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On the Semi-classical Method for Electron Scattering by Atoms

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Abstract

In applications of the semi-classical approximation to excitation of atoms by electron impact, it is commonly assumed that the trajectory of the incident electron can be taken to be a straight line. The validity of this assumption is tested by comparing cross sections obtained in a coupled channel model using either a straight line trajectory or a trajectory computed from an effective potential. It is found that as far as total cross sections are concerned the assumption of a straight line trajectory does not cause appreciable error for elastic scattering at incident energies above 200 eV and for inelastic scattering above 100 eV. The influence of the choice of trajectory on the angular distributions is discussed briefly.

Introduction

The semi-classical or 'impact parameter' approximation has been used in atomic collision problems for many years (Bransden 1970; McDowell and Coleman 1970). To illustrate the method, we can consider the excitation of a hydrogen atom by a projectile of charge Z and mass m (atomic units with $m_e = \hbar = e = 1$ are used throughout). Under suitable conditions it is possible to represent the motion of the projectile by a classical trajectory. These conditions are that the potential field in which the projectile moves should not vary appreciably over one wavelength and that the angular deflection of the projectile should be well defined. The first of these conditions can be stated roughly as

$$a \gg (mv)^{-1}, \tag{1}$$

where v is the velocity of the projectile and a the 'size' of the atomic field (several times a_0, the Bohr radius of the atom). The second condition is

$$\theta \gg \theta_c, \tag{2}$$

where θ is the angle of scattering and the critical angle θ_c is given by

$$\theta_c = (mva)^{-1}. \tag{3}$$

In the case of the excitation of an atom by protons or other heavy particles, the condition (1) is well satisfied at all energies above a few electron volts, and the critical angle θ_c is very small, so that (2) is satisfied over the range of θ accessible to experiment. For electron scattering, to reduce θ_c to less than $0 \cdot 1$ rad, taking $a \approx 1$ a.u., we require energies above 3 keV. Despite this, methods based on the semi-classical approximation appear to produce useful results at much lower energies so that the conditions (1) and (2) must be considered to be sufficient rather than necessary.

If $\boldsymbol{R}$ is the position vector of the projectile with respect to the nucleus of the target atom, the classical trajectory followed by the projectile can be written

$$\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{b}, t), \tag{4}$$

where $\boldsymbol{b}$ is a two-dimensional impact parameter vector in the scattering plane such that, as $t \to -\infty$, the trajectory coincides with the straight line (see Fig. 1)

$$\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t, \qquad \boldsymbol{b}.\boldsymbol{v} = 0. \tag{5}$$

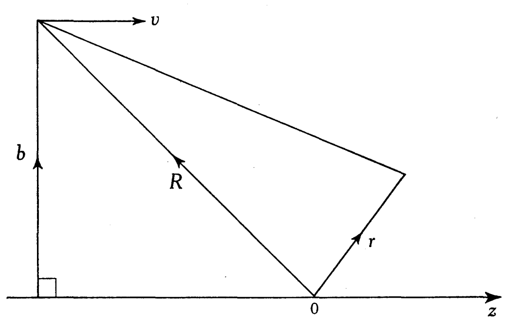

Fig. 1. Diagram of vectors involved in the atomic collision problem (see text for definitions).

The collision problem then consists in the solution of the time-dependent Schrödinger equation for the bound electron

$$(-\tfrac{1}{2}\nabla^2 + V(\boldsymbol{r}, t) - r^{-1})\Psi(\boldsymbol{r}, t) = \mathrm{i}\,\partial\Psi(\boldsymbol{r}, t)/\partial t, \tag{6}$$

where the interaction between the projectile and the target atom is

$$V(\boldsymbol{r}, t) = \{R(t)\}^{-1} - |\boldsymbol{R}(t) - \boldsymbol{r}|^{-1}. \tag{7}$$

It is not possible to solve equation (6) exactly, so various approximations have been devised; but before these can be applied, it is necessary to define the trajectory (4) followed by the projectile. It has been almost the universal practice* in electron scattering to make the rather drastic approximation of ignoring the deflection of the projectile and taking the trajectory to be the straight line (5).

It is the purpose of this paper to determine the energy above which the straight line trajectory approximation becomes accurate, by comparing cross sections for the excitation of the $n = 2$ levels of hydrogen computed from a straight line trajectory with those computed from a curved trajectory determined by assuming an effective potential between the projectile and target. For proton scattering by a neutral target the solution to this problem is well known (see e.g. Bransden 1972). The straight line approximation remains valid down to energies of about 1 keV, and for lower energies it is important to use a better approximation to the trajectory of the proton.

* Within the Glauber approximation to equation (6), combinations of two straight line trajectories have been proposed (see Gerjuoy and Thomas 1974) and an improved formulation allowing for different velocities of the projectile in different channels has been developed by Flannery and McCann (1974*a*).

Coupled Channel Model

To carry out numerical calculations of the 1s→2s and 1s→2p cross sections, the approximate method of solution of equation (6) must be defined and the trajectory (4) chosen. For our purpose it is not necessary to employ the most accurate methods of solution such as the second-order potential method of Bransden and Coleman (1972) or the pseudo-state expansion of Flannery and McCann (1974*b*), but it is sufficient to use an expansion in terms of the target eigenfunctions $\phi_n(\boldsymbol{r})$, retaining the four terms corresponding to the 1s, 2s, $2p_0$ and $2p_{\pm 1}$ levels, which will be labelled $n = 1$, 2, 3 and 4 respectively. The approximate wavefunction $\Psi(\boldsymbol{r}, t)$ then has the form

$$\Psi(\boldsymbol{r}, t) = \sum_{n=1}^{4} \phi_n(\boldsymbol{r}) \exp(-\mathrm{i}\varepsilon_n t)\, a_n(\boldsymbol{b}, t), \tag{8}$$

where ε_n is the energy of the nth level of the hydrogen target. For $t \to -\infty$, the probability amplitudes a_n must satisfy the boundary condition

$$a_n(\boldsymbol{b}, -\infty) = \delta_{n1}, \tag{9}$$

and at $t = +\infty$ the total cross sections for elastic scattering or excitation are given by

$$Q_n = 2\pi(v_n/v_1) \int_0^\infty |\, a_n(\boldsymbol{b}, +\infty) - \delta_{n1}|^2\, b \,\mathrm{d}b\,. \tag{10}$$

The equations which determine the $a_n(\boldsymbol{b}, t)$ are found by inserting the approximation (8) into equation (6) and projecting with the wavefunctions $\{\phi_n \exp(-\mathrm{i}\varepsilon_n t)\}$. We find

$$\mathrm{i}\frac{\partial a_n(\boldsymbol{b}, t)}{\partial t} = \sum_{j=1}^{4} V_{nj}(\boldsymbol{b}, t)\, a_j(\boldsymbol{b}, t) \qquad (n = 1, 2, 3, 4), \tag{11}$$

where

$$V_{nj}(\boldsymbol{b}, t) = \int \phi_n^*(\boldsymbol{r})\, V(\boldsymbol{r}, \boldsymbol{R})\, \phi_j(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} \exp\{\mathrm{i}(\varepsilon_n - \varepsilon_j)t\}\,. \tag{12}$$

Effective Potential and Trajectory

To represent the effective potential in which the incident electron moves, we have taken a combination of the static interaction $V_{11}(R)$ and the Buckingham polarization potential

$$V_{\mathrm{pol}} = -\alpha/2(r^2 + d^2)^2\,, \tag{13}$$

with $\alpha = 4{\cdot}5$ and $d = 1{\cdot}0$. The classical trajectory corresponding to the effective potential $W = V_{11} + V_{\mathrm{pol}}$ was found by numerical solution of Hamilton's equations.

Numerical Results and Discussion

The coupled equations (11) have been solved at incident energies $E = 25$, 50, 100 and 150 eV, with $R(t)$ given by (*a*) the straight line trajectory and (*b*) the effective nonlinear trajectory. The corresponding total cross sections are shown in Table 1, for elastic scattering ($Q_{1\mathrm{s}}$) and excitation of the $n = 2$ levels ($Q_{2\mathrm{s}}$, $Q_{2\mathrm{p}}$). It is seen that even at the very low energy of 25 eV, the total cross section for the strong optically allowed 1s→2p transition is quite insensitive to the choice of trajectory. In contrast, the cross sections for the weak 1s→2s transition do not agree in the two approximations within 10% until energies of greater than 50 eV are reached while, in the most sensitive case of elastic scattering, the two approximations still disagree by about 15% at 150 eV. The lack of sensitivity of the 1s→2p cross section to the choice of trajectory is due to the fact that the transition probability is small for small impact

Table 1. Total cross sections for electron scattering by hydrogen

The results shown are the total cross sections Q_n (in units of πa_0^2) calculated assuming (*a*) a straight line trajectory and (*b*) a curved trajectory

E (eV)	Q_{1s} (*a*)	Q_{1s} (*b*)	Q_{2s} (*a*)	Q_{2s} (*b*)	Q_{2p} (*a*)	Q_{2p} (*b*)
25	0·8923	1·590	0·128	0·169	1·171	1·134
50	0·519	0·739	0·088	0·099	0·959	0·937
100	0·285	0·348	0·052	0·055	0·685	0·674
150	0·186	0·227	0·037	0·038	0·534	0·528

parameters, and the important range of values of b for which $|a_{2p}|^2 b$ is significant is always in the region $b > 1$. For such values of b, the trajectory in the effective potential is practically a straight line and correspondingly the straight line approximation will provide accurate total 2p cross sections (cf. the comment on p. 459 of the monograph by Massey and Burhop 1969).

Table 2. Transition probabilities as a function of impact parameter

Results calculated for (*a*) a straight line trajectory and (*b*) a curved trajectory

Impact parameter b	1s (*a*)	1s (*b*)	2s (*a*)	2s (*b*)	2p (*a*)	2p (*b*)
$E = 50$ eV						
0·151	2·526	1·988	0·054	0·045	0·027	0·049
0·689	0·234	0·503	0·0339	0·0384	0·0392	0·0233
1·106	0·0459	0·1107	0·0180	0·0264	0·0491	0·0296
1·621	0·0079	0·0112	0·0070	0·0081	0·0592	0·0502
2·236[A]	0·0018	0·0020	0·0025	0·0025	0·0465	0·0476
$E = 100$ eV						
0·151	1·516	1·427	0·0332	0·0264	0·0108	0·0213
0·689	0·121	0·199	0·0212	0·0232	0·0179	0·0100
1·106	0·0227	0·0353	0·0116	0·0139	0·0242	0·0182
1·621	0·0035	0·0042	0·0046	0·0051	0·0280	0·0267
2·236[A]	0·00062	0·00064	0·0015	0·0015	0·0263	0·0264

[A] For values of b greater than 2·236, the approximations (*a*) and (*b*) coincide.

To get some idea of the angular range over which the straight line trajectory approximation is valid, the transition probabilities $(v_n/v_1)\,|\,\delta_{n1} - a_n(\boldsymbol{b}, \infty)\,|^2$ are shown in Table 2 as a function of the impact parameter b at 50 and 100 eV. As expected, for small values of b, which correspond to large angle scattering, the straight line trajectory approximation is inaccurate. On the other hand, for large b ($\geqslant 2$), the straight line approximation is very good.

By comparing elastic differential cross sections in a one-channel approximation in a partial wave and impact parameter formalism, Winters *et al.* (1974) showed that the impact parameter cross section agreed well with the partial wave cross section for small angle scattering $\theta \leqslant 30°$ for $E \geqslant 100$ eV. Taken together with the present results this suggests that the semi-classical approximation itself is accurate for energies as low as 100 eV for elastic scattering and the deficiencies at large angles arise from the assumption of a straight line trajectory. For inelastic scattering, our results suggest that the semi-classical method can be reliable for even lower energies and that, for the optically allowed transitions, the results are remarkably insensitive to the straight line approximation.

Conclusions

For a number of reasons, the semi-classical coupled equations are much easier to deal with numerically than the corresponding partial wave equations. This is not only because these equations are of first order but also because at higher energies, where very large values of l may be required, it is much more convenient to deal with the continuous impact parameter variable b rather than the discrete variable l. Some of this simplicity is lost when it is necessary to allow for the departure of the trajectory of the incident particle from a straight line. The present calculations indicate that for total inelastic cross sections the straight line approximation is accurate above 100 eV and, for elastic scattering, above 200 eV. As expected, the straight line trajectory will produce accurate differential cross sections in a limited angular range about the forward direction, at 100 eV extending to $\sim 25°$ for elastic scattering, and perhaps to 35° or 40° for excitation (Bransden and Winters 1975). To extend the region of validity of the impact parameter model over a larger angular range it is essential to allow for the curvature of the trajectory of the incident particle. In the present simple model, no allowance has been made for the effects of electron exchange; however, having established the region of validity of the semi-classical approximations, exchange effects can be included by using effective exchange potentials (Furness and McCarthy 1973; Bransden and Noble 1976) and corrections to the coupled channel model can be made by the second-order potential method of Bransden and Coleman (1972).

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