TRANSITION OF ELECTRONS TO A CONTINUOUS SPECTRUM

V. I. OSHEROV

Chemical Physics Institute, Academy of Sciences, U.S.S.R.

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The probability for the transition of an electron to a continuous spectrum with an arbitrary dispersion law is determined on the basis of the Landau-Zener approximation [1]. The dependence of the matrix elements of the interaction upon the momentum of the electron, which is important in this problem, is taken into account.

THE problem of calculating the probability of an electron transition from a bound state to the continuous spectrum arises, for example, in the theory of collisions when it is necessary to consider dissociation processes [2], and also in questions of the thermal ionization of impurity electrons in solid bodies [3]. The correct description of electron detachment in collisions of negative ions with atoms, as given by Demkov [2], corresponds to a particular idealized model using a δ-like potential for the bound state. Kubo [3] has found the transition probability only to first-order perturbation theory, and his subsequent attempt to go beyond this limitation [4] cannot be considered valid since he did not take into account the true nature of the spectrum in the final state (continuous spectrum) in this work. We employ a more general model than that used by Demkov [2], but set up the problem such that the result is applicable as well for ionization of negatively charged impurities in solid bodies.

Let us seek a wave function for the electron in the form

$$\Psi = c_0\psi_0 + \sum_{\mathbf{k}} c_{\mathbf{k}}\psi_{\mathbf{k}}, \tag{1}$$

where ψ_0 describes the bound (localized) electron state and $\psi_{\mathbf{k}}$ describes the wave function in the continuous spectrum (conduction band), so that if H_0 be the Hamiltonian neglecting the interaction of the terms V, then

$$H_0\psi_0 = E_0\psi_0, \qquad H_0\psi_{\mathbf{k}} = E_{\mathbf{k}}\psi_{\mathbf{k}}. \tag{2}$$

In (1) and (2) $\mathbf{k}$ is the momentum (quasimomentum) of the electron.

Let us make the following assumptions concerning our model: 1) the terms $E_{\mathbf{k}}$ are plane (corresponding forces equal to zero); 2) there are no interactions between these terms (this does not particularly limit the discussion, since it is possible in principle to take account of such interactions within the group of terms $E_{\mathbf{k}}$ separately and thereby improve the solution); 3) motion along the linear term E_0 is uniformly on a classical trajectory (this limitation is typical for the Landau-Zener approximation).

Without introducing new assumptions, one can obtain the following system of equations ($\hbar = 1$):

$$i\dot{c}_0 - ztc_0 - \Sigma\beta_{\mathbf{k}}c_{\mathbf{k}} = 0, \qquad i\dot{c}_{\mathbf{k}} - E_{\mathbf{k}}c_{\mathbf{k}} - \beta_{\mathbf{k}}c_0 = 0, \tag{3}$$

where $z = -vF$ (v is the classical velocity of the nuclei taking part in the process, F is the force on the term E_0), $\beta_{\mathbf{k}} = \langle\psi_{\mathbf{k}}V\psi_0\rangle$ is the off-diagonal matrix element of the interaction, assumed to be real for simplicity. The diagonal matrix elements of V renormalize the energies in the usual manner and will not be considered. This system of equations (3) has a solution in the form of the following contour integrals:

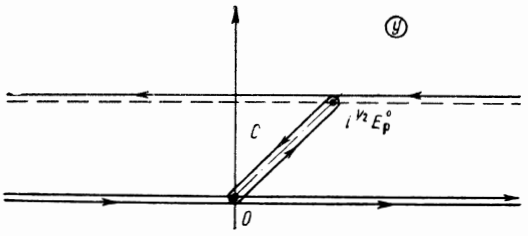
$$c_0(t) = A\int_C \exp(-x^2/2z + xt)\prod_{\mathbf{p}}(x + iE_{\mathbf{p}})^{-i\alpha_{\mathbf{p}}}dx,$$

$$c_{\mathbf{k}}(t) = -Ai\beta_{\mathbf{k}}\int_C \exp\left(-\frac{x^2}{2z} + xt\right) \times \frac{1}{x + iE_{\mathbf{k}}}\prod_{\mathbf{p}}(x + iE_{\mathbf{p}})^{-i\alpha_{\mathbf{p}}}dx. \tag{4}$$

Here

$$\alpha_{\mathbf{p}} = \beta_{\mathbf{p}}^2/z, \tag{5}$$

A is an arbitrary constant. Eq. (4) identically satisfies the second equation of (3), whereas substitution in the first of these equations results in a contour integral over the x-derivative of the integrand in $c_0(t)$. Therefore, if $c_0(t)$ is subsequently set equal to zero at the limits of the contour C or if its values at the limits are the same, then Eq. (4) will constitute a solution of system (3). The constant A and the contour C, however, must be chosen such that the initial conditions be satis-



fied, i.e.,

$$|c_0(-\infty)| = 1, \qquad c_k(-\infty) = 0.$$

For this purpose it is convenient to carry out a change of variables $x = -i^{1/2}y (z < 0)$. Then it is natural to take for C a path in the y plane (see the figure; E_p^0 is the upper limit of the continuous spectrum, which goes off to infinity for a purely continuous spectrum) which transforms into the contour for the appropriate parabolic-cylinder functions if $E_p^0 \to 0$ (the case of two terms).

When $t \to -\infty$, the coefficient $c_0(t)$ can be found by the method of steepest descents, and when $t \to +\infty$, it is sufficient simply to take the residue at the point $y = i^{1/2}E_k$. Now, writing

$$\prod_p (x + iE_p)^{-i\alpha_p} = \exp\left[-i\sum_p \alpha_p \ln(x + iE_p)\right],$$

we go over from the implied unity normalization of ψ_k to a δ-function normalization

$$\left(V^{-1}\sum_p \to \int d\mathbf{p}\right)$$

and, using the fact that

$$\ln(E_k - E_p) = P\int \frac{dE_k}{E_k - E_p} + i\pi\int \delta(E_k - E_p)\, dE_k,$$

we find for $dW(\mathbf{k}) = |c_k(\infty)|^2\, d\mathbf{k}$

$$dW(\mathbf{k}) = \gamma_k \exp\left(-\int\int^{E_k} \gamma_p \delta(E_k' - E_p)\, d\mathbf{p}\, dE_k'\right) d\mathbf{k},$$

$$\gamma_p = 2\pi\alpha_p. \qquad (6)$$

The integral over $\mathbf{p}$ can be taken by parts:

$$dW(\mathbf{k}) = \gamma_k \exp\left(-\int_{E_p = E_{k'}}^{E_k} \gamma_p \frac{dE_k'}{|\nabla E_p|}\, d\omega_p\right) d\mathbf{k}; \qquad (7)$$

Here $d\omega_p$ is the element of a square on the surface $E_p = E_k'$.

In the isotropic case

$$dW(\mathbf{k}) = \gamma_k \exp\left(-\int_0^k \gamma_{k'} d\mathbf{k}'\right) d\mathbf{k}. \qquad (8)$$

This distribution for $\gamma_k = \gamma$ and for a square dispersion law, in the sense of $\mathbf{k}$ dependence, agrees with the result found by Demkov, although, generally speaking, it is impossible to obtain complete agreement with the latter. The fact of the matter is that the principal theoretical parameter β in [2] must be found by using the equation

$$1 = \int \frac{A_p\, d\mathbf{p}}{E - E_p}, \qquad A_p = \frac{\beta_p^2}{E - E_0}. \qquad (9)$$

One can reduce Eq. (9) to a quadratic equation and introduce β at the price of an upper limit on the velocity v. Thus, the result (8), whose derivation did not presuppose a small E_p^0 (and the equation derived therefrom did not require an approximate solution) is free from the limitations associated with the Massey criterion.

Equation (8) includes the dependence of γ_k upon the momentum of the emitted electron, which eliminates the second limitation of Demkov's work [2], related to the δ-function model of the potential. Other conditions being equal, γ_k decreases with an increase in $\mathbf{k}$, leading to a slower decrease of $dW(\mathbf{k})/dk$ as $k \to \infty$. For example, under the following simplest assumptions regarding the wave functions $\psi_0 \sim e^{-\alpha r}$ and $\psi_k \sim e^{i\mathbf{k}\cdot\mathbf{r}}$ (V = const), the quantity dW(k) in general is not an exponential as $k \to \infty$:

$$dW(k) \sim k^{-6} dk, \quad k \to \infty.$$

If we define

$$\lim_{k\to\infty} \int_0^k \gamma_{k'}\, d\mathbf{k}' = \lambda, \qquad (10)$$

which is appropriate for a purely continuous spectrum, then Eq. (8) indicates that the total ionization probability will be

$$W = 1 - e^{-\lambda}. \qquad (11)$$

Depending upon the details of the interaction, λ is either ∞ or has a fixed finite non-zero value. In the first case, complete dissociation occurs, and in the second, the probability of a transition to the continuous spectrum has the form of the probability of the adiabatic Landau-Zener type transition, whereas the probability of remaining in a bound state is similar to that for the nonadiabatic transition. For the already mentioned simple model with a constant potential V, we have

$$\lambda = 4\pi^3 V/\hbar v F. \qquad (12)$$

For a transition to a band, the probability of remaining in a localized state is non-zero, and a situation is even likely (intersection of bands) wherein the argument of the exponential in (7) vanishes and, consequently, ionization does not occur.

Thus, the only limitation of the theory is a requirement resulting from the classical descrip-

tion of the nuclei participating in the process, namely that their kinetic energy be greater than the electron-detachment energy. Use of the classical description of the nuclei limits the theory to emitted electrons with not too great momenta.

The theoretical predictions of Demkov [2] can be supplemented by the following observation concerning the processes of thermal ionization in solids. As is known, the activation energy of this process depends strongly upon its thermal effect, which is determined by the difference in the electron energies in the initial and final states [3,4]. Thus far, it has been assumed that the principal contribution to this difference is made by electrons with $k = 0$. However, Eq. (7) shows that this is not the case. In general electrons are formed with quite large momenta, carrying away an approximate energy $(4\pi\gamma)^{-2/3}$ (for large F and not too large a band, in which case one can assume $\gamma_k = \gamma$) or an energy $\sim \alpha^2$ (for small F even with a wide band, in which case it is natural to utilize the model with a constant potential V). These quantities can be rather large, so that in the first case there results a strong dependence of the activation energy upon the nuclear velocity, ultimately leading to a transition which is non-exponential in the temperature, and in the second case the activation energy merely changes considerably.

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