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THE DISTORTION APPROXIMATION IN SCATTERING THEORY

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ABSTRACT

The distortion approximation for heavy particle collisions is developed from a molecular model.

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The Distortion Approximation in Scattering Theory

The distortion approximation [1] for collisions between atoms and ions at low and moderate energies is a refinement of the standard high energy approximation of Born. It was introduced as an alternative to the perturbed stationary state (molecular) approximation [2] , which has been found to have several serious defects [3] . Though the original derivation employed an atomic model, the distortion approximation is essentially a molecular model approximation. To discuss this we shall use the rectilinear path version of the impact parameter method.

1. SCATTERING THEORY

Let the target system be located at the origin of coordinates and let the incident system move with constant velocity v in the positive direction along a line distant ρ from the z axis. The structure of the target is represented by a Hamiltonian h , and the eigenfunctions of h are $\{\varphi_j\}$ with corresponding eigenvalues $\{\epsilon_j\}$. If $V(\underline{r},\underline{R})$ is the operator representing the interaction of the incident system and the target, $\underline{r}$ and $\underline{R}$ being the position vectors of the active target electron and incident system respectively, then

$$\{h + V(\underline{r}, \underline{R})\}\Psi = i\frac{\partial\Psi}{\partial t} \qquad (1)$$

describes the electron states of the complete scattering system. We now write (1) as

$$\{H_o + V^{od}\}\Psi = i\frac{\partial\Psi}{\partial t}, \tag{2}$$

with

$$H_o = h + V^d, \tag{3}$$

where V^d and V^{od} are the diagonal and off-diagonal parts of the operator V in the representation in which h is diagonal; that is,

$$V^d = \sum_n P_n V P_n, \qquad V^{od} = \sum_{\substack{n,m \\ n\neq m}} P_n V P_m, \tag{4}$$

where $P_n = |n\rangle\langle n|$ is a projection operator on to state $|n\rangle \equiv \varphi_n$ of the target system. It follows that

$$H_o \varphi_n = E_n^o(\underline{R})\, \varphi_n, \tag{5}$$

with

$$E_n^o(\underline{R}) = \epsilon_n + (\varphi_n, V\varphi_n). \tag{6}$$

Equation (5) describes the electron states in a molecule with eigenfunctions $\{\varphi_n\}$ and eigenvalues $\{E_n^o(\underline{R})\}$. The scattering system (2) therefore corresponds to this molecule subjected to a perturbation V^{od}.

We now expand the complete electron wave function Ψ in terms of the molecular eigenfunctions $\varphi_n(\underline{r})$ and eigenenergies $E_n^o(\underline{R})$, and write

$$\Psi(\underline{r},t) = \sum_n c_n(t;\rho,v)\,\varphi_n(\underline{r})\exp\left[-i\int^t E_n^o(\underline{R})\,dt\right]. \tag{7}$$

It follows from (2) and (7) that

$$iv\frac{\partial c_n}{\partial z} = \sum_s c_s(z;\rho,v)\,V_{ns}^{od}\exp\left[-i\omega_{sn}(z)\right], \tag{8}$$

where

$$z = vt, \tag{9}$$

$$\omega_{sn}(z) = \frac{1}{v}\int_{-\infty}^{z}(V_{ss}-V_{nn})\,dz + \frac{1}{v}(\epsilon_s-\epsilon_n)z, \tag{10}$$

$$V_{ns} = (\varphi_n, V\varphi_s) = \int \varphi_n^*(\underline{r})\,V\varphi_s(\underline{r})\,d\underline{r}, \tag{11}$$

$$V_{ns}^{od} = (\varphi_n, V^{od}\varphi_s) = (1-\delta_{ns})\,V_{ns}. \tag{12}$$

With initial conditions

$$C_0(-\infty;\rho,v) = 1\,, \quad C_s(-\infty;\rho,v) = 0 \ (s \neq 0)\,, \tag{13}$$

the cross section describing excitation from state 0 to state n is [4]

$$\sigma_{0n}(v) = 2\pi \int_0^\infty |C_n(\infty;\rho,v)|^2 \rho\, d\rho \quad (a_0^2)\,. \tag{14}$$

2. DISTORTION APPROXIMATION

A first approximation to the required solution of (8) is obtained by assuming that $C_0(z;\rho,v)$ is unity and that the other coefficients $C_s(z;\rho,v)$ $(s \neq 0)$ are so small that terms involving them may be neglected. This gives

$$iv \frac{\partial C_n}{\partial z} = V_{n0} \exp\left[-i\omega_{0n}(z)\right]\,, \tag{15}$$

and hence

$$iv\, C_n(\infty;\rho,v) = \int_{-\infty}^{\infty} V_{n0} \exp\left[-i\omega_{0n}(z)\right] dz\,. \tag{16}$$

The corresponding cross section is obtained by substituting (16) in (14). The result is identical to the distortion approximation of Bates [1] .

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