

The Nonadiabatic Sliding Model and its Application to δ -Electron Emission

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The ejection of target K electrons by projectiles which move with an arbitrary velocity v is calculated with the help of optimised basis states. These states are variationally determined by minimising the time-dependent monopole perturbation. As v increases, this prescription provides a continuous transition from molecular states to atomic states. It is demonstrated that a molecular description should not only be applied at low v , but also for very large energies of the ejected electron even if v is large. Calculations are performed for the collision systems Li+Ne and O+Al.

1. Introduction

For the treatment of electronic excitation in heavy-ion collisions [1] two models are commonly in use. At low collision velocity v , the molecular description is appropriate, where the electrons are allowed to adjust to the two-center potential at every time, while at high velocities the atomic picture can be applied. If, however, v is comparable to the orbiting velocity of the electron in its initial state, perturbation theory usually fails and the use of either the atomic or the molecular basis requires the inclusion of many states in a coupled channel calculation.

For this intermediate velocity region, variational theories offer the opportunity to reduce not only the large computational effort, but also to provide more insight into the physics of the collision process. Thereby, parameters are introduced into the electronic wavefunction and determined by minimising the matrix elements of the Hamilton operator. Kleber [2] has chosen a complex time-dependent parameter which is found from the solution of an Euler-Lagrange equation, and the electronic transition probability in zero order is given by the projection of the (time-dependent) wavefunction onto the desired final state. The first-order correction to it which is calculated from the transition matrix element of $H - i\partial/\partial t$ can, however, become quite large [3]. Thus, instead of using a wavefunction which is obtained from a classical equation of motion, it may be preferred to construct an optimal set of basis states from which the transition probability is calcu-

lated via a full quantum mechanical treatment. This basis is found from the minimisation of the coupling strength between the states. It can be characterised by velocity-dependent parameters which simulate the location and extension of the wavefunction [4], or by a real time-dependent parameter which describes the internuclear motion and serves as an indication of the nonadiabaticity of the collision process at fixed time [5].

The advantage of choosing parameters which depend only implicitly on time via the internuclear separation R as done in the sliding center model [6, 4], lies in the fact that they allow for a smooth interpolation between the united-atom and separated-atom limiting cases. This may compensate for the drawback that only the global nonadiabaticity can be extracted.

The sliding center model has recently been used for the interpretation of experimental results on the K-shell ionisation probability in asymmetric collisions [7, 8], where it was found that for protons colliding with heavy targets the atomic picture is satisfactory, while for higher projectile charges a molecular description is necessary when the adiabaticity parameter $v/(a_K E_{u.a.})$ falls below 0.5 (a_K is the K-shell radius and $E_{u.a.}$ the binding energy of the united atom).

However, the choice of the theoretical picture does not only depend on the asymmetry and the velocity of the collision system, but also on the energy of the

ejected electron. Recently, Bell has discovered by examining a large compilation of experimental data, that while the total K-shell ionisation cross sections scale with the projectile velocity [9], the differential cross sections for the emission of high-energy δ -electrons rather scale with the center of mass velocity. By using that the average internuclear distance \bar{R} which determines the transition to a given final state with energy transfer ΔE may be found from $\bar{R} \approx q_{\min}^{-1} = v/\Delta E$, Bell calculated the corresponding velocity $v(\bar{R})$ from the R - dependent location of the electron [6], and found good agreement with the data when this velocity was used in the scaling [10]. In this paper we want to give a theoretical foundation of this result by extending the sliding center model to high-lying electronic continuum states. The variational principle is reviewed in Sect. 2, and in Sect. 3 the differential cross section for electron emission is calculated in the first-order Born approximation by using the optimised basis states, and compared with results obtained from the atomic, the united-atom and the molecular description (Sect. 4). The conclusion is given in Sect. 5. Atomic units ($\hbar = m = e = 1$) are used throughout unless otherwise indicated.

2. Calculation of the Electronic States

We want to concentrate on collision systems where the projectile charge Z_P is sufficiently smaller than the target charge Z_T such that the ejection of K electrons is mainly due to direct excitation, while the contribution from multistep processes can be neglected. In this case, the transition probability is determined by only two electronic states, the initial state and the final state. Rearrangement collisions are not considered here.

In the independent electron model, the Hamiltonian H is governed by the two-center potential of the electron in the field of the projectile and target nucleus. For simplicity, we neglect screening and take it purely Coulombic. A parameter λ is introduced into H which determines how much of the time-dependent projectile field V_P is incorporated into the ‘unperturbed’ Hamiltonian H_0 [4]

$$H = H_0(\lambda) + (1 - \lambda)V_P \quad (2.1)$$

$$H_0(\lambda) = -\frac{1}{2}\Delta - \frac{Z_T}{|\mathbf{r} - \mathbf{x}|} + \lambda V_P - \mathbf{A}\mathbf{r}$$

$$V_P = -\frac{Z_P}{|\mathbf{r} - \mathbf{R} - \mathbf{x}|},$$

$$\mathbf{A} = \left(\frac{M_P}{M_P + M_T} - h \right) \dot{\mathbf{R}} - 2\dot{h}\dot{\mathbf{R}} - \dot{h}\mathbf{R}.$$

Here, we have denoted the origin of the electron by $\mathbf{x} = -h\mathbf{R}$ which is located a distance h from the target on the line connecting the projectile and target nuclei. As long as \mathbf{x} is not coinciding with the heavy particle center of mass, a recoil term $-\mathbf{A}\mathbf{r}$ has to be added which arises from the transformation to an accelerated coordinate system [11]. A classical trajectory $R(t)$ is assumed for the internuclear motion, and M_P , M_T is the mass of the projectile and target, respectively.

In order to construct a variational principle which determines the parameter λ , we recall that Demkov [12] has shown that the transition amplitude can be written in the form

$$a_{fi} = \langle \psi_f(\infty) | \psi_i(\infty) \rangle - i \int_{-\infty}^{\infty} dt \langle \psi_f(t) | H - i \frac{\partial}{\partial t} | \psi_i(t) \rangle \quad (2.2)$$

where $\psi_i(t)$ and $\psi_f(t)$ satisfy the boundary conditions to coincide with the initial state at $t = -\infty$ and with the final state at $t = +\infty$, respectively. When the functions $\psi_f(t)$ and $\psi_i(t)$ are exact solutions to the Schrödinger equation, the second term in (2.2) vanishes whereas the first term provides the exact transition amplitude. If, instead, trial functions are inserted, a_{fi} as calculated from (2.2) is stationary with respect to variations in $\psi_i(t)$ and $\psi_f(t)$ [12]. When these trial functions are chosen as eigenstates to some Hamilton operator H_0 , the first term in (2.2) vanishes due to the orthogonality of these states, such that the transition amplitude evaluated from (2.2) coincides with first-order perturbation theory

$$a_{fi} = -i \int_{-\infty}^{\infty} dt \langle \psi_f(t) | (H - H_0) - i \frac{\partial}{\partial t} | \psi_i(t) \rangle. \quad (2.3)$$

It follows immediately that also (2.3) is stationary with respect to variations in the wavefunctions and can thus be used for the variational determination of the ‘best’ wavefunctions.

In our case, the wavefunctions are characterised by the parameter λ . In order to make λ real, the absolute square of the transition amplitude has to be used as the variational functional. It also turns out that λ is very sensitive to strongly oscillating time-dependent phases of the wavefunctions which may lead to unphysical results. Rather than using (2.3), we therefore determine λ by dropping these phases, such that the variational functional consists in the time integral of the coupling strength alone [4]

$$\frac{d}{d\lambda} \int_0^{\infty} dt \langle \psi_f | (1 - \lambda)V_P - i \frac{\partial}{\partial t} | \psi_i \rangle \Big|^2 = 0 \quad (2.4)$$

where ψ_i and ψ_f do *not* contain time-dependent phases. Still, these functions may be viewed as (orthogonal) trial functions, such that the criterion of stationarity also applies to (2.4). The functions ψ_i and ψ_f depend on time via the internuclear separation R . As a consequence, they are symmetric with respect to time reversal, such that the time integral can be confined from 0 to ∞ .

The way how to determine λ may also be viewed as an extension of Stevenson's 'optimised perturbation theory' [13] to time-dependent problems. Stevenson obtains a fast convergence of the perturbation expansion of some physical observable by introducing a dummy variable into his theory. From the fact that the exact result must not depend on this variable, the 'best' approximation $A^{(n)}$ within a given order n of perturbation theory is found by requiring that the derivative of $A^{(n)}$ with respect to the variable be zero or minimal. This criterion of 'minimal sensitivity' determines the variable and consequently $A^{(n)}$. In the example discussed here ($n=1$), Stevenson's prescription can thus be mathematically confirmed by a variational principle, similarly as for time-independent problems when $n=1$.

The minimisation of the coupling strength given in (2.4) provides a balance between the two operators $(1-\lambda)V_p$ and $\partial/\partial t$. The limiting cases are readily identified: For slow collisions where $\partial/\partial t \rightarrow 0$, λ must tend to 1 to reduce the potential perturbation, which means that the full potential is incorporated into H_0 . For fast collisions, the effect of $\partial/\partial t$ can only be reduced by choosing $\lambda \rightarrow 0$ such that ψ_i and ψ_f become time-independent (atomic picture).

In the general case, ψ_i and ψ_f are eigenfunctions to a two-center potential. However, these states are difficult to handle, especially when continuum states are involved. Therefore we approximate the eigenfunctions to H_0 by another variational calculation. For the ground-state wavefunction ψ_i , we use a spherically symmetric one-center function characterised by a parameter Z

$$\psi_i(\mathbf{r}) = \frac{1}{\sqrt{\pi}} Z^{3/2} e^{-Zr}. \quad (2.5)$$

The parameters $Z(\lambda, R)$ together with $x(\lambda, R)$ which has been introduced into H_0 are determined by minimising the ground-state expectation value of $H_0(\lambda)$ with respect to z and x [6]. The resulting two coupled equations for Z and x can easily be solved for fixed λ if the variables $\rho = ZR$ and $x = hR$ are introduced

$$Z = \lambda Z_p e^{-2\rho(1-h)} [1 + 2\rho(1-h)] + Z_T e^{-2\rho h} [1 + 2\rho h], \quad (2.6a)$$

$$\frac{Z_T}{\lambda Z_p} = \frac{h^2}{(1-h)^2} \cdot \frac{1 - e^{-2\rho(1-h)} [2\rho(1-h) + 2\rho^2(1-h)^2 + 1]}{1 - e^{-2\rho h} [2\rho h + 2\rho^2 h^2 + 1]} \quad (2.6b)$$

by finding $h(\rho)$ from (2.6b) and then $Z(\rho)$ from (2.6a) which subsequently determines $R = \rho/Z$. The limiting values for Z and h can be directly deduced from (2.6): For $R \rightarrow 0$, $Z = (\lambda Z_p + Z_T)(1 - 2R^2 \lambda Z_p Z_T)$,

$$h = \lambda Z_p / (\lambda Z_p + Z_T) + 3(Z_T \lambda^2 Z_p^2 - \lambda Z_p Z_T^2) R / (2(\lambda Z_p + Z_T)^2),$$

which coincide with the 'united atom' charge and the 'center of charge' (with Z_p reduced by λ) at $R = 0$, whereas for $R \rightarrow \infty$, $Z = Z_T - (9\lambda^2 Z_p^2) / (8Z_T^5 R^4)$ and $h = (3\lambda Z_p / (4Z_T^4 R^3))$, denoting the case where the electron is localised on the target.

For the approximation of the final wavefunction ψ_f , we make use of the fact that it is orthogonal to ψ_i and take it as a Coulomb wave to the same charge $Z(\lambda, R)$.

When calculating λ from (2.4) with these functions, it is important to note that the $\partial/\partial t$ operator affects only the monopole part of the final state because ψ_i is chosen to be spherically symmetric. In order to retain the balance between the two operators in (2.4), it is therefore also necessary to disregard any contribution of higher multipoles of ψ_f when the matrix element of V_p is evaluated. An improvement would consist in introducing more parameters into ψ_i which allow for higher partial waves and thus for a better adjustment to the (non-spherical) two-center potential.

The numerical details for the evaluation of (2.4) are given in the next section in connection with the calculation of the differential cross section. For the test system $\text{Li} \rightarrow \text{Ne}$ which has an asymmetry of $Z_p/Z_T = 0.3$, and which is light enough to make a nonrelativistic calculation meaningful, the parameter λ is shown in Fig. 1 as a function of the projectile velocity relative to the united-atom orbiting velocity $v_{u.a.} = Z_p + Z_T$. The impact parameter of the collision process was taken to be zero. At fixed energy E_f of the emitted electron, λ decreases monotonically from 1 (molecular basis) to zero (atomic basis) when v increases, with the steepest descent at $v \approx v_{u.a.}$ when E_f equals the united-atom energy $E_{u.a.}$. For large values of E_f , λ remains close to 1 even at higher velocities.

This behaviour becomes more evident in Fig. 2 where at fixed v , λ is shown as a function of E_f . While at $v \ll v_{u.a.}$, the basis is close to the molecular one for any E_f , it is *not true* that for $v \gg v_{u.a.}$, the

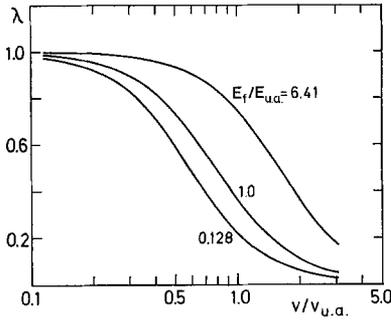


Fig. 1. Variational parameter λ as a function of the collision velocity relative to the united-atom orbiting velocity $v_{u.a.}$, calculated for K-shell ionisation of Ne by Li impact. The curves are for electronic energies E_f of 0.2 keV, 1.56 keV and 10 keV, respectively

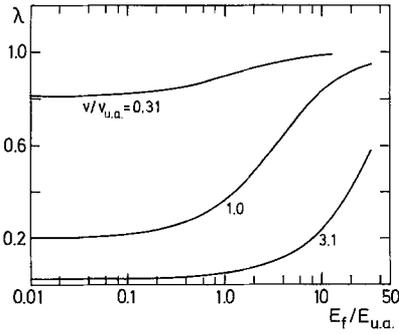


Fig. 2. Variational parameter λ as a function of the electron energy relative to the united-atom binding energy $E_{u.a.}$, calculated for K-shell ionisation of Ne by Li impact. Curves are shown for collision velocities of 4, 13 and 40 atomic units, respectively

basis is always well represented by the atomic one. Instead, for sufficiently high E_f , λ will eventually approach 1, irrespective of the magnitude of v . The transition from the atomic to the molecular basis occurs approximately at $E_f \approx v^2$ for this collision system.

This behaviour can easily be understood from (2.4) by noting that the matrix element of the operator $\partial/\partial t$ can be transformed into a matrix element of $-\partial H_0/\partial t(E_f - E_i)^{-1}$ where E_i is the energy of the initial state. For $E_f \gg |E_i|$, this matrix element is thus proportional to v/E_f . From this it follows that a large E_f has the same consequence on λ as a small v .

3. Calculation of the Differential Cross Section

In first-order Born approximation, the transition amplitude for the ejection of δ -electrons from the K-shell is given by

$$a_{fi} = -i \int_{-\infty}^{\infty} dt \langle \psi_f | \frac{Z}{r} - \frac{Z_T}{|\mathbf{r}-\mathbf{x}|} - \frac{Z_P}{|\mathbf{r}-\mathbf{R}-\mathbf{x}|} - \mathbf{A} \cdot \mathbf{r} - i \frac{\partial}{\partial t} | \psi_i \rangle e^{iF(t)} F(t) = \int_0^t dt (E_f - E_i(t)) \quad (3.1)$$

where ψ_i and ψ_f are solutions of $\tilde{H}_0 = -\Delta/2 - Z/r$, such that the difference between H_0 and \tilde{H}_0 has been included as perturbation.

It is convenient to make a partial wave expansion of both ψ_f and the two-center Coulomb field [11] and introduce the form factor integrals

$$Q_l(R) = \int_0^{\infty} dq [Z_P j_l(q(R-x)) + (-1)^l Z_T j_l(qx) - Z \delta_{l,0}] F_l(q, Z) F_l(q, Z) = \int_0^{\infty} r^2 dr r^l e^{ik_f r} {}_1F_1(l+1-i\eta, 2l+2, -2ik_f r) j_l(qr) e^{-Zr} \quad (3.2)$$

where the term $-Z \delta_{l,0}$ arises from the monopole field Z/r in (3.1). Further, \mathbf{k}_f is the momentum of the ejected electron, $\eta = Z/k_f$, j_l is a spherical Bessel function and ${}_1F_1$ a confluent hypergeometric function. The contribution from the Coulomb potentials in (3.1) can then be written in the following way

$$a_{fi}^c = -\frac{8\sqrt{2}}{\pi} \sum_{lm} (-i)^{l+1} \frac{(2k_f)^l}{(2l+1)!} Y_{lm}(\hat{\mathbf{k}}_f) \cdot \int_{-\infty}^{\infty} dt C_l(Z) Q_l(R) e^{iF(t)} Y_{lm}^*(\hat{\mathbf{R}}) C_l(Z) = Z^{3/2} e^{i\pi/2} |\Gamma(l+1+i\eta)| e^{i\sigma_l} \quad (3.3)$$

where $\sigma_l = \arg \Gamma(l+1-i\eta)$ is the Coulomb phase shift.

The internuclear coordinate $\mathbf{R}(t)$ is determined from the Rutherford hyperbola. Choosing a coordinate system where the z-axis is perpendicular to the line connecting the two nuclei at the distance of closest approach (i.e. at $t=0$), the spherical harmonics $Y_{lm}(\hat{\mathbf{R}})$ exhibit symmetry properties with respect to time reversal. For example, $Y_{10}(\hat{\mathbf{R}}) = (3/4\pi)^{1/2} R_z/R$ is odd in t , while $Y_{11}(\hat{\mathbf{R}}) = -(3/8\pi)^{1/2} R_x/R$ is even in t . One can make use of this symmetry by reducing the time integration interval to one from 0 to ∞ .

The contributions to a_{fi} from the time derivative and from the recoil field in (3.1) are easily evaluated. The result is

$$\begin{aligned}
a_{fi}^t &= -i \frac{4\sqrt{2}}{\pi} \int_0^\infty dt C_0(Z) \dot{Z} \\
&\quad \cdot \left[(Z - ik_f)^{-4} \left(1 + \frac{2ik_f}{Z - ik_f} \right)^{-2+i\eta} \right] \sin F(t) \\
a_{fi}^r &= \frac{16\sqrt{2}}{3} k_f \sum_m Y_{1m}(\hat{\mathbf{k}}_f) \int_{-\infty}^\infty dt Z C_1(Z) \\
&\quad \cdot \left[\frac{1}{Z + ik_f} \frac{1}{(Z - ik_f)^5} \left(1 + \frac{2ik_f}{Z - ik_f} \right)^{-2+i\eta} \right] \\
&\quad \cdot \left\{ \left(\frac{M_p}{M_p + M_T} - h \right) \ddot{R} Y_{1m}^*(\hat{\mathbf{R}}) - 2\dot{h} \dot{R} Y_{1m}^*(\hat{\mathbf{R}}) \right. \\
&\quad \left. - \ddot{h} R Y_{1m}^*(\hat{\mathbf{R}}) \right\} e^{iF(t)} \quad (3.4)
\end{aligned}$$

where the latter expression can also be reduced to an integral from 0 to ∞ by using that \ddot{R}_z and \dot{R}_x are odd, and \dot{R}_x , \ddot{R}_z even in t .

For the differential cross section, the square of a_{fi} has to be integrated over impact parameter b . When the direction of the emitted electron is not observed, there is an additional integral over Ω_{k_f} , such that one obtains, taking into account the presence of two K-electrons

$$\frac{d\sigma}{dE_f} = 4\pi k_f \int_0^\infty b db \int d\Omega_{k_f} |a_{fi}^c + a_{fi}^t + a_{fi}^r|^2 \quad (3.5)$$

which reduces with the help of

$$\int d\Omega_{k_f} \left| \sum_{lm} Y_{lm}(\hat{\mathbf{k}}_f) A_{lm} \right|^2 = \sum_{lm} |A_{lm}|^2$$

to an incoherent sum of the multipole contributions. If one is interested in the doubly differential cross section, the functions $Y_{lm}(\hat{\mathbf{k}}_f)$ have to be rotated through half the scattering angle at each impact parameter, such that the ejection angle ϑ_f coincides with the experimentally observed angle between \mathbf{k}_f and the beam axis \mathbf{v} .

4. Numerical Methods and Results

While the form factor $F_l(q, Z)$ reduces to a simple analytic expression for nonrelativistic wavefunctions, the integration over q in the form factor integral $Q_l(R)$ has to be done numerically. We have calculated $Q_l(R)$ at fixed values of R until it converged to the large- R behaviour which for $l \leq 1$ is given by

$$\begin{aligned}
Q_0(R) &\sim R^{-4} \\
Q_1(R) &\sim R^{-2}, \quad R > R_c \quad (4.1)
\end{aligned}$$

and used a spline-like interpolation routine for the calculation of $Q_l(R)$ for $R \leq R_c$. For the time inte-

grals in (2.4), (3.3) and (3.4) it is convenient to introduce a pseudo-linear coordinate which is obtained from the usual hyperbolic coordinate w by means of $\tau = \varepsilon \exp w$, such that

$$\begin{aligned}
t &= \frac{d}{v} \left(\frac{\tau}{2} - \frac{\varepsilon^2}{2\tau} + \ln \frac{\tau}{\varepsilon} \right) \\
R &= d \left(1 + \frac{\tau}{2} + \frac{\varepsilon^2}{2\tau} \right) \\
R_x &= d \left(\frac{\tau}{2\varepsilon} + \frac{\varepsilon}{2\tau} + \varepsilon \right) \\
R_z &= d \sqrt{\varepsilon^2 - 1} \left(\frac{\tau}{2\varepsilon} - \frac{\varepsilon}{2\tau} \right) \quad (4.2)
\end{aligned}$$

with $d = Z_p Z_T / (2E_{cm})$ (E_{cm} is the center of mass scattering energy) and $\varepsilon = (1 + (b/d)^2)^{1/2}$. The τ integral extends from ε to infinity. Fast convergence is obtained if it is split when τ corresponds to $R \approx 3a_K$, and the second part done with a much larger step width than the inner part.

The energy phase factor $F(t)$ defined in (3.1) is evaluated simultaneously with the transition matrix element at each successive instant of time, thus avoiding the evaluation of an additional integral. Thereby, we used for the energy E_i of the initial state the following formula

$$\begin{aligned}
E_i(R) &= \theta \left\{ \frac{Z^2}{2} - \lambda Z_p \left[\frac{1}{(1-h)R} \right. \right. \\
&\quad \left. \left. - e^{-2ZR(1-h)} \left(\frac{1}{(1-h)R} + Z \right) \right] \right. \\
&\quad \left. - Z_T \left[\frac{1}{Rh} - e^{-2ZRh} \left(\frac{1}{Rh} + Z \right) \right] \right\} \\
\theta &= \theta_s + \frac{Z - Z_T}{Z_p} (\theta_u - \theta_s) \quad (4.3)
\end{aligned}$$

which is obtained from the ground state expectation value of H_0 modified by the screening constant θ for which a linear interpolation in Z is chosen, such that the limiting values $\theta(Z_T) = \theta_s$, $\theta(Z_p + Z_T) = \theta_u$ are obtained. θ_s and θ_u are the ratios of the experimental binding energy to the hydrogenic energy.

For the determination of the wavefunctions, we have taken a Slater screened nuclear charge. The functions $Z(R)$, $h(R)$ and $E_i(R)$ are calculated with the help of interpolation routines. For large R , the corresponding analytic expressions were chosen. In the case of $E_i(R)$, one finds from (4.3), $E_i(R) = \theta_s (-Z_T^2/2 - \lambda Z_p/R) + O(R^{-4})$. The derivatives dZ/dR , dh/dR and d^2h/dR^2 entering into (3.4) are directly expressed in terms of h , Z and R by means of a differentiation of the implicit equations (2.6).

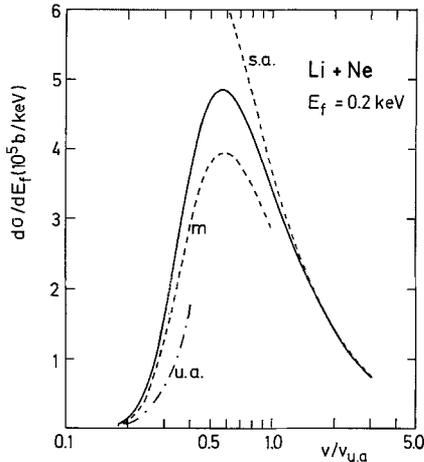


Fig. 3. Differential cross section for K-shell ionisation of Ne by Li impact as a function of collision velocity at $E_f = 0.2$ keV. Shown are the results from the sliding center calculation (full curve), from the separated-atom and molecular calculation (broken curves) and from a united-atom calculation (chain curve)

The differential cross section for the ejection of a K electron from Ne by Li impact is shown in Fig. 3 as a function of the collision velocity. The electronic energy $E_f = 0.2$ keV is chosen rather small such that it represents an important contribution to the total cross section. At very high velocities, the sliding center theory coincides with the result of an atomic calculation which can be obtained by setting $\lambda = 0$ or rather by using the standard formulas of an SCA calculation [11]. It is clearly seen that a description with fixed target wavefunctions fails when v falls below Z_T , i.e. the orbiting velocity of a K electron.

In the limit of very low velocities v , the theory coincides with a molecular calculation, obtained by choosing $\lambda = 1$. Then, at very small internuclear distances, the location of the electron distribution is in the center of charge which roughly coincides with the center of mass, such that the recoil contribution to the transition amplitude should approximately be zero. Incidentally, the recoil field gives a rather large contribution when the whole internuclear trajectory is taken into account. This follows from the behaviour of $h(R)$ which varies linearly with R (for $R \rightarrow 0$) and therefore departs rather fast from the center of charge. Thus, also the velocity of the electronic rest frame changes rapidly from the center of charge velocity to the lab velocity when the two nuclei separate. Which velocity eventually will be decisive for the electronic excitation process depends on the average internuclear separation $\bar{R} = v/\Delta E$ [10].

The recoil contribution is, however, largely cancelled by the dipole term of the Coulomb potential for

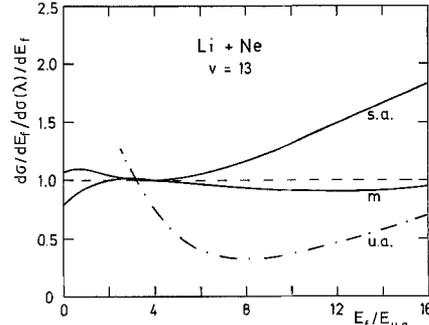


Fig. 4. Differential cross section for K-shell ionisation of Ne by Li impact, calculated in the separated-atom description and the molecular description (full curves) as well as in the united-atom picture (chain curve), relative to the differential cross section $d\sigma(\lambda)/dE_f$ from the sliding center model as a function of electron energy

these small collision velocities. It is therefore important to include the recoil term in the transition amplitude. For high velocities, on the other hand, the recoil is negligible because then the internuclear trajectory is well represented by a straight line.

An approximation to the molecular theory which has been applied quite frequently, consists in replacing the molecular functions by time-independent united atom functions localised at the center of charge [14]. The result of such a calculation is also shown in Fig. 3. It deviates from the molecular theory even at rather low velocities for the small E_f considered here.

We also have calculated the dependence of the differential cross section on the electronic energy at fixed velocity. As $d\sigma/dE_f$ decreases by about seven orders of magnitude in the energy region considered here, we have preferred to plot in Fig. 4 the ratio of the differential cross section calculated in the various limiting cases relative to the sliding center result. For an intermediate velocity ($v/v_{u.a.} = 1$), the separated atom description breaks down at energies about ten times the target K-shell binding energy, whereas the molecular theory works rather well except for the lowest E_f . On the other hand, very high energies are required to make a united-atom description reasonable.

At an energy of about 3–4 times the united atom binding energy, all theories give rather close results. An inspection of this energy region reveals that it corresponds to the binary encounter peak which for zero electron emission angle has its maximum at $E_f = E_i + vk_f$. The cross section in this region is mainly determined from a binary collision of a free electron with the projectile. This makes its independence of the various descriptions plausible.

In our calculations, only monopole and dipole tran-

sitions have been included. They give the dominant contribution to the differential cross section except in a rather extended region around the binary encounter peak. A comparison with an atomic SCA calculation [15] for the Li+Ne system at $v=v_{u.a.}$ shows that the higher multipoles give a 10% contribution at the smallest electron energies, but a rather constant enhancement by nearly a factor of 2 for $1 \lesssim E_f/E_{u.a.} \lesssim 20$. The influence of higher l decreases, however, when v is lowered.

In order to give an idea how the sliding model compares with experiment, we have calculated the δ -electron distribution for the system $O^{16}+Al$ at a collision velocity $v=11.2$ which is nearly equal to the target K-shell orbiting velocity. For this system, data are available from Bell and coworkers [10, 16] for the doubly differential cross section. These data imply a sum over electrons emitted from all shells, but at the high energies E_f considered, K-shell ionisation provides the dominant contribution. The L-shell electrons are estimated to account for about 10–30% of the experimental intensity. Therefore, a comparison with theoretical K-shell cross sections is meaningful.

Similarly as for the Li+Ne case, monopole and dipole transitions account only for about half the cross section in the energy region between 15 and 50 keV, which we have found by comparing $d^2\sigma/dE_f d\Omega_f$ in the separated-atom case with calculations [10] using the Trautmann-Rösel code [17]. It is seen from Fig. 5 that these calculations show a fall-off with E_f which is much steeper than the experimental data. The united-atom curve shown in this figure has been calculated with $l \leq 1$ transitions only, but has been multiplied by a factor of 2 to account for the contributions from the higher multipoles. Its slope is closer to the data, but a factor of 3 is missing in intensity.

The calculations within the sliding model also shown in Fig. 5 should only be considered as approximate results. Contrary to the calculations which use a fixed charge for the electronic wavefunctions, the Coulomb phases $\exp(i\sigma_l)$ which depend on Z introduce a strong oscillatory behaviour into the time integrals. This is of little consequence for the singly differential cross section $d\sigma/dE_f$. However, for the doubly differential cross section $d^2\sigma/dE_f d\Omega_f$ where the relative phases are decisive, it turns out that the inclusion of only $l \leq 1$ transitions leads to strong variations in the slope of $d^2\sigma/dE_f d\Omega_f$ which will only be washed out if all relevant multipole transitions are included. Thus we have calculated the angular averaged cross section $(4\pi)^{-1}d\sigma/dE_f$ and multiplied it (besides the factor 2 for higher l -transitions) with the ratio of the doubly to the averaged

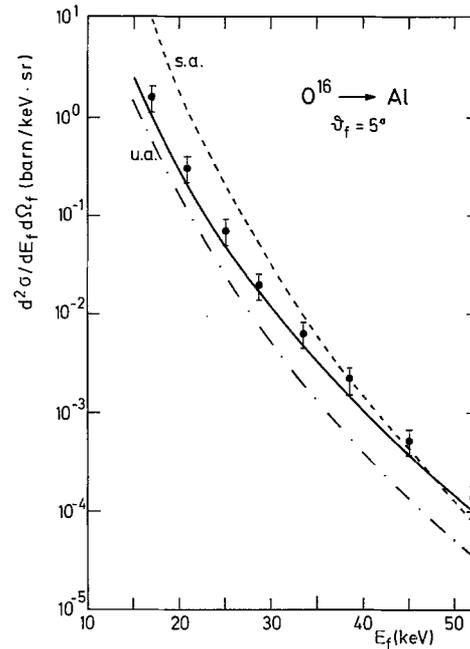


Fig. 5. Cross section for δ -electron production in 50 MeV O^{16} colliding with Al at an electron emission angle $\vartheta_f = 5^\circ$ as a function of E_f . The full curve gives the K-shell ionisation within the sliding center model, the chain curve is the result of the united-atom picture, the broken curve is done with the Trautmann-Rösel SCA code [10], and the data are from Bell et al. [10]

singly differential cross section obtained in the united-atom limit (which falls from 1.9 to 1.6 for $\vartheta_f = 5^\circ$ when E_f increases from 15 to 50 keV). We would like to point out that for this rather symmetric collision system the nonadiabaticity parameter λ is already 0.9 for $E_f = 15$ keV which is about 3 times the united-atom binding energy (increasing to 0.97 for $E_f = 50$ keV), thus showing that a molecular description is appropriate. However, the difference between the sliding result and the united-atom calculation indicates that in this intermediate velocity region, molecular wavefunctions should be used, rather than the time-independent united-atom functions.

5. Conclusion

For the calculation of K-shell ionisation electronic states have been used which were obtained from minimising the transition matrix elements. By studying the dependence of the differential cross section $d\sigma/dE_f$ on collision velocity and energy of the ejected electrons, the applicability of various standard models could be tested. As expected, it was found that for high collision velocities and those electron energies which determine the total cross section σ ,

the electron can well be described by (target-centered) target wavefunctions, while for slow collisions molecular wavefunctions have to be used, where care should be taken that for collision systems with moderate Z_P/Z_T , a description with united-atom wavefunctions located at the center of charge should only be applied when v is very low.

However, at high velocities, the separated-atom picture breaks down if E_f is very much larger than the binding energy of the initial electronic state. Then, even in these fast collisions, a molecular theory has to be used. This contradicts the obvious picture that the electrons will never have time to adjust to the two-center field. Rather, the relevant internuclear distances are so small, that the target electron nevertheless is strongly perturbed by the projectile. For increasing v , the electron energy required for a molecular description increases very fast, $E_f \sim v^2$, and not linearly with v what would be expected from a mere inspection of the minimum momentum transfer $q_{\min} = \Delta E/v$. This may be viewed as a compromise which takes into account the shortening of the collision time with growing v .

Test calculations have been performed for the collision system Li+Ne the asymmetry of which ($Z_P/Z_T=0.3$) is low enough to make a Born calculation meaningful, but high enough to allow for a proper distinction between the united-atom and the separated-atom description. This distinction is still more evident for the system $O^{16} + Al$ ($Z_P/Z_T=0.6$). A comparison with existing experimental data shows promising agreement if the sliding model is used.

A deficiency of the choice of a simple monopole variational wavefunction in our model calculations is that dipole transitions which are rather important for the higher impact parameters, are not included in the determination of the parameter λ which expresses the nonadiabaticity of the collision process. Therefore, especially if the ionisation of higher shells is considered, one should choose variational wavefunctions which are a better approximation to the two-center potential in order to obtain quantitative results. Qualitatively, however, the above mentioned behaviour will remain unaffected.

In cases where a first-order treatment is not sufficient, e.g. for systems with level matching, the optimised basis states can be used in multistep calculations. Even then, the determination of the parameter λ through minimising the coupling strength between the initial and final state is reasonable, not only because (for fixed λ) the eigenstates to $H_0(\lambda)$ are orthogonal, but also because the initial and final

states have a dominant influence on the transition amplitude.

An improvement is likely to be achieved if, in the spirit of Stevenson's work, the important intermediate states are allowed to contribute to the choice of λ . Thereby, while keeping the final state $\psi_f(t)$ as eigenstate to $H_0(\lambda)$ in the defining equation (2.2) for the transition amplitude, the initial state $\psi_i(t)$ may be chosen to include higher-order terms in the perturbation $(1-\lambda)V_p$. As long as care is taken that the overlap term $\langle \psi_f(\infty) | \psi_i(\infty) \rangle$, if nonzero, is retained in the transition amplitude, the variational principle still holds, such that λ can be found from making the higher-order transition probability stationary. However, this will drastically increase the numerical effort.

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