_2 laser has been actively stabilized to within 1 kHz of the observed line center of an I_2 hyperfine component.

We report a new Doppler-free stimulated-emission spectroscopic technique using a cw optically pumped laser (OPL). The molecule under study forms the gain medium of the OPL. The technique can also be used to generate a set of laser frequency standards covering a substantial spectral range. We have demonstrated this technique by observing narrow hyperfine-structure (hfs) features in an I_2 OPL with linewidths of less than 1 MHz which allowed us to perform high-resolution spectroscopic measurements. In addition, we have stabilized an I_2 OPL to one of the I_2 hyperfine-structure transitions.

This method of stimulated-emission spectroscopy may be compared with Doppler-free two-photon schemes[1,2] which require the use of two tunable lasers, a pump and a probe. The wavelength coverage in such schemes is limited by the tuning range of the probe laser. The OPL method described here involves only one tunable laser, since the OPL is effectively its own probe. Moreover, the wavelength coverage, in principle, ex-

