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Abstract

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TRANSITION OF AN ELECTRON INTO THE CONTINUOUS SPECTRUM

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For the first time, the solution of the problem of transition into the continuous spectrum for the case of electron detachment in the collision of a negatively charged ion with an atom was found by Yu. N. Demkov (^{1}). The Massey parameter was assumed to be much larger than unity, the system of atoms was replaced by a point singularity at the origin of coordinates (as a result, the total probability of detachment was obtained close to unity), and the motion of the nuclei was treated classically (this did not allow the result to be extended to the case of slow collisions or the distribution of fast electrons to be found).

In order to remove the indicated restrictions, let us consider the quantum problem of the motion of the nuclei in the interaction of one linear term with a continuum. Assuming the terms $E_{\mathbf{k}}$ ($\mathbf{k}$ is the electron momentum), corresponding to the motion of the electron in the continuous spectrum, not interacting with one another and having zero slope, we write the following system of quantum equations for the motion of the nuclei (see, in this connection, (^{2})):

$$\frac{1}{2}\varphi''_{xx}(\mathbf{k},x) + (E - E_{\mathbf{k}})\varphi(\mathbf{k},x) + \beta_{\mathbf{k}}\varphi_0(x) = 0,$$

$$\frac{1}{2}\varphi''_0(x) + (E + Fx)\varphi_0(x) + \sum_{\mathbf{k}}\beta_{\mathbf{k}}\varphi(\mathbf{k},x) = 0 \qquad (1)$$

($\hbar = 1$, nuclear mass $M = 1$); which must be solved with the following boundary conditions: unit flux density in the state $\varphi_0(x)$ as $x \to -\infty$, and absence of flux in all states $\varphi(\mathbf{k},x)$ as $x \to -\infty$. F is the force associated with the sloping term along which the nuclei initially moved ($x \to -\infty,\ F < 0$), $\beta_{\mathbf{k}}$ is the interaction of the sloping term and the term $E_{\mathbf{k}}$, assumed real. The energy $E = Mv^2/2$ is measured from the lower boundary of the continuous spectrum.

It is convenient to solve system (1) in the momentum representation (^{2}). Writing

$$\varphi(\mathbf{k}, x) = A \int_C e^{ipx} a_{\mathbf{k}}(p)\, dp,$$

$$\varphi_0(x) = A \int_C e^{ipx} a_0(p)\, dp,$$

where A is a constant determined from the boundary conditions, and the contour C passes slightly below the real axis, we find a system of equations for $a_{\mathbf{k}}(p), a_0(p)$, which is easily solved,

$$a_0(p) = \exp\left\{-\frac{i}{F}\left[\frac{p^3}{6} - Ep + \sum_{\mathbf{k}'} \beta_{\mathbf{k}'}^2 \frac{1}{\sqrt{2(E - E_{\mathbf{k}'})}} \ln \frac{p + \sqrt{2(E - E_{\mathbf{k}'})}}{p - \sqrt{2(E - E_{\mathbf{k}'})}}\right]\right\},$$

$$a_{\mathbf{k}}(p) = -\frac{2a_0(p)}{-p^2 + 2(E - E_{\mathbf{k}})}.$$

Now one must return to the x-representation. To find $\varphi(\mathbf{k}, x)$ $(x \to \infty)$, it is sufficient to take the residues at the poles of $a_{\mathbf{k}}(p)$ lying above the contour C. One immediately obtains the following result: if $E < 0$ or $0 < E <$

For $E_k > E$, $\varphi(\mathbf{k}, x)$ decreases exponentially as $x \to \infty$, the corresponding flux is zero and, consequently, no free electrons can arise with energy greater than the energy of the nuclei participating in the process. For $E_k < E$ we take into account normalization to flux, replace summation over $\mathbf{k}$ by integration, and for

$$dW(\mathbf{k}, E) = \lim_{x \to \infty} \frac{1}{\Delta E} \int |\varphi(\mathbf{k}, x)|^2 \, dE \, d\mathbf{k} \tag{2}$$

(the integration over E is carried out over a small neighborhood ΔE of the point E and eliminates the rapid oscillations of $\varphi(\mathbf{k}, x)$, $x \to \infty$) with an isotropic dispersion law E_k we find

$$dW(\mathbf{k}, E) = \gamma_k(E) e^{-R(\mathbf{k}, E)} d\mathbf{k} \qquad (E_k < E), \tag{3}$$

where

$$R(\mathbf{k}, E) = \int_0^k \gamma_{k'}(E)\, d\mathbf{k}', \qquad \gamma_k(E) = \pi \frac{(2M)^{1/2} \beta_k^2}{\hbar |F| (E - E_k)^{1/2}}. \tag{4}$$

(3) may be supplemented by the expression

$$dW(\mathbf{k}, E) = 0 \qquad (E < 0,\ 0 < E < E_k). \tag{5}$$

A remarkable feature of (3) is that this relation leads to an anomalous dependence of the total probability $\widetilde{W}(E)$ of detachment on the energy of the nuclei. Indeed, $W(E)$, defined by the expression

$$W(E) = \int_0^\infty dW(\mathbf{k}, E), \tag{6}$$

as is seen from (3) and (5), has the form

$$W(E) = 1 - e^{-\lambda(E)}. \tag{7}$$

Here

$$\lambda(E) = R(\mathbf{k}, E)_{E_k = E}. \tag{8}$$

It should now be taken into account that even the maximum energy in the part of the electronic wave packet that has not had time to spread out during the collision time is much smaller than E. Therefore one may regard $\widetilde{W}(E)$ as the sum of the probability of a double passage through the turning region and W, i.e.

$$\widetilde{W}(E) = 1 - e^{-2\lambda(E)}. \tag{9}$$

To find $\lambda(E)$ suitable over the entire range of energy variation, it is necessary to know more or less in detail the form of β_k. To find the latter one should pass in (3) to the classical limit and compare the resulting expression with that arising in a classical treatment of the motion of the nuclei from the very beginning. Then it becomes clear that $\beta_k = \langle \psi_k V \psi_0 \rangle$ (ψ_k, ψ_0 are electronic wave functions, V is the interaction). For example, for the model:

$$\psi_k = \frac{1}{\sqrt{2\pi}} e^{i\mathbf{kr}}, \qquad \psi_0 = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha r}, \qquad V = \text{const}$$

$$\lambda(E) = \frac{8\pi^3 V^2}{\hbar^2 |F|} (mM)^{1/2} a^2 (\alpha^2 + a^2)^{-3/2} \left(1 + 2\frac{\alpha^2}{\alpha^2 + a^2} + 5\frac{\alpha^4}{(\alpha^2 + a^2)^2}\right),$$

m is the electron mass, $a^2 = 2mE/\hbar^2$.

In the quantum limit $E \ll \hbar^2\alpha^2/2m$

$$\lambda(v) = \frac{2^6 \pi^3 (mM)^{3/2} V^2}{\hbar^4 |F| \alpha^3} \, v^2;$$

In the classical case, $\lambda(v)$ has the form characteristic of the Landau–Zener relation

$$\lambda(v) = 8\pi^3 \frac{V^2}{\hbar v \, |F|} \left(E \gg \frac{\hbar^2 \alpha^2}{2m} \right).$$

At $E \simeq 0.6 E_0$ ($E_0 = \hbar^2 \alpha^2 / 2m$ is the binding energy), $\lambda(E)$ and, consequently, $\widehat{W}(E)$ have a maximum. For large $\lambda_{\max}$, $\widehat{W}(E)$ has a pronounced resonance character. For close masses of the colliding nuclei, in order to observe the resonance the energy of the incident atom must somewhat exceed the electron binding energy.

Such anomalous behavior of $\widehat{W}(E)$ is obtained also for other models and, probably, can be observed experimentally.

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CITED LITERATURE

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Note: Figure translations are in progress. See original paper for figures.

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