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Transitions from a discrete level to the continuous spectrum upon adiabatic variation of the potential

E. A. Solov'ev

Leningrad State University
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An adiabatic approximation describing transitions between a molecular term and the continuous spectrum is developed. The motion of the nuclei is assumed to be classical. The developed approximation is utilized for an investigation of the processes which take place during the collision of a negative ion with a neutral atom. A universal distribution with respect to the momenta of the emitted electrons is obtained for this case, this distribution being valid for all momenta. The effect of the formation of a quasistationary s-term on the low-energy part of the spectrum of the emitted electrons is considered. The probability of populating the discrete levels of the system via the continuous spectrum is calculated. Possible applications of the approximation developed in this work to other problems in the theory of atomic collisions are discussed.

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1. INTRODUCTION

One of the important problems in the theory of atomic collisions is the problem of the interaction of a molecular term with the continuous spectrum when, on the one hand, the motion of the nuclei can be regarded as classical and, on the other hand, as sufficiently slow. The goal of the theory is a calculation of the populations of the discrete terms and the momentum distribution of the electrons which are emitted into the continuous spectrum. The results obtained in this field are basically connected with either the exactly soluble model of Demkov–Osherov[1] or else with an assumption concerning the smallness of the interaction between the term and the continuous spectrum.[2] The interaction of a term with the continuous spectrum is not small in the majority of experimentally important cases. At the same time the models describe only the low-energy part of the spectrum of the emitted electrons, where one can abstract from the specific features of the utilized models, and do not permit one to investigate certain effects connected with reverse motion of the system with respect to the term. Thus, the existing theory does not give a complete description of the cited processes. In this connection an approach which does not contain any restrictions on the form of the Hamiltonian and the behavior of the terms, but only utilizes the smallness of the colliding particles' velocity, is of interest. Such a problem is solved in the present article.

The approximation developed in Sec. 2 is not related to either model representations or to an assumption concerning the smallness of the interaction of a term with the continuous spectrum. It is asymptotically exact with respect to the small parameter v which characterizes the time rate of change of the electronic Hamiltonian. The electron wave function is sought in the form of an integral over the energy E of the adiabatic wave functions, in the same way as this is done in the Demkov–Osherov model. Such an approach differs from that adopted in the theory of nonadiabatic transitions between discrete terms[3] by the fact that the expansion in terms of states of the instantaneous Hamiltonian is still integrated over E. This difference has a simple physical meaning. The integration over the energy allows one to uniquely take into consideration the retardation, which is unimportant for transitions between discrete levels due to the localized nature of the wave functions.

In Secs. 3 and 4 the approximation is utilized in order to investigate the processes which take place during the collision of a negative ion with a neutral atom. In spite of the fact that the theory is most highly developed for this case, the approximation developed in this article enables us to obtain a number of new results. The momentum distribution is calculated for the reaction involving the detachment of an electron, the result being valid for all momenta of the emitted electrons (the previously obtained results only pertain to the low-energy part of the spectrum of the emitted electrons). The influence of the turning point of the s-term and of the formation

of a quasistationary s-term on the momentum distribution is considered. It is shown that upon close approach of a turning point to the boundary of the continuous spectrum, the momentum distribution is significantly altered even in the low-energy regime. In a certain sense this effect is analogous to the Breit–Wigner effect[4] in potential scattering. The probability of multiple capture of the emitted electrons for the s-term was calculated in the article by Demkov.[5] In Sec. 4 this quantity is calculated when the term has an arbitrary orbital quantum number in the vicinity of the boundary of the continuous spectrum. There the probability of populating the other states of the system via the continuous spectrum is calculated; as far as we know this calculation has not previously been made. The process of populating the terms via the continuous spectrum has a resonance character for terms which cross the boundary of the continuous spectrum, and should lead to appreciable cross sections in the inelastic channels of the reaction. The possible applications of the proposed treatment are not at all limited to the examples mentioned; they are briefly discussed in Sec. 5.

2. THE ADIABATIC APPROXIMATION FOR THE WAVE FUNCTION

Taking the motion of the nuclei into account classically leads to the time-dependent Schrödinger equation for the electronic wave function $\Psi(\mathbf{r}, t)$ ($\mathbf{r}$ denotes the set of electron coordinates). The electron Hamiltonian $\hat{H}$ depends on the time only through the internuclear distances appearing in it. For the construction of the adiabatic approximation, let us choose a certain parameter v characterizing the time rate of change of the Hamiltonian: $\hat{H}=\hat{H}(vt)$. For slow motion of the nuclei, v is small, and in this case it is natural to use the eigenfunctions $\varphi_n(\mathbf{r}, t)$ ($\tau=vt$) and the corresponding eigenvalues $E_n(\tau)$ (molecular terms) of the instantaneous electron Hamiltonian. With the aid of the functions $\tau_n(E)$, reciprocal to the functions $E_n(\tau)$, let us change in $\varphi_n(\mathbf{r}, \tau)$ to the variable E:

$$\varphi_n(\mathbf{r}, E)=\varphi_n(\mathbf{r}, \tau)\,|_{\tau=\tau_n(E)}.$$

We shall seek the wave function in the form ($\hbar=1$)

$$\Psi(\mathbf{r}, t)=\sum_n \int_{L_n} f_n(E)\varphi_n(\mathbf{r}, E)e^{-iEt}\,dE.$$

The functions $f_n(E)$ are subject to determination from the nonstationary Schrödinger equation, which takes the following form:

$$\sum_n \int_{L_n} [\hat{H}(\tau)-\hat{H}(\tau_n(E))]f_n(E)\varphi_n(\mathbf{r}, E)e^{-iEt}\,dE=0. \tag{1}$$

The choice of the integration contours will be discussed below. Equation (1) does not contain the complete electron Hamiltonian, but only its time-dependent part $V(\mathbf{r}, \tau)$. Multiplying Eq. (1) by $e^{i\varepsilon t}$ and integrating over the time, we obtain

$$\sum_n V(\mathbf{r}, \tau_n(\varepsilon))f_n(\varepsilon)\varphi_n(\mathbf{r}, \varepsilon)=\sum_n \int_{L_n} \mathcal{V}(\mathbf{r}, q)\varphi_n(\mathbf{r}, \varepsilon+vq)f_n(\varepsilon+vq)\,dq, \tag{2}$$

$$\mathcal{V}(\mathbf{r}, q)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} V(\mathbf{r}, \tau)e^{-iq\tau}\,d\tau.$$

This equation is already suitable for the construction of an asymptotic expansion of the functions $f_n(\varepsilon)$ with respect to the small parameter v. We note that $V(\mathbf{r}, \tau_n(\varepsilon))$, $\mathcal{V}(\mathbf{r}, q)$, and $\varphi_n(\mathbf{r}, \varepsilon)$ do not contain v. Let us represent the functions $f_n(\varepsilon)$ in the form

$$f_n(\varepsilon)=\begin{cases}\exp\left(\frac{i}{v}\int^{\varepsilon}\theta(\varepsilon')\,d\varepsilon'\right), & n=p\\ v\eta_n(\varepsilon)\exp\left(\frac{i}{v}\int^{\varepsilon}\theta(\varepsilon')\,d\varepsilon'\right), & n\neq p\end{cases}.$$

The selection of the state with $n=p$ is associated with that formulation of the problem when only the state with label p is occupied as $t\to-\infty$. With regard to the functions $\theta(\varepsilon)$ and $\eta_n(\varepsilon)$, let us assume that as $v\to 0$ they do not have any singularities and are finite. The admissibility of this assumption is evident from the self-consistency of the equations derived below for these functions $\varphi_n(\mathbf{r}, \varepsilon+vq)$ and $f_n(\varepsilon+vq)$ on the right-hand side of Eq. (2) in terms of the small parameter v. Limiting ourselves to the linear terms, we obtain

$$V(\mathbf{r}, \tau_p(\varepsilon))\varphi_p(\mathbf{r}, \varepsilon)+v\sum_{n\neq p}\eta_n(\varepsilon)V(\mathbf{r}, \tau_n(\varepsilon))\varphi_n(\mathbf{r}, \varepsilon)=V(\mathbf{r}, \theta(\varepsilon))\varphi_p(\mathbf{r}, \varepsilon)$$
$$-\frac{iv}{2}\varphi_p(\mathbf{r}, \varepsilon)\frac{d\theta(\varepsilon)}{d\varepsilon}\frac{\partial^2 V(\mathbf{r}, \theta)}{\partial\theta^2}-iv\frac{\partial\varphi_p(\mathbf{r}, \varepsilon)}{\partial\varepsilon}\frac{\partial V(\mathbf{r}, \theta)}{\partial\theta}$$
$$+v\sum_{n\neq p}\eta_n(\varepsilon)V(\mathbf{r}, \theta(\varepsilon))\varphi_n(\mathbf{r}, \varepsilon). \tag{3}$$

We shall seek the solution of Eq. (3) (in analogy to the quasiclassical approximation) in the form of an expansion of the functions $\theta(\varepsilon)$ and $\eta_n(\varepsilon)$ in terms of the parameter v. Let us represent $\theta(\varepsilon)$ in the form

$$\theta(\varepsilon)=\mu(\varepsilon)+v\nu(\varepsilon),$$

here in $\eta_n(\varepsilon)$ one should retain the first term of the expansion $\eta_n^0(\varepsilon)$. In order to calculate these functions to higher order, it is necessary to take the following terms of the expansion on the right-hand side of Eq. (2) into account. Equating to zero the coefficients associated with different powers of v in Eq. (3), we obtain

$$V(\mathbf{r}, \mu(\varepsilon))-V(\mathbf{r}, \tau_p(\varepsilon))=0, \tag{4}$$

$$\varphi_p(\mathbf{r}, \varepsilon)\frac{\partial V(\mathbf{r}, \mu)}{\partial\mu}\nu(\varepsilon)=\frac{i}{2}\varphi_p(\mathbf{r}, \varepsilon)\frac{d\mu(\varepsilon)}{d\varepsilon}\frac{\partial^2 V(\mathbf{r}, \mu)}{\partial\mu^2}$$
$$+i\frac{\partial\varphi_p(\mathbf{r}, \varepsilon)}{\partial\varepsilon}\frac{\partial V(\mathbf{r}, \mu)}{\partial\mu}+\sum_{n\neq p}\eta_n^0(\varepsilon)[V(\mathbf{r}, \tau_n(\varepsilon))-V(\mathbf{r}, \mu(\varepsilon))]\varphi_n(\mathbf{r}, \varepsilon). \tag{5}$$

From Eq. (4) it follows that $\mu(\varepsilon)=\tau_p(\varepsilon)$. Multiplying (5) by $\varphi_p(\mathbf{r}, \varepsilon)$ and integrating over $\mathbf{r}$, we obtain the following equation for the determination of $\nu(\varepsilon)$:

$$\left\langle\varphi_p\left|\frac{\partial V}{\partial\mu}\right|\varphi_p\right\rangle\nu(\varepsilon)=\frac{i}{2}\frac{d\mu}{d\varepsilon}\left\langle\varphi_p\left|\frac{\partial^2 V}{\partial\mu^2}\right|\varphi_p\right\rangle+i\left\langle\varphi_p\left|\frac{\partial V}{\partial\mu}\right|\frac{\partial\varphi}{\partial\varepsilon}\right\rangle. \tag{6}$$

Here the fact that the summation over $n\neq p$ in Eq. (5) is orthogonal to φ_p has been used. It is not difficult to verify this with the aid of the time-dependent Schrödinger equation. The matrix elements are taken without complex conjugation in order to preserve analyticity in ε. In addition, since the integrals over $\mathbf{r}$ formally diverge for arbitrary ε, the matrix elements should be calculated as suggested in[6]. On the right-hand side of Eq. (6) stands the derivative with respect to ε of the matrix

element

$$\left\langle \varphi_p \left| \frac{\partial V}{\partial \mu} \right| \varphi_p \right\rangle,$$

which is equal to $d\varepsilon/d\mu$ according to the theorem of Gell-Mann and Feynman. Taking this into consideration, we obtain the function $\nu(\varepsilon)$ in the form

$$\nu(\varepsilon) = \frac{i}{2}\frac{d}{d\varepsilon}\ln\left(\frac{d\varepsilon}{d\mu}\right) = -\frac{i}{2}\frac{d}{d\varepsilon}\ln\left[\frac{d\tau_p(\varepsilon)}{d\varepsilon}\right].$$

The projection of Eq. (5) onto other states leads to the equations from which the functions $\eta_n^0(\varepsilon)$ are determined. These functions are related to higher-order corrections to the wave function than the functions $\mu(\varepsilon)$ and $\nu(\varepsilon)$; therefore, we shall not discuss their calculation. Thus, in the assumed approximation the wave function appears in the following form:

$$\Psi(\mathbf{r},t) = N\int_L \left[\frac{d\tau_p(E)}{dE}\right]^{1/2} \varphi_p(\mathbf{r},E)\exp\left\{\frac{i}{v}\int_{E_p}^{E}\tau_p(\varepsilon)\,d\varepsilon - iEt\right\}dE, \qquad E_p = \lim_{\tau\to-\infty} E_p(\tau). \tag{7}$$

As $t \to -\infty$ the integral in Eq. (7) is evaluated by the method of steepest descents; in accordance with the initial condition chosen above, $\Psi(\mathbf{r},t)$ goes over into the wave function $\varphi_p(\mathbf{r},E_p)$ and the normalization factor $N = (2\pi v)^{-1/2}$. It is not difficult to see how retardation is taken into consideration in the wave function (7). For large values of $\mathbf{r}$, $\varphi_p \sim \exp(i\sqrt{2E}\,r)$, and the saddle point E' is found from the equation

$$\tau_p(E') - vt + vr/\sqrt{2E'} = 0.$$

The interpretation of this relationship is quite obvious: it indicates that the wave packet of the emitted electrons is formed from electrons which, having received a momentum $k' = \sqrt{2E'}$ at the instant of time $t' = v^{-1}\tau_p(E')$ turn out to be at a distance $r = k'(t - t')$ at the instant of time t, and is determined by the form of the Hamiltonian at the instant of time t', but not at t.

In a real physical situation the terms of the system are even functions of the time. As a consequence of this, the function $\mu(\varepsilon)$ has two branches: $\tau_p^-(E)$ and $\tau_p^+(E)$ corresponding to the approach and separation of the atoms, where

$$\tau_p^-(E) = -\tau_p^+(E).$$

The function $f_p(E)$ is now represented in the form of two terms:

$$f_p(E) = A\left\{\left[\frac{d\tau_p^-}{dE}\right]^{1/2}\exp\left[\frac{i}{v}\int_{E_p}\tau_p^-\,d\varepsilon\right] + B\left[\frac{d\tau_p^+}{dE}\right]^{1/2}\exp\left[\frac{i}{v}\int_{E_p}\tau_p^+\,d\varepsilon\right]\right\}. \tag{8}$$

The function $f_p(E)$ in the form (8) contains only the main terms of the asymptotic expansion with respect to the parameter v. The coefficients A and B, which are related to the Stokes constants, change abruptly on the Stokes lines, which emerge from the turning points $E_0 = E_p(0)$. In the vicinity of a turning point

$$\tau_p(E) = \text{const}\cdot(E - E_0)^{1/2},$$

and the behavior of the function $f_p(E)$ coincides with the behavior of the quasiclassical wave function in the vicinity of the turning point. By virtue of this, it is at once seen that here the Airy equation serves as the standard equation. Therefore, the steady asymptotic form of the function $f_p(E)$, which is valid in the neighborhood of the point E_0, is expressed in terms of the Airy function $\Phi(x)$. In this connection the wave function satisfying the initial condition has the following form:

$$\Psi(\mathbf{r},t) = \sqrt{\frac{2}{\pi v}}\,e^{-\sigma(E_p)}\int_L\left[\frac{d\tau_p^-}{dE}\right]^{1/2}(v\sigma(E))^{1/6}\Phi\left(\left[\frac{3}{2}\sigma(E)\right]^{2/3}\right) \times\varphi_p(\mathbf{r},E)\,e^{-iEt}\,dE, \qquad \sigma(E) = \frac{i}{v}\int_{E_0}^{E}\tau_p^-(\varepsilon)\,d\varepsilon. \tag{9}$$

When the turning point is close to the real E axis, the coefficient B changes upon a transition from $E > \mathrm{Re}\,E_0$ to $E < \mathrm{Re}\,E_0$ and is analogous to the reflection coefficient in the quasiclassical approximation:

$$B = \begin{cases} 0, & E > \mathrm{Re}\,E_0 \\ \exp\left[\frac{i}{v}\int_{E_p}^{E_0}[\tau_p^-(\varepsilon) - \tau_p^+(\varepsilon)]\,d\varepsilon\right], & E < \mathrm{Re}\,E_0 \end{cases} \tag{10}$$

The coefficient $A = (2\pi v)^{-1/2}$ does not change on the real E axis.

3. ELECTRON DETACHMENT

The approximation (7) is valid for the wave function if the functions $E_p(\tau)$ and $\tau_p(E)$ do not have any singularities. The wave function (9) takes into consideration the reverse motion of the system along a term, i. e., a branch point of the function $\tau_p(E)$. The branch points of the functions $E_p(\tau)$, which are related to the crossing of terms,[1,3] are also physically important. These characteristics may be taken into account within the framework of the present approximation. However, it is sufficient to use the wave function in the form (9) for the calculation of the momentum distribution for the electron detachment reaction (ionization associated with the collision of a negative ion with a neutral atom). In this case Rydberg crowding is not present at the boundary of the continuous spectrum, and there is no need to consider the crossing of terms. For the construction of the momentum distribution we shall, for the sake of simplicity, confine our attention to an investigation of a spherically symmetric one-electron Hamiltonian $\hat{H}(\tau)$.[1)] Since the angular variables are separable, by wave functions we shall mean only their radial part.

Let us consider the time-dependent matrix element

$$W(r,t) = \int_0^\infty \Psi_0^*(r,k)\,\Psi(r,t)\,r^2\,dr = \langle \Psi_0(k) | \Psi(t)\rangle, \tag{11}$$

where $\Psi_0(r,k)$ is the wave function of the continuous spectrum with momentum k of the asymptotic Hamiltonian $\hat{H}(\tau \to +\infty)$. The function

$$F(k) = \lim_{t\to\infty}|W(k,t)|^2$$

represents the momentum distribution of the emitted electrons. Using expression (9) for the wave function, let us write the matrix element in the form

$$W=\sqrt{\frac{2}{\pi v}}e^{-\sigma(E_p)}\int_L\left[\frac{d\tau_p^-}{d\varepsilon}\right]^{1/2}(v\sigma(\varepsilon))^{1/4}\Phi\left(\left[\frac{3}{2}\sigma(\varepsilon)\right]^{2/3}\right)w(k,\varepsilon)e^{-i\varepsilon t}\,d\varepsilon. \tag{12}$$

Here $w(k,\varepsilon)=\langle\Psi_0(k)|\varphi_p(\varepsilon)\rangle$. For large values of r the functions $\Psi_0(r,k)$ and $\varphi_p(r,\varepsilon)$ have the asymptotic forms

$$\Psi_0(r,k)=\frac{1}{\sqrt{2\pi r}}\{\exp(ikr+i\delta)-\exp(-ikr-i\delta)\},$$
$$\varphi_p(r,\varepsilon)=\frac{C(\varepsilon)}{r}\exp(i\sqrt{2\varepsilon}\,r), \tag{13}$$

where δ is the phase shift, and $C(\varepsilon)$ is the analytic continuation, in the complex ε plane, of the coefficient in front of $\exp(i\sqrt{2\varepsilon}r)/r$ in the bound-state wave function $\varphi_p(r,\varepsilon)$, which is normalized to unity for $\varepsilon<0$. With (13) taken into account, one can write

$$w(k,\varepsilon)=-i\frac{C(\varepsilon)}{\sqrt{2\pi}}\left\{\frac{e^{i\delta}}{\sqrt{2\varepsilon}+k}-\frac{e^{-i\delta}}{\sqrt{2\varepsilon}-k}\right\}+w_0(k,\varepsilon). \tag{14}$$

The function $w_0(k,\varepsilon)$ has no poles.

As $t\to-\infty$ the contour L in the right half-plane of ε borders the negative imaginary axis, and the integral over this portion of the contour tends to zero. A saddle point $\varepsilon'=E_p$ exists in the left half-plane; however, this does not give a contribution since the functions $\Psi_0(r,k)$ and $\varphi_p(r,E_p)$ are eigenfunctions of the same Hamiltonian and $w(k,E_p)=0$. Thus, $W(k,t)\to0$ and $t\to-\infty$, which agrees with the initial condition for the problem. For the same reason the saddle point doesn't give a contribution as $t\to+\infty$. In the right half-plane of ε the contour L is deformed upward, and a residue arises associated with the first term in (14), but the integral over the remaining part of the contour tends to zero. Thus, the momentum distribution is determined by only the asymptotic behavior in r of the wave functions

$$F(k)=\frac{4k^2}{v}\left|e^{-\sigma(E_p)}\left[\frac{d\tau_p^-}{dE}\right]^{1/2}(v\sigma(E))^{1/4}C(E)\Phi\left(\left[\frac{3}{2}\sigma(E)\right]^{2/3}\right)\right|^2. \tag{15}$$

The momentum distribution (15) is valid in the adiabatic approximation for all values of k and takes into account the reverse motion of the system along the term. When the point E_0 is located close to the real E axis, the Airy function leads to oscillations in $F(k)$ which are related to interference of the electrons ionized upon approach and separation. The existence of oscillations of this type was indicated in the article by Ostrovskii,[9] where they were obtained in an exactly soluble model with a Hamiltonian having only a continuous spectrum and in its background a quadratically time-dependent quasistationary term with constant width. If the turning point is found far from the real axis of E, i.e.,

$$|\sigma(\mathrm{Re}\,E_0)|\gg1,$$

in $F(k)$ we should confine ourselves to the leading term in the asymptotic form of the Airy function. Then

$$F(k)=\frac{k^2}{v}\left|\left[\frac{d\tau_p^-}{dE}\right]^{1/2}C(E)\exp\left\{\frac{i}{v}\int_{E_p}^{E}\tau_p^-(\varepsilon)\,d\varepsilon\right\}\right|^2. \tag{16}$$

In the Demkov–Osherov model the exponential in the momentum distribution coincides with the exponential in formula (16), but the pre-exponential factor is different and is equal to $v^{-1}\mathrm{Im}\,\tau_p(E)$, which is a reflection of the specific properties of this model. Both pre-exponential factors agree in the low-energy region, if the term does not have any singularities in this region. It is not difficult to confirm this by using formula (16) and the results of[10].

If the Hamiltonian is not spherically symmetric, after an expansion of $\varphi_p(\mathbf{r},E)$ in terms of spherical harmonics

$$\varphi_p(\mathbf{r},E)=\sum_{l,m}\varphi_p^{lm}(r,E)\,Y_{lm}(\theta,\varphi)$$

and the introduction of the functions

$$C_{lm}(E)=\lim_{r\to\infty}re^{-ikr}\varphi_p^{lm}(r,E),$$

we obtain

$$|C(E)|^2=\sum_{l,m}|C_{lm}(E)|^2.$$

One can find the function $C(E)$ in the first-order approximation by simulating the interaction of a weakly bound electron with neutral cores with the aid of zero-radius potentials.[11] For low energies it can be evaluated in the general case:

$$C(E)=\begin{cases}\sqrt{2k}, & l=0\\ a_{pl}k^l, & l\neq0\end{cases}. \tag{17}$$

Here the a_{pl} are constants which depend on the specific form of the potential. The result (17) in implicit form is contained in[2].

The problem of the interaction of an s-term with the continuous spectrum was investigated in the articles by Demkov[5] and Devdariani.[12] The specific properties of the zero-radius potential, which was utilized in these articles, did not allow one to take account of the influence of a coalescence point for the zeroes of the Jost function and the formation of a quasistationary s-term on the momentum distribution. The coalescence point frequently turns out to be close to the boundary of the continuous spectrum and, as is shown below, may significantly influence the behavior of $F(k)$ at low energies. Let us take

$$\tau_p^-(E)=-[(k_0-k)(k_0^*+k)]^{1/2}. \tag{18}$$

Here $k_0=\tau_0+i\varkappa$ and $(-k_0^*)$ are the turning points in the k plane. Such an approximation describes bound and virtual states which move with variation of the time along the imaginary k axis in opposite directions to each other and after coalescence at the point $i\varkappa$ at the instant of time $v^{-1}\tau_0$, they diverge in opposite directions in parallel to the real k axis as far as the turning points. Then the motion takes place in the opposite direction. With $C(E)=\sqrt{2k}$ and τ_p^- in the form (18), the momentum distribution

$$F(k)=\frac{2k^2}{v}\left|\frac{\varkappa}{[(k_0-k)(k_0^*+k)]^{1/2}}\exp\left\{-\frac{i}{v}\int_0^k[(k_0-k')(k_0^*+k')]^{1/2}k'\,dk'\right\}\right|^2 \tag{19}$$

coincides, for $k<|k_0|$, with the result obtained in[5,12]. If $|k_0|$ is small, expression (19) also describes the re-

gion $k > |k_0|$. As usual the argument of the exponential behaves like k^3, but the coefficient associated with k^3 differs by the factor $|k_0\varkappa^{-1}| > 1$. In this region the pre-exponential factor reaches a constant value. All this leads to a more rapid decrease of $F(k)$.

Now let us discuss the behavior of the momentum distribution as $k \to \infty$. The nature of the decrease of $F(k)$ is primarily determined by the argument of the exponential, that is, by the behavior of $\tau_p(E)$ as $E \to \infty$. Since the function $E_p(\tau)$ tends to a finite limit as $\tau \to \infty$, it is natural to consider two versions of the dependence $E_p(\tau)$: The first version is when $E_p(\tau)$ is a bilinear function of τ, and the second version is when $E_p(\tau)$ exponentially approaches the asymptotic value:

$$E_p(\tau) = E_p + \exp(-\sqrt{\tau^2+\rho^2})$$

(ρ is a constant analogous to the impact parameter). In the first case $\tau_p(E)$ tends to a finite limit corresponding to the pole of the function $E_p(\tau)$, and the argument of the exponential is a linear function of E. In the second case $\tau_p(E) \approx \ln E + n\pi i$ ($n = 0, 1, 2, \ldots$), which again leads to a linear dependence of the real part of the argument of the exponential on the energy. It is clear from general considerations that such behavior should develop at energies $E > |E_p|$.

4. POPULATION OF THE DISCRETE LEVELS VIA THE CONTINUOUS SPECTRUM

Let us consider the population of the states $\varphi_p(r, E_p)$ when relation (10) is valid for the coefficient B. Evaluation of the integral in the wave function (9) by the method of steepest descents for large positive values of t and finite values of r gives

$$\Psi(r,t) = \exp\left\{\frac{i}{v}\int_{E_p}^{E_0}[\tau_p^-(\varepsilon) - \tau_p^+(\varepsilon)]\,d\varepsilon - iE_p t\right\}\varphi_p(r, E_p).$$

It is natural to call the quantity

$$Q = \left|\exp\left\{\frac{i}{v}\int_{E_p}^{E_0}[\tau_p^-(\varepsilon) - \tau_p^+(\varepsilon)]\,d\varepsilon\right\}\right|^2$$

the survival probability, since this is the probability of the system's motion along the term without decay. After integration by parts of the integral in Q, we obtain

$$Q = \exp\left\{-2\int_{t_0}^{t_0+T}\Gamma_p(t)\,dt\right\}, \qquad (20)$$

where $\Gamma_p(t) = |\operatorname{Im} E_p(vt)|$ denotes the width of the term, t_0 denotes the time of the term's emergence into the continuous spectrum, and T denotes the time during the course of which the term was quasistationary. This result is natural and was previously cited without proof in[13,14].

Population of the state $\varphi_p(\mathbf{r}, E_p)$ also occurs as a result of multiple capture of emitted electrons. This process is divided into two stages: The first stage is the transition from the initial term to the continuous spectrum, and the second stage is the capture of an electron from the continuous spectrum into a bound state, i.e., in each stage we have the problem of the interaction of a single discrete level with the continuous spectrum, which was considered in Sec. 3. For small values of v, the capture probability is determined by the low-energy part of the emitted electrons' spectrum. Since a low-energy electron is captured only in that emerging bound state, having an even smaller energy, the capture process is resonant in nature. In this connection it is not important whether the electron is captured in the bound state corresponding to the initial term or in any other emerging state.

The probability of multiple capture for the s-term was calculated in the article by Demkov.[5] Using the momentum distribution (16) and $C(E)$ in the form (17), let us calculate the probability of multiple capture for arbitrary $l \neq 0$. Following[5], we obtain

$$P = a_{pl}^4 \frac{(2l+1)!!\pi}{2v^2 T^{2l+3}}\left[\frac{d\tau_p^-}{dE}\Big|_{E=0}\right]^2. \qquad (21)$$

Using the average width Γ of the term and assuming that $v \sim T^{-1}$, let us ascertain those cases in which it is necessary to take the survival probability into consideration. If

$$\Gamma T < (l+1/2)\ln T,$$

the population of the term is described by formula (20). However, if the width of the term is large or the velocity v is very small, population of the term takes place due to the capture of ionized particles.

Resonance capture of electrons from the continuous spectrum also takes place in other bound states, if the terms $E_n(\tau)$ corresponding to them cross the boundary of the continuous spectrum. By carrying out essentially the same calculations as in the derivation of formula (21), we obtain the following formula for the probability of capture in the state $\varphi_n(\mathbf{r}, E_n)$:

$$P_{np} = a_{pl}^2 a_{nl}^2 \frac{(2l+1)!!\pi}{2v^2 T_{np}^{2l+3}}\left(\frac{d\tau_p}{dE}\frac{d\tau_n}{dE}\right)\Big|_{E=0} \qquad (22)$$

where T_{np} denotes the time between emergence of the initial term E_p into the continuous spectrum and emergence of the term E_n from the continuous spectrum. Capture in those states, whose terms do not cross the boundary of the continuous spectrum, has a subbarrier character, and the capture probability is exponentially small.

5. CONCLUSION

The wave function (9), whose derivation results from simple and natural assumptions, permits us to obtain rather complete information about electronic transitions. This not only pertains to transitions to the continuous spectrum, but also to transitions between discrete and quasistationary levels. The presence of several terms in the problem appears as the presence of several branches of the analytic function $E(\tau)$. This question, just like the question of the interaction of a molecular term with Rydberg crowding, was not touched upon here and may be the object of a separate investigation. However, we note that since the wave function (7) coincides with the exact solution as applied to the Demkov–Osherov

model (see the Appendix), the approach used in the article by Demkov and Osherov[11] for consideration of nonadiabatic transitions between terms and in the article by Demkov and Komarov[15] in the problem concerning ionization in a Coulomb field may be utilized within the framework of the present approximation for the solution of these problems in the general case. It is of interest to take the following corrections to the wave function (7) into consideration, these corrections being related to the effect of momentum transfer. One can apparently construct an approximation analogous to the one proposed here allowing for the quantum motion of the nuclei. In this connection, of course, it is necessary to consider the given Green's functions which describe the motion of the nuclei in the potentials $E_n(R)$.

The momentum distribution is expressed in terms of the functions $C(E)$ and $\tau_p(E)$, which in principle can be derived from the experimental data. The following question arises in this connection: Is it possible to re-establish the system's Hamiltonian from the known functions $C(E)$ and $\tau_p(E)$? A similar inverse problem was investigated for the Demkov–Osherov model in the article by Demkov and Ostrovskiĭ,[16] where it was shown that assignment of the time-independent part of the Hamiltonian is sufficient for the reconstruction of a nonstationary separable potential from ionization data.

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APPENDIX

Let us show in what way the exact solution in the Demkov–Osherov model can be represented in the form (7). The solution of the nonstationary Schrödinger equation with a linearly time-dependent separable potential $t|\varphi\rangle\langle\varphi|$ has the form[11]

$$\Psi(\mathbf{r},t)=\frac{1}{\sqrt{2\pi}}\int_L \frac{\hat{G}(E)|\varphi\rangle}{\langle\varphi|\hat{G}(E)|\varphi\rangle}\exp\left\{i\int_0^E\langle\varphi|\hat{G}(\varepsilon)|\varphi\rangle^{-1}d\varepsilon-iEt\right\}dE, \quad (A.1)$$

where $\hat{G}(E)=(\hat{H}_0-E)^{-1}$ is the Green's operator and $\hat{H}_0$ is the stationary part of the Hamiltonian. It is not difficult to verify that the eigenfunctions $\chi(r,E)$ of the instantaneous Hamiltonian are expressed in the following way:

$$\chi(\mathbf{r},E)=-t(E)\hat{G}(E)|\varphi\rangle\langle\varphi|\chi\rangle. \quad (A.2)$$

The function

$$t(E)=\langle\varphi|\hat{G}(E)|\varphi\rangle^{-1} \quad (A.3)$$

is reciprocal to the function $E(t)$. In the present case the Gell-Mann–Feynman relation takes the form

$$dE(t)/dt=\langle\varphi|\chi\rangle^2. \quad (A.4)$$

Allowing for Eqs. (A.2), (A.3), and (A.4), the wave function (A.1) may be written down in the following way:

$$\Psi(\mathbf{r},t)=\frac{1}{\sqrt{2\pi}}\int_L\left[\frac{dt(E)}{dE}\right]^{1/2}\chi(\mathbf{r},E)\exp\left\{i\int_0^E t(\varepsilon)d\varepsilon-iEt\right\}dE,$$

i.e., in the form (7). Thus, the approximation constructed in this article leads to exact results in the Demkov–Osherov model.

[1)]The limitation associated with spherical symmetry is unimportant in the region of small energies, where one can always ascribe a definite orbital quantum number l to a state.[7] The influence of inner-shell electrons on the detachment of a weakly bound electron was investigated in the article by Dalidchik.[8]

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